An Overview of Simultaneous Strategies for Dynamic Optimization

Lorenz T. Biegler
Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh 15213, PA
lb01@andrew.cmu.edu

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Abstract

Simultaneous approaches for dynamic optimization problems are surveyed and a number of emerging topics are explored. Also known as direct transcription, this approach has a number of advantages over competing dynamic optimization methods. Moreover, a number of industrial applications have recently been reported on challenging real-world applications. This study provides background information, summarizes the underlying concepts and properties of this approach, discusses recent advances in the treatment of discrete decisions and, finally, illustrates the approach with two process case studies.

1 Introduction

With growing appreciation of dynamic simulation in computer aided process engineering, reliable and efficient optimization tools have also become more important for these systems. Dynamic optimization studies have been used for a number of *offline* tasks, including transitions between desired operating conditions, operating profiles for batch process operation, design and

operating studies in response to disturbances and upsets, parameter estimation, model development and discrimination for dynamic systems, and the design of control systems. *Online* tasks include the solution of optimization problems for control and identification, particularly in model predictive control (MPC). For particularly nonlinear processes, such as polymer processes, nonlinear models are essential to capture the dynamics of the process. As a result, several applications of Nonlinear MPC strategies have been reported for these processes.

For the purpose of this study, we consider the optimization problem stated in the following form:

$$\min_{z(t),u(t),p} \varphi(z(t_f)) \tag{1a}$$

$$s.t. \quad \frac{dz(t)}{dt} = f(z(t), y(t), u(t), p), \quad z(t_0) = z_0 \tag{1b}$$

$$g(z(t), y(t), u(t), p) = 0 \tag{1c}$$

$$g_f(z(t_f)) = 0 \tag{1d}$$

$$\begin{aligned} u_L \leqslant u(t) \leqslant u_U \\ y_L \leqslant y(t) \leqslant y_U \\ z_L \leqslant z(t) \leqslant z_U \end{aligned} \tag{1e}$$

The "unknowns" in this optimization problem are the *differential state variables* $z(t)$, *algebraic variables* $y(t)$, *control variables* $u(t)$, all functions of the scalar "time" parameter $t \in [t_0, t_f]$, as well as *time-independent parameters* p. As constraints we have the differential and algebraic equations (DAEs) given by (1b)-(1d) and we assume without loss of generality that the DAE system (1b,1c) is index one.

As shown in Figure 1, a number of approaches can be taken to solve (1a)-(1e). Currently, DAE optimization problems are solved using a variational approach or by various strategies that apply nonlinear programming (NLP) solvers to the DAE model. Until the 1970s, these problems were solved using an *indirect* or *variational approach*, based on the first order necessary conditions for optimality obtained from Pontryagin's Maximum Principle [67, 25]. For problems without inequality constraints, these conditions can be written as a set of DAEs. Obtaining a solution to these equations requires careful attention to the boundary conditions. Often the state variables have specified initial conditions and the adjoint variables have final conditions; the

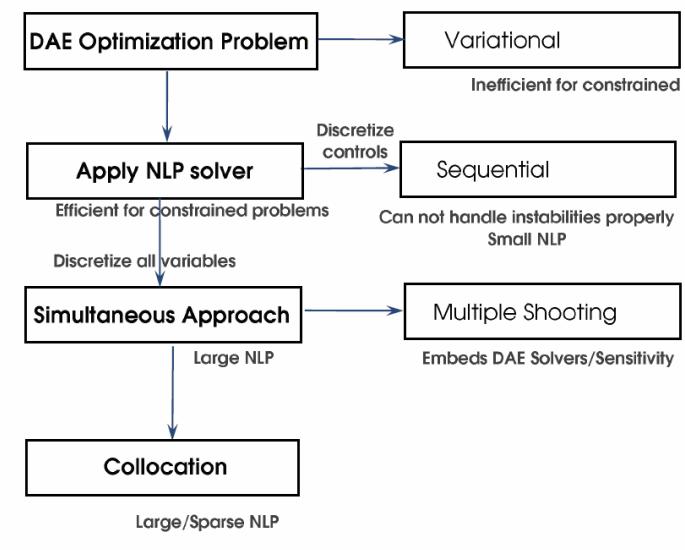

Figure 1: Solution strategies for dynamic optimization

resulting two-point boundary value problem (TPBVP) can be addressed with different approaches, including single shooting, invariant embedding, multiple shooting or some discretization method such as collocation on finite elements or finite differences. A review of these approaches can be found in [26]. On the other hand, if the problem requires the handling of active inequality constraints, finding the correct switching structure as well as suitable initial guesses for state and adjoint variables is often very difficult. Early approaches to deal with these problems can be found in [25].

Methods that apply NLP solvers can be separated into two groups, *sequential* and the *simultaneous* strategies. In the *sequential methods*, also known as *control vector parameterization*, only the control variables are discretized. In this formulation the control variables are represented as piecewise polynomials [86, 87, 5] and optimization is performed with respect to the polynomial coefficients. Given initial conditions and a set of control parameters, the DAE model is solved within an inner loop controlled by an NLP solver; parameters representing the control variables are updated by the NLP solver itself. Gradients of the objective function with respect to the control coefficients and parameters are calculated either from direct sensitivity equations of the DAE system or by integration of the adjoint equations. Several

efficient codes have been developed for both sensitivity methods including DDASAC, DASPK and CVODES.

Sequential strategies are relatively easy to construct and to apply as they contains the components of reliable DAE solvers (e.g., DASSL, DASOLV, DAEPACK) as well as NLP solvers (NPSOL, SNOPT). On the other hand, repeated numerical integration of the DAE model is required, which may become time consuming for large scale problems. Moreover, it is well known that sequential approaches have properties of single shooting methods and cannot handle open loop instability [2, 36]. Finally, path constraints can be handled only approximately, within the limits of the control parameterization. More information on these approaches can be found in [26].

Multiple shooting is a simultaneous approach that inherits many of the advantages of sequential approaches. Here the time domain is partitioned into smaller time elements and the DAE models are integrated separately in each element [21, 22, 54]. Control variables are parametrized as in the sequential approach and gradient information is obtained for both the control variables as well as the initial conditions of the states variables in each element. Finally, equality constraints are added to the NLP to link the elements and ensure that the states are continuous across each element. As with the sequential approach, inequality constraints for states and controls can be imposed directly at the grid points. For piecewise constant or linear controls this approximation is accurate enough, but path constraints for the states may not be satisfied between grid points.

In the simultaneous approach, also known as *direct transcription*, we discretize both the state and control profiles in time using collocation of finite elements. This approach corresponds to a particular implicit Runge-Kutta method with high order accuracy and excellent stability properties. Also known as fully implicit *Gauss* forms, these methods are usually too expensive (and rarely applied) as initial value solvers. However, for boundary value problems and optimal control problems, which require implicit solutions anyway, this discretization is a less expensive way to obtain accurate solutions. On the other hand, the simultaneous approach leads to large-scale NLP problems that require efficient optimization strategies [15, 18, 29]. As a result, these methods directly couple the solution of the DAE system with the optimization problem; the DAE system is solved only once, at the optimal point, and therefore can avoid intermediate solutions that may not exist or may require excessive computational effort.

In the next section we formulate the simultaneous approach and summa-

rize its main advantages and characteristics. Section 3 then reviews nonlinear programming strategies that solve the resulting problem. Section 4 provides a survey of process applications with the simultaneous approach along with a case study dynamic optimization of a crystallizer. Section 5 then extends this approach with a discussion of discrete decisions along with a batch distillation case study that highlights the salient features within the previous sections. Conclusions and directions for future work are given in Section 6.

2 Formulation and Characteristics of the Simultaneous Approach

The DAE optimization problem can be converted into an NLP by approximating state and control profiles by a family of polynomials on finite elements ($t_0 < t_1 < \ldots < t_N = \theta$). These polynomials can be represented as power series, sums of orthogonal polynomials or in Lagrange form. Here, we use the following monomial basis representation for the differential profiles, which is popular for Runge-Kutta discretizations:

$$z(t) = z_{i-1} + h_i \sum_{q=1}^{K} \Omega_q \left(\frac{t - t_{i-1}}{h_i} \right) \left. \frac{dz}{dt} \right|_{i,q}. \tag{2}$$

Here z_{i-1} is the value of the differential variable at the beginning of element i, h_i is the length of element i, $dz/dt_{i,q}$ is the value of its first derivative in element i at the collocation point q, and Ω_q is a polynomial of order K, satisfying

$$\begin{aligned} \Omega_q(0) &= 0 \qquad && \text{for } q = 1, \ldots, K \\ \Omega_q'(\rho_r) &= \delta_{q,r} \qquad && \text{for } q, r = 1, \ldots, K \end{aligned}$$

where ρ_r is the location of the r^{th} collocation point within each element. Continuity of the differential profiles is enforced by

$$z_i = z_{i-1} + h_i \sum_{q=1}^{K} \Omega_q(1) \left. \frac{dz}{dt} \right|_{i,q}. \tag{3}$$

Based on our experience in a number of studies, we prefer Radau collocation points because they allow constraints to be set at the end of each element and

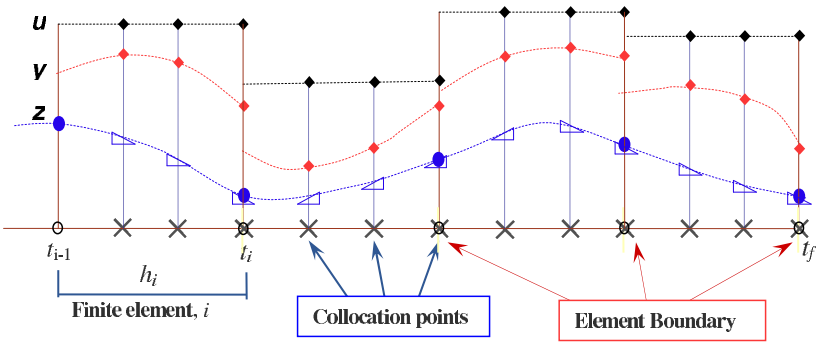

Figure 2: Collocation on finite elements. The diamonds represent u and y at collocation points. The triangles represent dz/dt at collocation points and the circles represent z at element boundaries, where discontinuity is allowed in u and y, although continuity of z is retained.

to stabilize the system more efficiently if high index DAEs are present. In addition, the control and algebraic profiles are approximated using a Lagrange basis representation which takes the form:

$$y(t) = \sum_{q=1}^{K} \psi_q \left(\frac{t - t_{i-1}}{h_i} \right) y_{i,q} \tag{4}$$

$$u(t) = \sum_{q=1}^{K} \psi_q \left(\frac{t - t_{i-1}}{h_i} \right) u_{i,q}. \tag{5}$$

Here $y_{i,q}$ and $u_{i,q}$ represent the values of the algebraic and control variables, respectively, in element i at collocation point q. ψ_q is the Lagrange polynomial of degree K satisfying

$$\psi_q(\rho_r) = \delta_{q,r} \qquad \text{for } q, r = 1, \ldots, K.$$

From (2), the differential variables are required to be continuous throughout the time horizon, while the control and algebraic variables are allowed to have discontinuities at the boundaries of the elements. As seen from Figure 2, (2) allows bounds on the differential variables to be enforced directly at element boundaries, using z_i. These can also be enforced at all collocation points by writing additional point constraints.

Substitution of equations (2)-(5) into (1a)-(1e) leads to the following NLP.

$$\min_{\frac{dz}{dt}_{i,q}, u_{i,q}, y_{i,q}, p} \quad \varphi(z_N) \tag{6a}$$

$$s.t. \quad \frac{dz}{dt}_{i,q} = f(z_{i,q}, y_{i,q}, u_{i,q}, p), \tag{6b}$$

$$z_{i,q} = z_{i-1} + h_i \sum_{q'=1}^{K} \Omega_{q'}(\rho_q) \tag{6c}$$

$$g(z_{i,q}, y_{i,q}, u_{i,q}, p) = 0 \quad i = 1, \ldots N, q = 1, \ldots K \tag{6d}$$

$$z_i = z_{i-1} + h_i \sum_{q=1}^{K} \Omega_q(1) \quad i = 1, \ldots N \tag{6e}$$

$$g_f(z_N) = 0 \tag{6f}$$

and for $i = 1, \ldots N, q = 1, \ldots K$:

$$\begin{aligned} u_L &\leqslant u_{i,q} \leqslant u_U \\ y_L &\leqslant y_{i,q} \leqslant y_U \\ z_L &\leqslant z_{i,q} \leqslant z_U \end{aligned} \tag{6g}$$

This NLP can be rewritten as:

$$\min_{x \in \mathcal{R}^n} \quad f(x) \tag{7}$$

$$s.t. \quad c(x) = 0 \tag{8}$$

$$x_L \leqslant x \leqslant x_U \tag{9}$$

where $x = \left(\frac{dz}{dt}_{i,q}, z_i, y_{i,q}, u_{i,q}, t, p\right)^T$, $f : \mathcal{R}^n \longrightarrow \mathcal{R}$ and $c : \mathcal{R}^n \longrightarrow \mathcal{R}^m$.

The simultaneous approach has a number of advantages over other approaches to dynamic optimization:

1. Control variables are discretized at the same level as the state variables the Karush Kuhn Tucker (KKT) conditions of the simultaneous NLP are consistent with the optimality conditions of the discretized variational problem, and, under mild conditions, convergence rates can be shown (see [75, 33, 40]) . More recently, we have extended these properties to Radau collocation. In [46, 47], convergence rates were derived that relate NLP solutions to the true solutions of the infinite dimensional optimal control problem.

2. As with multiple shooting approaches, simultaneous approaches can deal with instabilities that occur for a range of inputs. Because they can be seen as extensions of robust boundary value solvers, they are able to "pin down" unstable modes (or increasing modes in the forward direction). This characteristic has benefits on problems that include transitions to unstable points, optimization of chaotic systems [22] and systems with limit cycles and bifurcations, as illustrated in [36].

3. Simultaneous methods also allow the direct enforcement of state and control variable constraints, at the same level of discretization as the state variables of the DAE system. As was discussed in [47], these can present some interesting advantages on large-scale problems.

4. Finally, recent work has shown [13, 48, 47] that simultaneous approaches have distinct advantages for singular control problems and problems with high index path constraints.

Nevertheless, simultaneous strategies require the solution of large nonlinear programs, and specialized methods are required to solve them efficiently. These NLPs are usually solved using variations of Successive Quadratic Programming (SQP). Both full space and reduced space options exist for these methods. Full space methods take advantage of the sparsity of the DAE optimization problem. They are best suited for problems where the number of discretized control variables is large [15]. Here, second derivatives of the objective function and constraints are usually required, as are measures to deal with directions of negative curvature in the Hessian matrix [88]. Betts [12] provides a detailed description of the simultaneous approach with full space methods, along with mesh refinement strategies and case studies in mechanics and aerospace. On the other hand, reduced-space approaches exploit the structure of the DAE model and decompose the linearized KKT system; second derivative information is often approximated here with quasi-Newton formulae. This approach has been very efficient on many problems in process engineering that have few discretized control variables (say $\leqslant$ 1000) [10, 16, 27]. We will sketch our current NLP algorithm, IPOPT, in the next section and discuss both full- and reduced-space options.

3 Solving large-scale NLPs

We now consider methods for the solution of the NLP resulting from the simultaneous formulation. Because of the large problem size, large number of inequalities and a potentially large number of degrees of freedom, we find that NLP (7)-(9), can be solved quite efficiently using the IPOPT algorithm [88] for large-scale nonlinear programming. This algorithm follows a barrier approach, where the bound constraints (9) are replaced by logarithmic barrier terms which are added to the objective function to give:

$$\begin{aligned} \min \varphi(x) = f(x) - \hat{\mu} \textstyle\sum_{i=1}^{n} \ln(x^{(i)} - x_L^{(i)}) & \\ -\hat{\mu} \textstyle\sum_{i=1}^{n} \ln(x_U^{(i)} - x^{(i)}) & \quad (10) \\ s.t. \qquad c(x) = 0 & \quad (11) \end{aligned}$$

with a barrier parameter $\hat{\mu} > 0$. Here, $x^{(i)}$ denotes the i^{th} component of the vector x. Since the objective function of this barrier problem becomes arbitrarily large as $x^{(i)}$ approaches either of its bounds, a local solution $x_*(\hat{\mu})$ of this problem lies in the interior of this set, i.e., $x_U > x_*(\hat{\mu}) > x_L$. The degree of influence of the barrier is determined by the size of $\hat{\mu}$, and under mild conditions $x_*(\hat{\mu})$ converges to a local solution x_* of the original problem (7)-(9) as $\hat{\mu} \to 0$. Consequently, a strategy for solving the original NLP is to solve a sequence of barrier problems (10)-(11) for decreasing barrier parameters $\hat{\mu}_l$, where l is the counter for the sequence of subproblems.

IPOPT follows a primal-dual approach and applies a Newton method to the resulting KKT conditions, leading to solution of the following linear system at iteration k:

$$\begin{bmatrix} H_k + \Sigma_k & A_k^T \\ A_k & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \lambda^+ \end{bmatrix} = - \begin{bmatrix} \nabla \varphi(x_k) \\ c(x_k) \end{bmatrix} \quad (12)$$

where we use the convention, $X = diag(x)$, etc., H_k is the Hessian of the Lagrangian function $\nabla_{xx} f(x_k) + c(x_k)^T \lambda_k$, $A_k = \nabla c(x_k)$ and $\Sigma_k = (V_a^k)^{-1}(X_k - X_L) + (V_b^k)^{-1}(X_U - X_k)$ is the barrier term. Exact first and second derivatives for this method can be evaluated in a number of ways, including automatically through the AMPL interface [38]. Global convergence of the Newton method is promoted by a novel filter line search strategy; detailed analysis shows both global convergence and fast local convergence properties. More information on IPOPT can be found in Wächter and Biegler [88]. In the next section, we note that this Newton-based approach provides

a number of opportunities for decomposition and tailoring to the structure of the dynamic optimization problem.

The simultaneous approach also offers opportunities to exercise flexibility and exploit structure, particularly in the Newton step (12) and solution of this linear system. Here we are presented with three options:

- Apply a *range and null space decomposition* to (12); this leads to the *reduced space approach.*
- Apply a *direct, sparse symmetric linear solver* to (12), leading to a full space approach. This approach takes advantage of widely used sparse matrix software.
- Apply an iterative linear solver to the indefinite system (12). This takes advantage of problem specific preconditioners to exploit the structure of the A matrix in (12) [20]. More information on this approach can be found in [19]

The reduced space approach has been developed and demonstrated in a number of studies [18, 27, 29]. Here the variables are partitioned into m dependent (Y space) and $n - m$ independent (Z space) variables. The independent variable space occupies the null space of A_k^T. The combined set of these variables spans the full space. Note that the control variables and parameters are not necessarily the independent variables. With this partition $A_k^T = [C_k \mid N_k]$, where the $m \times m$ basis matrix C_k is nonsingular, we define the matrices $Z_k^T = [-N_k^T C_k^{-T} \mid I]$ and $Y_k^T = [I \mid 0]$ and that Note that Z_k satisfies $A_k^T Z_k = 0$ and is therefore a null space basis matrix for A_k^T. The search direction can now be written as $d_k = Y_k d_Y + Z_k d_Z$. The range space direction d_Y is determined by solving:

$$d_Y = -C_k^{-1} c_k, \tag{13}$$

and the null space direction d_Z is obtained from (12) after substituting for d and invoking $A_k^T Z_k = 0$:

$$d_Z = -[Z_k^T (H_k + \Sigma_k) Z_k]^{-1} \left(Z_k^T \nabla \varphi(x_k) + w_k \right). \tag{14}$$

with $w_k = Z_k^T (H_k + \Sigma_k) Y_k d_Y$. Calculation of both the range space step and the null space basis is aided by exploiting the structure of $A^T = [C \mid N]$,

given by:

$$\left[\begin{array}{cccccc|ccccc}
I & & & & & & & & & & \\
T^1 & C^1 & & & & & N^1 & & & & \\
I & \widehat{C}^1 & -I & & & & \widehat{N}^1 & & & & \\
 & & T^2 & C^2 & & & & N^2 & & & \\
 & & I & \widehat{C}^2 & -I & & & \widehat{N}^2 & & & \\
 & & & & T^3 & C^3 & & & N^3 & & \\
 & & & & & \ddots & & & & \ddots &
\end{array}\right]$$

Here linear solutions that require matrix C proceed by factoring C^i for each element i sequentially. This follows in the same manner as in the forward solution of DAEs and the associated sensitivity equations, with the exception that A^T can first be stabilized to enforce dichotomy (see [28] for a detailed analysis of this approach).

The reduced space approach is especially advantageous for dynamic optimization problems with few degrees of freedom. It has been implemented in the DynoPC package [53] and has been used to solve a wide variety of large problems [53, 18, 52] quite efficiently. Moreover, Li, Wozny and coworkers [43, 55] have proposed feasible path extensions of this approach (instead of (13) the nonlinear collocation equations are solved at each time step) with excellent performance on large scale problems. Finally, this approach has been developed further further [68, 61] by modifying the implicit Runge-Kutta discretization and adjusting element lengths to ensure accurate state profiles.

However, as the degrees of freedom increase, determination of Z, calculation of d_Z and especially computation of $Z_k^T \Sigma_k Z_k$ in (14) become expensive. This property was demonstrated in [47] on results for the dynamic optimization of a distillation column with up to 1,215,970 variables (see also, [89]). A number of options were considered for the calculation of d_Z in (14), but, for computation on single processor computers, all of these grow polynomially with the degrees of freedom.

Nevertheless, the reduced space approach has the advantage that the information in (12) can be constructed and stored element-by-element and parallel processors can be used to great advantage in the computation of (14) and (13). Future work will therefore concentrate on reduced-space decomposition procedures that exploit parallelism for large problems.

4 Applications of the Simultaneous Approach

Along with the advances described above, there have been a large number of applications of the simultaneous approach. These were prompted by early studies in the 70s and early 80s [84, 64, 62, 21, 17] and a realization that these methods were especially suitable for unstable systems and systems with path constraints. In particular, the simultaneous approach has been applied widely in aeronautical and astronautical applications. A cursory literature search reveals about 200 publications that apply simultaneous approaches in this area. Specific applications include the collision avoidance for multiple aircraft [14, 70] and underwater vehicles [80], trajectories for satellites and earth orbiters [78, 32] and the design of multiple paths and orbits for multibody dynamics [24], including interplanetary travel [11]. An overview of these applications is given in [12]. Moreover, the SOCS (Sparse Optimal Control Software) [12] package, commercial software developed marketed by Boeing Corporation, has been widely used for these and other engineering applications.

In process engineering, applications of the simultaneous approach include the design and optimal operation of batch processes. These include optimization of operating policies for fermentors [33] and bioreactors [77], flux balance models for metabolic systems [51, 60, 73], batch distillation columns [58, 65], membrane separators [34], polymerization reactors [36, 44], crystallization [52], freeze-drying processes [23] and integrated multi-unit batch processes [16]. Other off-line applications include parameter estimation of reactive systems [83, 35], design of periodic separation processes including pressure swing adsorption [63] and simulated moving beds [50, 49], optimal grade transitions in polymer processes [30, 36], reactor network synthesis [7, 66] and economic performance analysis of batch systems [57].

On-line applications include dynamic data reconciliation algorithms for batch processes [1, 56], state estimation and process identification [82], optimal startup policies for distillation columns [71], optimal feed policies for direct methanol fuel cells [91] and a number of algorithms and case studies for nonlinear model predictive control (NMPC)[79, 39]. Moreover, commercial applications of NMPC include several applications at ExxonMobil and ChevronPhillips, which use the NLC package and NOVA solver by PAS, Inc. [76, 92]. Other software implementations of the simultaneous approach include *DynoPC* [53], a Windows-based platform, as well as the *OptimalControlCentre* [39] and *dynopt* [31] packages, both developed in MATLAB.

4.1 Crystallization Case Study

To illustrate the simultaneous approach on a process application, we consider the dynamic optimization of a crystallizer described with a simple population balance model. Conventional crystallization kinetics are characterized in terms of two dominant phenomena: nucleation and crystal growth. These are competing phenomena that both consume desired solute material during the crystallization process. To obtain larger (and fewer) crystals, nucleation needs to be minimized, and the goal of the optimization is to find operating strategies that will allow us to minimize this phenomenon. To do this, we determine a profile for the cooling jacket temperature.

The dynamic optimization problem for the crystallizer consists of a DAE model, a lower bound of the jacket temperature as a function of the solute concentration and an objective to maximize the crystal length. This objective also corresponds to minimizing the surface area in order to obtain higher purity of the crystals. The dynamic optimization problem can be stated as:

$$\max_{z(t),u(t),p} L_s(t_f) \tag{15}$$

$$\frac{dL_s}{dt} = K_g L_s^{0.5} \Delta T^{1.1} \tag{16}$$

$$\frac{dN}{dt} = B_n \Delta T^{5.72} \tag{17}$$

$$\frac{dL}{dt} = N\frac{dL_s}{dt} + L_0\frac{dN}{dt} \tag{18}$$

$$\frac{dA}{dt} = 2\alpha N\frac{dL_s}{dt} + L_0^2\frac{dN}{dt} \tag{19}$$

$$\frac{dV_c}{dt} = 3\beta A\frac{dL_s}{dt} + L_0^3\frac{dN}{dt} \tag{20}$$

$$\frac{dM}{dt} = 3(W_{s0}/L_{s0}^3)L_s^2\frac{dz_1}{dt} + \rho V\frac{dV_c}{dt} \tag{21}$$

$$\frac{dC}{dt} = -\frac{dM}{dt}/V \tag{22}$$

$$\frac{dT}{dt} = K_c\frac{dM}{dt} - (K_e/(wC_p))(T - T_j) \tag{23}$$

$$\phi(C) \leqslant T_j \in [10^oC, 100^oC] \tag{24}$$

where L_s is the mean crystal size, N is the number of nuclei per liter of solvent, L is the total length of the crystals per liter of solvent, A is the total

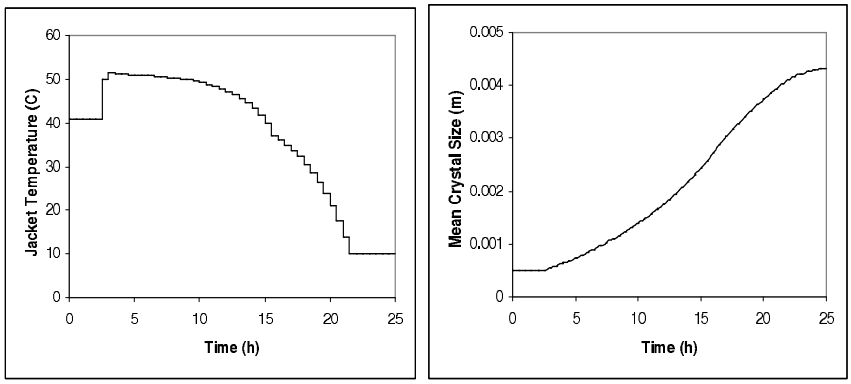

Figure 3: Optimal cooling and crystal size profiles for crystallizer

surface area of the crystals per liter of solvent, V_c is the total volume of the crystals per liter of solvent, C is the solute concentration, M is the total mass of the crystals, V is the volume of the solvent, L_0 is the initial crystal size, W_{so} is the mass of seeds added, L_{so} is the mean size of the seeds, ρ is the true specific gravity of the crystals, and α, β are shape factors for area and volume of the crystals, respectively. These and the remaining parameter values, K_g, B_n, w, C_p, K_c and K_e are reported in [52].

The most important aspect of this problem is how the control profile impacts the process. The control variable is the jacket temperature, T_j, which has a lower bound, $\phi(C)$, that changes dynamically with the concentration of the solute. The function $\phi(C)$ is calculated based on a polynomial relationship between concentration and equilibrium temperature.

Applying the simultaneous approach to this model with 3 point Radau collocation and fifty finite elements leads to an NLP with 1900 variables and 1750 equality constraints. Using DynoPC [53], the optimal solution was obtained in 12.5 CPUs (1.6 MHz IBM laptop) with 105 iterations of the reduced space version of IPOPT. The optimal profiles of the mean crystal size and the jacket temperature are given in Figure 3. Note that the mean crystal size increased by over eight times in 25 h. Also, in order to maximize the crystal size, the jacket cooling profile must first *increase* to reduce the number of nucleating particles. Further information on this optimization study can be found in [52, 89].

5 Discrete Decisions

Discrete events occur in many dynamic simulation and optimization problems. In chemical processes, examples of this phenomena include phase changes in equilibrium systems, changes in modes in the operation of safety and relief valves, vessels running dry or overflowing, discrete decisions made by control systems and explosions due to accidents. These actions can be reversible or irreversible and should be modeled with appropriate logical constraints. Modeling discrete events is discussed in [5]; these events are often triggered by an appropriate discontinuity function which monitors a change in the condition and leads to a change in the state equations. These changes can be reformulated either as binary decision variables [6] or by using complementarity conditions (with nonnegative continuous variables $x^{(i)}$ and $x^{(j)}$ alternately set to zero). These additional variables can then be embedded within optimization problems.

The incorporation of binary variables leads to mixed integer optimization problems. Here, several studies have considered the solution of Mixed Integer Dynamic Optimization (MIDO) problems. In particular, Avraam et al. [4] developed a complete discretization of the state and control variables to form a mixed integer nonlinear program. More recently, a number of MIDO algorithms were developed and compared with the simultaneous approach [37] in order to select optimal control strategies. Alternately Allgor and Barton [3] and Bansal et al. [8] apply sequential strategies and discretize only the control profile. For this approach, careful attention must paid to calculation of sensitivity information for discrete decisions triggered in time.

On the other hand, many discrete decisions for hybrid systems can be modeled through complementarity relations [42, 85]. Furthermore, complementarity conditions can be considered in a straightforward way through barrier methods [72] to yield an NLP. This class of problems can be generalized to Mathematical Programs with Equilibrium Constraints (MPECs) of the following form:

$$\begin{aligned}
\min_{x \in \mathcal{R}^n} \quad & f(x) && \text{(25a)}\\
s.t. \quad & c(x) = 0 && \text{(25b)}\\
& x_L \leqslant x \leqslant x_U && \text{(25c)}\\
& 0 \leqslant \hat{x} \perp \bar{x} \geqslant 0 && \text{(25d)}\\
& && \text{(25e)}
\end{aligned}$$

with $x^T = [\tilde{x}^T\ \hat{x}^T\ \bar{x}^T]$. Applications of MPECs have long been recognized in game theory, transportation planning, economics and engineering design; a broad survey of these applications can be found in [41, 59]. In process engineering, these problems stem from bilevel and multilevel optimization problems as well as optimization of hybrid (discrete and continuous) systems [81]. Included in this class are optimization problems with phase equilibrium constraints, as in equilibrium stage processes [69], and cellular models based on metabolic pathways [73].

To solve the MPEC, we could apply a primal-dual interior point approach, but the KKT matrix corresponding to (12) is singular at all points that satisfy (25d). To deal with this characteristic, we rewrite (25d) as $\hat{X}\bar{x} \leqslant \hat{\mu}e$, where $\hat{\mu}$ is the barrier parameter whose sequence goes to zero. We have incorporated this MPEC reformulation into the IPOPT code along with algorithmic modifications to treat the complementarity constraints more efficiently. The implementation compares well against competing barrier algorithms [69, 72] and performs well on distillation optimization problems with disappearing vapor and liquid phases on equilibrium stages, as well as on a number of other applications [73, 45].

5.1 Example Problem: Batch Distillation

To illustrate the application of MPECs to dynamic optimization, we present an example developed in [71], that deals with the cold startup of a batch distillation unit. These models have also been considered in [90]. Consider a batch distillation column with a charge of 8 kmol of a 58/42 mixture of benzene and toluene in the bottom of the column. The column operates at 1 bar and consists of 12 trays, including the reboiler and condenser. The maximum reboiler heat duty is set to 600 kJ/hr and the minimum holdup for the trays and condenser are 0.3 and 0.5 kmol, respectively. The control variables in the column operation are the distillate flowrate, D and the reboiler heat duty, Q_r. At initial time, the tray holdups are set to zero and startup of the column is posed as a free end-time problem which maximizes the average rate of product withdrawn over the time of operation t_f as follows:

$$\max \quad \frac{1}{t_f}\left(\int_0^{t_f} D(t)dt + M_{12}^l(t_f)\right) - \epsilon\frac{1}{t_f}\int_0^{t_f}(Q_r(t) - Q_r^{\max})^2 dt \qquad (26)$$

$$
\begin{aligned}
s.t. \quad \tfrac{dM_1}{dt} &= L_2 - V_1 - L_1 \\
\tfrac{dM_i}{dt} &= V_{i-1} + L_{i+1} - V_i - L_i \quad i = 2, \ldots 11 \\
\tfrac{dM_{12}}{dt} &= V_{11} - D - L_{12}
\end{aligned} \tag{27}
$$

$$
\begin{aligned}
M_1 \tfrac{dx_{1,j}}{dt} &= L_2(x_{2,j} - x_{1,j}) - V_1(y_{1,j} - x_{1,j}) \\
M_i \tfrac{dx_{i,j}}{dt} &= V_{i-1}(y_{i-1,j} - x_{i,j}) + L_{i+1}(x_{i+1,j} - x_{i,j}) - V_i(y_{i,j} - x_{i,j}) \quad i = 2, \ldots 11 \\
M_{12} \tfrac{dx_{12,j}}{dt} &= V_{11}(y_{11,j} - x_{12,j})
\end{aligned} \tag{28}
$$

$$
\begin{aligned}
M_1 \tfrac{dh_1^l}{dt} &= L_2(h_2^l - h_1^l) - V_1(h_1^v - h_1^l) + Q_r \\
M_i \tfrac{dh_i^l}{dt} &= V_{i-1}(h_{i-1}^v - h_i^l) + L_{i+1}(h_{i+1}^l - h_i^l) - V_i(h_i^v - h_{i,j}^l) \quad i = 2, \ldots 11 \\
M_{12} \tfrac{dh_{12}^l}{dt} &= V_{11}(h_{11}^v - h_{12}^l) - Q_c
\end{aligned} \tag{29}
$$

$$
\begin{aligned}
y_{i,j} &= \beta_i K_{i,j}(T_i, P_i, x_i) x_{i,j} \quad j \in COMP \\
0 &= \sum_{j \in COMP} y_{i,j} - \sum_{j \in COMP} x_{i,j} \\
\beta_i &= 1 - \alpha_i^l + \alpha_i^v \\
0 \leqslant M_i^l &\perp \alpha_i^l \geqslant 0 \\
0 \leqslant M_i^v &\perp \alpha_i^v \geqslant 0
\end{aligned} \tag{30}
$$

$$
\frac{x_{12,C_6H_6} M_{12}^l(t_f) + \int_0^{t_f} x_{12,C_6H_6} D(t) dt}{M_{12}^l(t_f) + \int_0^{t_f} D(t) dt} \geqslant 0.95 \tag{31}
$$

where M_i, L_i, V_i are the holdup, liquid flowrate and vapor flowrate on the i^{th} tray, respectively, $x_{i,j}, y_{i,j}$ represent the liquid and vapor compositions on the i^{th} tray, respectively, h_i^v, h_i^l represent the specific enthalpies of the vapor and liquid streams from tray i, Q_r and Q_c are the reboiler and condenser heat loads and $\epsilon > 0$ is a small parameter serving to regularize the problem. In the above formulation, the total product at final time is defined as the sum of the condenser holdup at final time and the total distillate withdrawal over time. The total product that is withdrawn from the column is required to have a certain purity of benzene as indicated by the last constraint of the optimization problem (31). Finally, additional algebraic equations are added to define the specific enthalpies in terms of temperature and to relate conditions between the tray holdups M_i and liquid flowrate L_i. Note that we modeled the tray holdup by ignoring the vapor component. As described in [71], this leads to a DAE model of index 2. In particular, the vapor flowrate, $V_i(t)$, an algebraic variable, appears nowhere in the algebraic equations. As a result, this system had to be reformulated to index 1 in [71].

From (30), we note that the complementarity constraints allow the liquid phase to disappear [71], so that:

$$\begin{array}{ll} M_i^l, M_i^v > 0 & \text{then } \beta_i = 1 \\ M_i^l = 0 < M_i^v & \text{then } \beta_i \leqslant 1 \\ M_i^l > 0 = M_i^v & \text{then } \beta_i \geqslant 1. \end{array} \tag{32}$$

The optimal control problem is discretized over 30 elements with 2 collocation points leading to a problem with 22226 variables and 20125 constraints including 2040 complementarity constraints. The problem solved to a tolerance of 10^{-5} in the optimality conditions using a 2.2 GHz Intel Pentium IV processor running *Linux* as the operating system. Intuitively, one would expect the optimal startup solution to exhibit total reflux and a heat duty profile at its upper bound. However, this is not possible for this example, as the trays are deliberately undersized. Setting Q_r to the upper bound would lead to complete depletion of the charge *before holdups would be established and the purity could be satisfied.* As a result, an intermediate reboil profile needs to be determined.

Solution of the optimization problem yields an optimal operating time of 28.8 hours. The profiles of liquid holdup and reflux flow for the optimal solution are shown in Figures 4 and 5. The trays have no holdup initially so no liquid flows from the trays until the liquid holdup is at least equal to the minimum threshold. The vapor from the bottom is completely condensed on tray 12 and refluxed to the column at initial time. This increases the holdup on the trays in decreasing order of tray number. Also, fluctuations in the liquid holdup correspond to the times at which the vapor flowrate is lowered and this decreases with reboiler heat duty, Q_r, shown in Figure 6. The control profiles lie strictly between bounds over a significant portion of the time of operation, and the solution exactly matches the purity constraint on benzene at final time.

6 Conclusions and Future Directions

With increasing demands for the analysis and exploitation of dynamic behavior in processes systems, dynamic optimization has become increasingly important, both for off-line and on-line applications. This paper presents a general overview of simultaneous approaches to dynamic optimization problems. Over the past two decades, simultaneous approaches have been applied

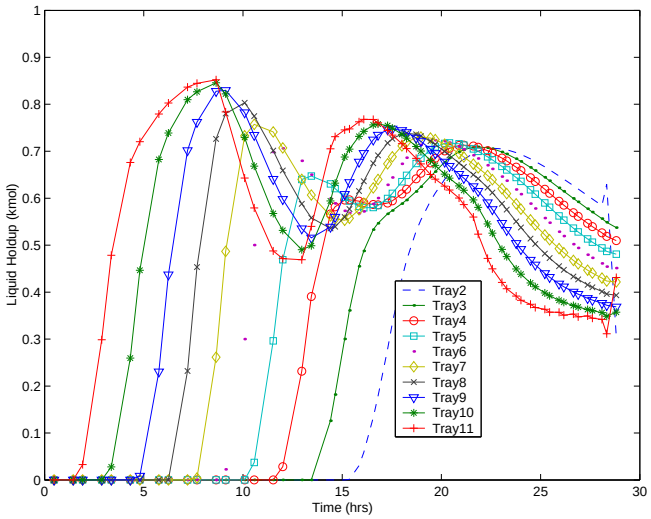

Figure 4: Liquid tray holdups in batch column

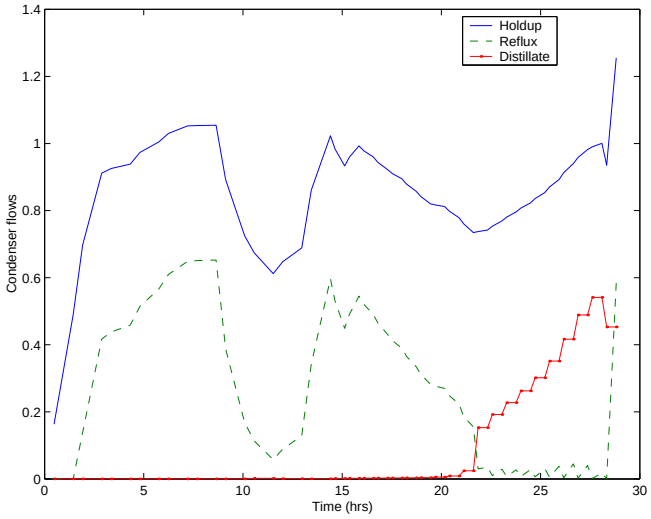

Figure 5: Liquid holdup and flow from condenser in batch column

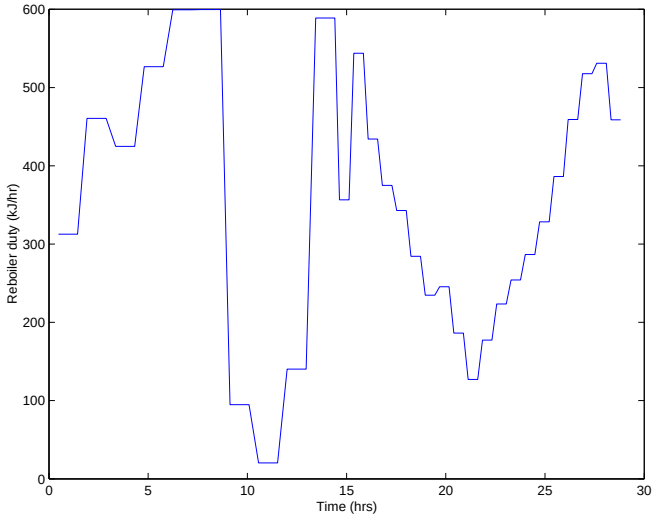

Figure 6: Optimal reboiler duty in batch column

in hundreds of literature studies. By discretizing both the state and control variables with a stable, high order implicit Runge-Kutta scheme and forming large-scale nonlinear programs, these approaches allow the rapid determination of accurate solution profiles with fewer time steps (finite elements) than with sequential methods that apply standard ODE solvers. Moreover, the simultaneous strategy has clear advantages in the treatment of path constraints and unstable dynamic systems.

Recent work in numerical analysis and mathematical programming has led to highly efficient large-scale NLP solvers to handle the discretized dynamic optimization problem, thus leading to to fast solutions. Moreover, the approach also offers flexibility with respect to the formulation, decomposition and solution of large-scale NLP problems. Finally, accurate first and second derivatives can be obtained cheaply from the NLP, thus providing an essential element for superior performance of the NLP solution strategy.

Future work with simultaneous dynamic optimization lies in the solution of large-scale NLPs with efficient decomposition strategies that take advantage of structure and lend themselves to parallel computing. Additional work is also required for ill-conditioned optimal control problems, in particular, singular problems and high index path constrained problems. These problem types present difficulties for all optimal control strategies. For si-

multaneous methods, they lead to ill-conditioning of the linear system (12). To overcome this drawback, unbiased regularization strategies are proposed and demonstrated in [47] for singular control problems. On the other hand, ill-conditioning due to path constrained problems seems to be benign as discussed and demonstrated in [48, 13].

The treatment of discrete decisions has only recently been considered with simultaneous approaches. In particular, we have found that complementarity constraints and the resulting MPEC formulations can deal with large sets of discrete decisions that result from temporal discretizations. Nevertheless, careful formulation of MPEC problems still needs to be explored. A promising approach develops complementarity constraints from switching conditions that arise from convex inner-level NLPs. However, the properties of these formulations still need to be analyzed. Moreover, reformulation techniques that convert the MPEC to a well-posed NLP have been described and analyzed in [74]. These need to be evaluated in the context of dynamic optimization.

Finally, the above dynamic optimization problems lead to solution profiles with function and derivative discontinuitues (jumps and kinks over time). Within the simultaneous approach, accurate solutions with these features require the incorporation of moving finite elements based on error criteria both in state variable representation and in optimality conditions. Interesting preliminary results in this area are described in [47, 18]. Ongoing work with moving elements extends this approach to a broader range of problems.

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