RESEARCH PROPOSAL

IN SITU ADAPTIVE TABULATION FOR REAL-TIME CONTROL

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1 Introduction

The three most significant obstacles to nonlinear model predictive control (NMPC) applications are nonlinear model development, state estimation, and rapid, reliable solution of the control algorithm in real time (Qin and Badgwell, 2000). This proposal outlines an attempt to overcome the last two obstacles through a computational reduction technique formerly developed for turbulent combustion simulations (Pope, 1997). This technique, called *in situ* adaptive tabulation (ISAT), is a storage and retrieval method to reduce the computational time of open loop simulations of continuous dynamic first principles models. In direct multiple shooting implementations of NMPC (Binder et al., 2001; Tenny et al., 2002) open loop simulations are performed many times until an optimal trajectory of inputs is found. Also, in sequential state estimation (dynamic data reconciliation) many open loop simulations are performed until an approximation to the unmeasured states is obtained (Liebman et al., 1992). Since the open loop simulations occupy a majority of the computational effort, ISAT has potential to greatly improve the speed of state estimation and dynamic optimization.

Other methods have been proposed as storage and retrieval methods for NMPC. Three of these include dynamic programming (Luus and Okongwu, 1999), artificial neural networks, and approximations to the explicit linear quadratic regulator (LQR) for constrained systems (Bemporad et al., 2001; Pistikopoulos et al., 2002). The explicit LQR solution is a piecewise mapping of linear approximations to the exact solution with constraints. This work is a storage and retrieval method for the optimization solution, not for the model dynamics. Therefore, this work will not be directly compared in subsequent sections.

Neural nets are an effective tool to build and deploy nonlinear models from plant historical data. However, when neural nets are built from first simulations of a first principles model, much of the extrapolative power of the model is lost. ISAT is an alternative to neural nets for building discrete nonlinear models from continuous nonlinear models.

The remainder of the proposal is organized as follows. Section 2 gives a summary of three methods of storage and retrieval that can be used to solve optimal control problems. These three methods include dynamic programming, neural nets, and the proposed ISAT approach. Section 3 includes illustrative examples that compare neural nets and ISAT and control of a distillation column. Section 4 includes a description of future work that will be performed, followed by a summary in section 5.

2 Previous Work

The simulation of continuous nonlinear models can pose a significant computational challenge for control applications. Two general classifications of methods to reduce the computational cost of integrating the model are model reduction and computational reduction.

The main types of model reduction for nonlinear dynamic models are projection methods, proper orthogonal decomposition (POD), perturbation methods, and model simplification (Marquardt, 2001). A recent development with a projection method is the balancing of covariance matricies (Hahn et al., 2003). This method reduces a nonlinear model to a variable subspace that captures the most important input to output dynamics. POD, on the other hand, generates an optimal input to state reduced model (Zhang et al., 2003). Perturbation methods are useful for models where there is a large separation of time scales allowing the fast dynamics to be eliminated (Vora and Daoutidis, 2001). Model simplification is a general classification of methods that includes linearization.

The aim of computational reduction is different than that of model reduction. In model reduction, the focus is on reducing the order of the system while maintaining the most important dynamics. In computational reduction, the goal is to retain all of the system dynamics while substantially lowering the computational cost. This review of previous work focuses on computational reduction for the simulation of nonlinear models. Three computational reduction approaches relevant to process control are dynamic programming, neural nets and ISAT. All three methods use storage and retrieval of training data to reduce the computation effort to generate the model response. General criteria to benchmark storage and retrieval methods were given by Pope (1997).

1. The CPU time required to create the stored trajectories
2. The memory required for the stored trajectories
3. Inaccuracies in the retrieved mapping (e.g., interpolation errors)
4. The CPU time required to retrieve the mapping
5. The degree to which the technique is generally applicable and can be automated

In the following three sections, dynamic programming, neural nets and ISAT are evaluated by these criteria.

2.1 Dynamic Programming

Dynamic programming was originally proposed by Bellman to solve optimal control problems (Bellman, 1962). The goal of dynamic programming is to find an optimal 'cost-to-go' function, which can be used to solve for an optimal trajectory of inputs as a function of initial states. A major drawback to this method is the "curse of dimensionality", coined by Bellman. The size of the problem grows proportional to N^D, where N is the length of the discretized control horizon and D is the number of states in the model. Other difficulties with dynamic programming are multivariable interpolation and “the menace of the expanding grid”. Recent approaches such as sequential reinforcement learning avoid dynamic programming dimensionality problems by operating on states as they occur sequentially (Barto, 1997). Also, neuro-dynamic programming (Peroni et al., 2003; Bertsekas, 2002) overcomes the curse of dimensionality by approximating the cost-to-go function with a neural net.

2.2 Neural Nets

Neural nets are an effective tool to represent nonlinear models. Neural nets are networks of adaptable nodes which, through a process of learning from task examples, store experimental knowledge and make it available for later use (Aleksander and Morton, 1995). The flexibility and general applicability of neural nets have been demonstrated by diverse applications across many fields of study. Kohonen nets are used in classification and fault detection, n-tuple nets in image processing and vision, and both multi-layer perceptrons and radial basis functions are used in signal processing and control (Warwick, 1995). Neural nets are an effective tool to incorporate historical data for use in state estimation and control, although filtering and preconditioning the plant data are often time-consuming tasks (Qin, 1997). One limitation of neural nets is the inability to extrapolate outside the training domain. Because of the history of success in control applications, we will compare neural net performance in evaluating ISAT.

2.3 ISAT in Turbulent Combustion

Detailed combustion models typically include reactants, products, and reaction intermediates that result from hundreds of reactions. These reaction timescales can range from 10^{-9} sec to 1 sec. Models with a large range of timescales produce a stiff system that is difficult to integrate.

Analytical and numerical tools have been developed to optimally reduce the kinetic models. Some of these tools include a sensitivity analysis or principal component analysis and species lumping procedures (Tomlin et al., 1997). Another tool is computational singular perturbation (CSP) as a formal way to apply partial-equilibrium approximations on an *a priori* basis (Lam and Goussis, 1988).

Many of the methods for creating reduced mechanisms rely on steady-state or partial-equilibrium approximations. However, the reduced mechanisms are generally limited to a range of temperature, pressure, and/or species’ concentrations, known as the thermochemical space. Outside of this defined space, large errors can occur. To overcome this deficiency, Mass and Pope proposed a new method for reducing chemical kinetics based on intrinsic low-dimensional manifolds (ILDM) (Maas and Pope, 1992a and 1992b). However, the ILDM method also had the following drawbacks (Yang and Pope, 1998).

1. Storage requirements increase dramatically as the manifold dimension increases.
2. The entire thermochemical space must be calculated for a fixed dimensional manifold that cannot be easily adapted when a higher dimensional manifold is required.
3. For higher dimensional manifolds, the work to retrieve information is not trivial.
4. There is a lack of dynamic error control.

Pope developed ISAT to overcome the shortcomings of the ILDM method (Pope, 1997). The ISAT method calculates and stores the data *in situ* rather than as a preprocessing step. Thus, only areas of the thermochemical space that are accessed are included in the database. Another benefit of ISAT is the addition of error control that guarantees with a high probability that the retrieved data is within a specified error tolerance. In a turbulent flame simulation, a reduction by a factor of 1000 in the computational effort was demonstrated (Pope, 1997).

Consider how ISAT reduces computational time of the chemistry integrations in turbulent flames. As a first step, the chemistry integration is isolated from other physical simulations, such as mixing, by one of many splitting schemes. During the course of the simulation, integration queries consisting of initial states ($x_{initial}$), an integration time (Δt), and an error tolerance for x_{final} (ε_{tol}) are sent to ISAT many times. ISAT returns the final states (x_{final}) of the chemistry integration within the specified error tolerance (see Figure 1).

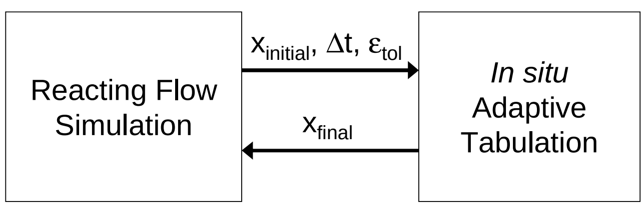

Figure 1 - Reacting Flow Simulation with ISAT

For a NMPC application, the splitting is accomplished by choosing a sequential optimization approach rather than a simultaneous approach. In the simultaneous approach, the inputs and states are solved together after the state derivatives are transformed to states through direct collocation (Binder, 2001). An advantage of the simultaneous approach is that computational effort is not wasted on computing accurate state solutions for suboptimal input solutions. An advantage of the sequential approach is that sub-optimal solutions are available for real-time requirements. Generally, however, the simultaneous approach is generally faster than the sequential approach. ISAT reduces the computational time for the sequential approach by approximating state solutions with stored integrations.

For NMPC the optimizer may also require sensitivities when updating the inputs during the optimization. The computation of sensitivities can be very expensive, especially for large models. ISAT already calculates and stores sensitivities so the sensitivity (A) can be returned with the integration (see Figure 2).

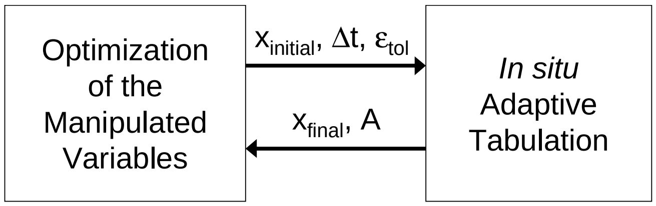

Figure 2 - NMPC with ISAT

For turbulent combustion simulations the sensitivities are not used. For sequential NMPC, the sensitivities are valuable in saving computational effort. In this way ISAT is actually better suited for process control than for the original application for which it was developed!

Once ISAT receives an integration request, it performs one of three scenarios. In the first scenario, the query ($\phi = x_{initial}$) is inside a region of accuracy termed the ellipsoid of accuracy (EOA), centered about a close stored record, ϕ_1 (see Figure 3). This scenario is extremely fast because a stored integration serves as an approximation to the integration query.

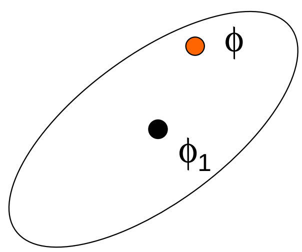

Figure 3 - ISAT Retrieval

In the second scenario, the query is outside the EOA but inside the final state error tolerance. In this case, the EOA is expanded to include the new initial state (see Figure 4). An integration of the chemistry model must be performed to determine if the final states are within the specified error tolerance. For this scenario, there is no computational advantage of ISAT over direct integration.

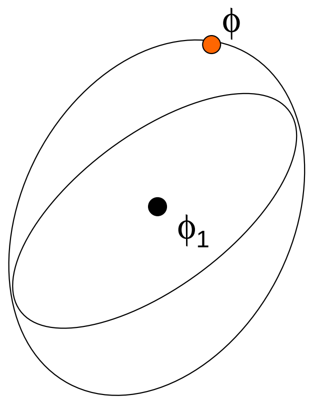

Figure 4 - ISAT Growth

In the final scenario, the query is outside the EOA and outside the final state integration tolerance. A new ISAT record is added with an initial EOA based on the state sensitivity matrix. This is the most computationally challenging of the three scenarios as the sensitivities of each variable are computed.

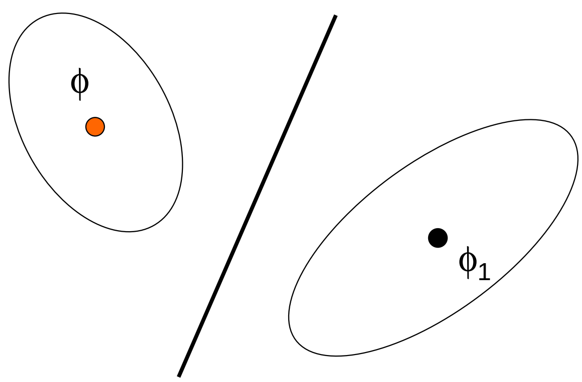

Figure 5 - ISAT Addition

As the database of integrations is built, the time required to find a close record grows. Sequential searching requires O(N) operations where N is the number of records stored in the database. An alternative to sequential searching is through a binary tree structure that requires $O(\log_2(N))$ operations. The binary tree has a structure shown in Figure 6.

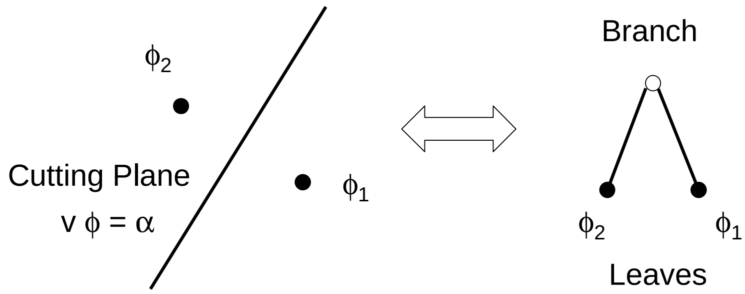

Figure 6: Binary Tree Structure

The cutting plane is defined by the vector v and scalar α shown in Equations 1 and 2, respectively.

$$v = \phi_2 - \phi_1 \tag{1}$$

$$\alpha = v^T \left(\frac{\phi_2 + \phi_1}{2} \right) \tag{2}$$

When $v^T\phi_i$ is less than α, ϕ_i is closer to ϕ_1 and when $v^T\phi_i$ is greater than α, ϕ_2 should be chosen as the closer record. If ϕ_i is closer to ϕ_1, but still not within the specified tolerance, then ϕ_i is integrated to ϕ_f and the tree is grown (see Figure 7).

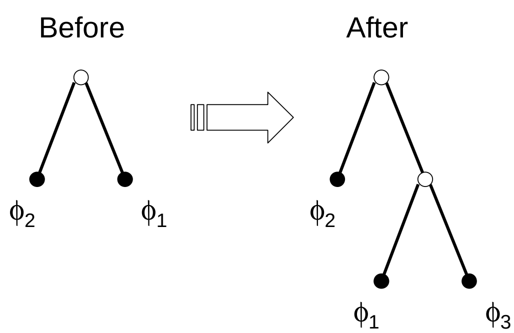

Figure 7: Binary Tree Growth

Since Pope first published the ISAT method, there have been numerous applications of ISAT in combustion to simulations that were previously quite formidable. Saxena and Pope (1998, 1999) simulated a piloted jet diffusion flame of CH_4-air with 16 species and 41 reactions. A significant speedup was not reported because the chemistry calculations took only 60% of the total CPU time. Shah and Fox (1999) performed CFD simulations of methane thermochlorination reactors involving 38 species with a speedup of 138 over direct integration. They also mentioned that ISAT has been successfully applied to a mechanism with 116 species and 447 reactions, although no further details were given. Xu and Pope (2000) performed another simulation of piloted jet flames of methane with a parallel implementation of ISAT with an estimated speedup of 40. It is likely that ISAT will be used more frequently with its recent integration into the popular CFD software, Fluent™ (Fluent, 2003).

There has been some interest in reducing the storage requirements for ISAT. Tang and Pope developed an extension that combines ISAT and model reduction through rate-controlled constrained equilibrium, abbreviated ISAT-RCCE (Tang and Pope, 2002). ISAT-RCCE as applied to a mechanism with 32 species and 175 reactions shows a speedup factor of 500 over direct integration. Another method to reduce storage was proposed by Chen et al. (2000). The ISAT database is replaced by a neural net, thereby reducing the storage requirement from ~100 MB to ~1 MB. Even though there is a savings in memory, there is a loss of error control. The authors mention that by using a neural net, extrapolation would produce unpredictable results and that ISAT should be used for points outside the training domain.

3 Illustrative Examples

ISAT was implemented in MATLAB based on Pope's original work (Pope, 1997). In the first example, the computational reduction of ISAT is tested for full and reduced ODE and DAE models. In the second example, neural nets and ISAT are compared in open loop and closed loop step tests.

3.1 ISAT Applications in NMPC

As a proof of concept, ISAT was implemented in a simple direct single shooting implementation of NMPC in MATLAB. This implementation was tested with three distillation column models that have similar dynamics but have a range of states and form. To reduce the computational time, the control and prediction horizons were limited to 2 times and 3 times the sampling interval, respectively. In addition, the sampling interval was purposely lengthened to capture only a coarse response of the system. The focus of this implementation is not the optimality of the NMPC routine, but as a test of potential for the future application of ISAT in more efficient NMPC algorithms. A list of each model along with some basic properties is shown in Table 1.

Table 1 - Distillation Models

ID	Model Description	Type	States
1	Distillation column with constant relative volatility and reduced with balanced empirical gramians	ODE	5
2	Distillation column with constant relative volatility	ODE	32
3	Distillation column	DAE	64

The two ODE models of a 30 tray binary distillation column are from Hahn and Edgar (2002) while the DAE model is a slight modification by dropping the assumption of constant P/P_i^{sat} and using the Wilson equations for the VLE relationships. Combining model reduction through model reduction and computational reduction through ISAT exploits the strengths of both methods. Generally, the model reduction step decreases the number of dynamic variables but does not have sufficient computational speed-up. Computational reduction is more effective with a low number of dynamic variables and can reduce the computational time significantly. Figure 8 provides an overview of the combined approach.

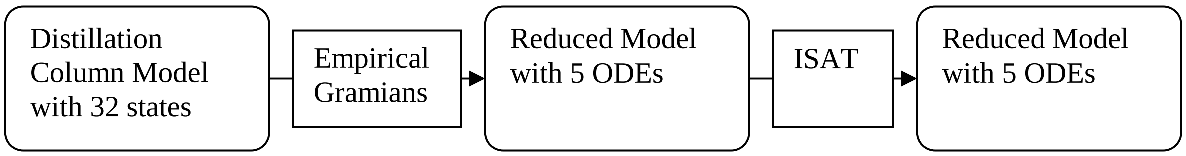

Figure 8: Combining Model Reduction and Computational Reduction

For each model, a set point tracking simulation was performed to build the ISAT database. Once sufficient training was performed, a closed loop step test was performed as a test of ISAT computational reduction. A soft constraint limited the reflux ratio to a range of between 2 and 4. For each model two plots are displayed of the closed loop step test (see Figures 9-12). Computational times are from a Windows version of MATLAB 5.3 running on a 2000 MHz Celeron processor.

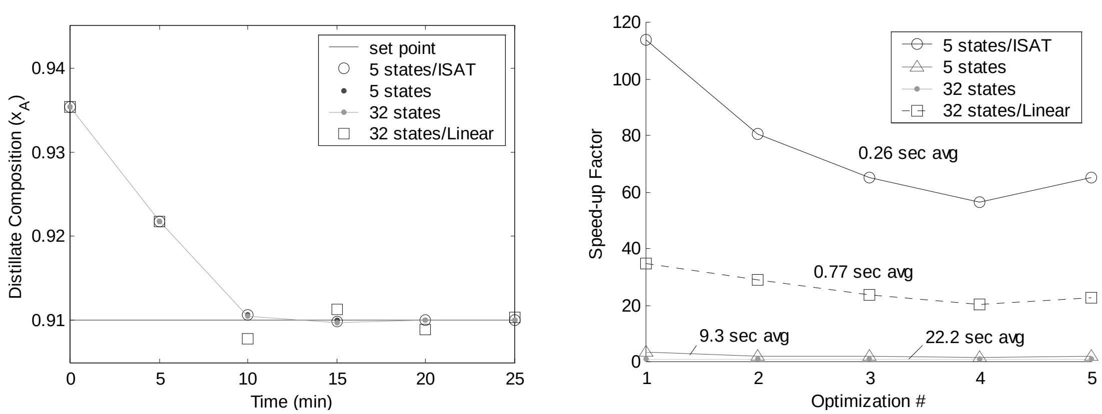

Figure 9 - Model 1 Closed Loop Response

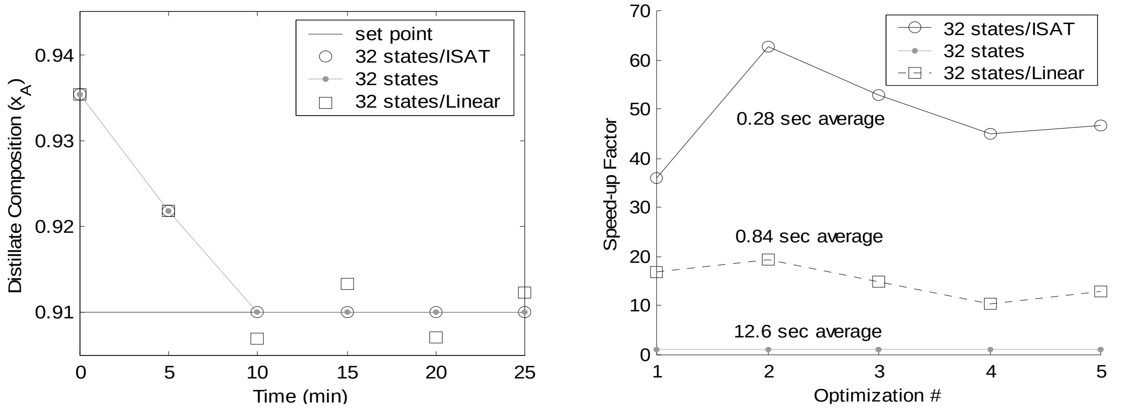

Figure 10 - Model 2 Closed Loop Response

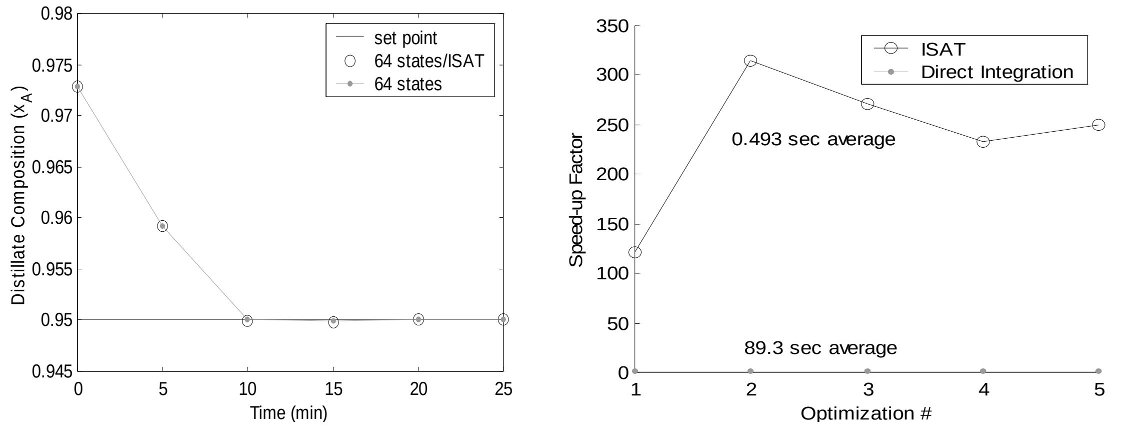

Figure 11 - Model 3 Closed Loop Response

For this distillation column example, ISAT maintains the accuracy of the nonlinear controller while achieving the speed of linear MPC. The average computational speedups were 85, 45, and 181 for models 1, 2, and 3, respectively. For models 2 and 3, the speedup was below average on the first optimization. This was due to ISAT growths that were slower than ISAT retrievals. Another observation is that the speedup drops after the second optimization. In this case, ISAT does not slow down, but the full state NMPC routine is faster because steady state is reached and the optimization is faster.

3.2 Neural Net vs. ISAT

As an illustrative example, ISAT and a neural net are compared in an open loop step test and a closed loop control application. The example model was a dual CSTR model (see Figure 12) with 1 manipulated variable (heat addition to the first tank), 6 states, and 1 controlled variable (temperature of the second reactor). The model was developed by Hahn and Edgar (2002) as a benchmark model for nonlinear model reduction. Appendix A contains a more detailed description of the model.

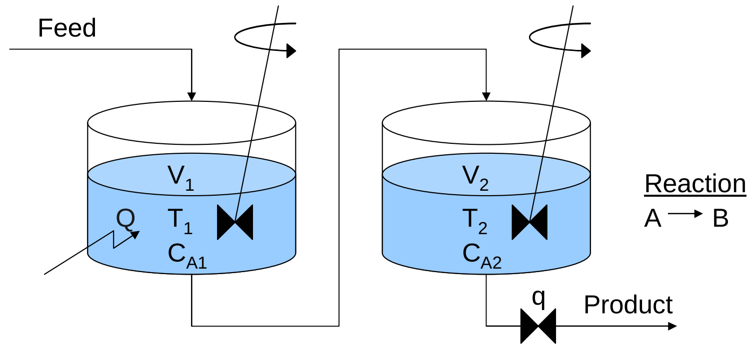

Figure 12 - Dual CSTR

The data were gathered from ISAT training. For the sake of comparison, the neural net used the ISAT training data. The neural net was constructed with one hidden layer of a hyperbolic tangent sigmoid transfer function and an output layer of a linear transfer function (Figure 13).

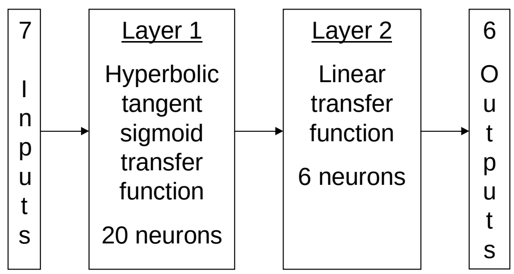

Figure 13 - Neural Net Structure

The neural net was trained for over an hour of CPU time with a 2000 MHz Celeron processor using ~1600 data sets. Before the training, the data were appropriately scaled for efficient implementation in the neural net. Figure 14 shows a large open loop step test, one that is outside those found in the training data. In this step test, the cooling is increased to the point that the irreversible reaction is extinguished and a large temperature step results.

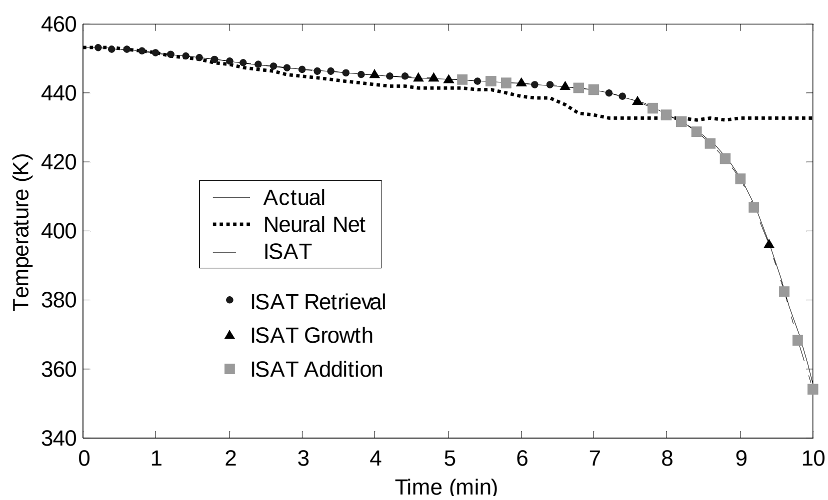

Figure 14 - Open Loop Step Test

Up to about 5 minutes of simulation, the neural net and ISAT perform similarly. To this point both were accessing data that were within the training domain. Beyond 5 minutes ISAT is superior in agreement with the non-reduced model due to a built in error checking strategy. Before 5 minutes, the ISAT method shows that it performs mostly retrievals indicated by the round dots. Once ISAT detects large errors from retrievals, it starts adding and growing records, indicated by the squares and triangles, respectively. If the step response were to extend further in time to a new steady state, the points would again become dots, indicating database retrievals.

ISAT and the neural net were compared in a closed loop simulation with a 'small' step change inside the training domain (Figure 15).

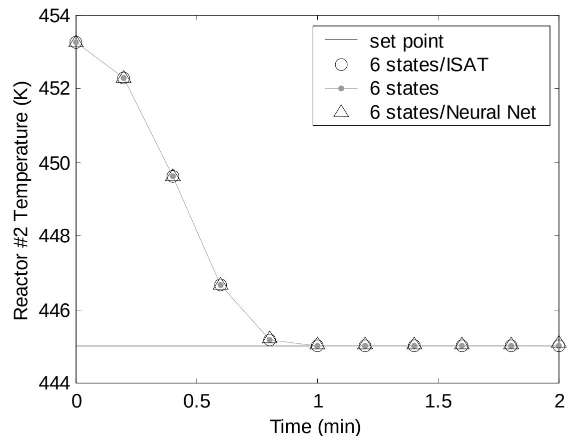

Figure 15 - Small Closed Loop Step Test

All three responses show excellent agreement as they reach the new set point along the same trajectory. Next, a 'large' step change was performed to access a region of state space outside of the training domain (see Figure 16).

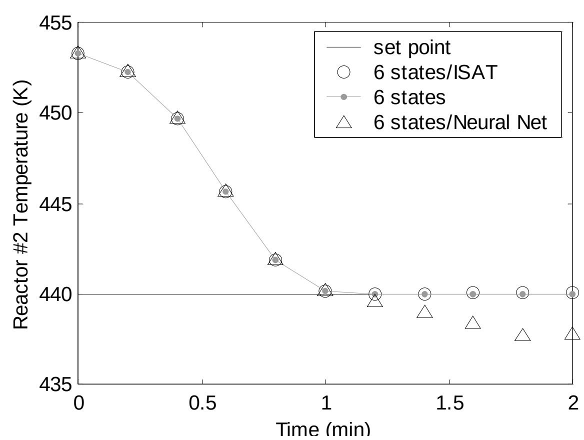

Figure 16 - Large Closed Loop Step Test

For this step change, the neural net controller eventually becomes unstable. This is because the neural net does not have the capability to extrapolate outside of the data that was used to train it. In this respect, the ISAT method is superior because it detects when it has gone outside of the training domain and integrates the model to generate and add new data to the training set.

4 Future Work

ISAT was originally developed to reduce the overall simulation time. In contrast, for NMPC the controller must act faster than the process that is being controlled. Large time delays can cause stability problems, undesirable plant performance, and loss of profitability. Therefore, ISAT for NMPC must be designed to meet real-time requirements. This may include strategies such as delaying sensitivity computations by one sampling step, generating feasible sub-optimal solutions within the required time, or developing a linear MPC controller to operate as a backup in case the nonlinear MPC controller does not find a solution within the required time. These options will be evaluated to generate optimal control policies considering limited computational resources. Four potential applications of ISAT include dynamic optimization, dynamic data reconciliation, adaptive control, and reactive distillation control. These four areas are discussed in the following sections.

4.1 Dynamic Optimization

ISAT will be implemented in Fortran for use with the Octave NMPC toolbox (Tenny et al., 2002) or MUSCOD-II (Leinweber et al., 2002). The NMPC toolbox implements a sequential direct multiple shooting approach to dynamic optimization. The N-step finite-horizon NMPC problem formulation is given by the following.

$$\min_{x,u,\eta} \Phi(x,u,\eta) \quad s.t. \quad x_0 \text{ given}, \; x_{k+1} = F(x_k, u_k), \; Du_k \le d, \; Gx_k - \eta_k \le g, \; \eta_k \ge 0 \qquad (3)$$

In this problem formulation, Φ (the cost function) is typically quadratic in x (states), u (inputs), and η (state constraint violations) and therefore strictly convex. The source of nonlinearity comes from the model function $F(x_k,u_k)$ that is solved by integrating the DAE model. ISAT fits into the NMPC scheme by storing and retrieving integrations of the model.

Previous experience with the NMPC toolbox in Octave revealed that sensitivity calculations were so expensive that a finite-difference Hessian required an inordinate amount of time. Other Hessian updating procedures also suffered from problems such as the inability to maintain sparsity or failure due to unpredictable causes. An unexplored feature of ISAT is the ability to provide an approximation of the sensitivities. Since ISAT computes and stores sensitivities internally, a new method will be developed to update the Hessian. This method will optimally exploit the information from the stored sensitivities and include error control.

Chemical process models may include hundreds of algebraic and differential equations that would make the computation of sensitivities computationally infeasible. Before ISAT can be applied successfully, the most important process dynamics must be extracted through model reduction. Proper orthogonal decomposition (POD) or balanced empirical gramians are optimal in that the reduced model is optimal given the reduced order. As a preprocessing step, simulation data will used to compute an optimal eigenfuction basis for the differential states. The algebraic states are not reduced through model reduction. One possible strategy to reduce the algebraic states is through sequential reinforcement learning (Barto, 1997). The algorithm will transform the algebraic states into an explicit function of the reduced differential states. This strategy will also allow training of a neural net to occur sequentially as new data are generated from ISAT.

4.2 Dynamic Data Reconciliation

Data reconciliation is necessary for NMPC when modeled states are not directly measured or data uncertainty is high due to noise (Liebman et al., 1992). ISAT can be employed in a sequential direct multiple shooting approach to data reconciliation. The N-step finite-horizon problem formulation is given by the following.

$$\min_{x,\eta} \Phi(x,\eta,y) \overset{def}{=} \sum_{k=-N}^{-1} \left[C(x_k, y_k) + \Xi(\eta_k) \right] + C(x_0, y_0) + \Xi(\eta_0) \quad s.t. \tag{4a}$$

$$y \ given, u \ given, \ x_{k+1} = F(x_k, u_k), \ Gx_k - \eta_k \le g, \ \eta_k \ge 0 \tag{4b}$$

This formulation is similar to the dynamic optimization problem but instead of finding optimal inputs, optimal states are found that agree with the measured data (y). The terminal constraint was added to allow a different cost function for the most current measurement. With model-plant mismatch, the most current measurement should be the most reliable and should therefore receive a greater weighting in the optimization.

ISAT will be used in data reconciliation by storing and retrieving integrations of the nonlinear model. As in dynamic optimization, the state sensitivities stored in ISAT can be used to provide an approximation of the Hessian. Data reconciliation must occur before dynamic optimization in order to provide an estimate of the initial states (x_0). It is critical for a real-time controller to operate faster than the dynamics of the process it is controlling. ISAT will be applied in the Octave NMPC toolbox for dynamic data reconciliation and optimization to reduce the computational cost necessary for real-time control.

4.3 Nonlinear Adaptive Control

The dynamics of a controlled process can change due to fouling, disturbances, unusual operating states, ambient variations, and changes in product specifications (Seborg et al., 2004). When the process dynamics change significantly, an adaptive controller is automatically tuned to provide satisfactory closed loop performance. Adaptive control can be achieved in the NMPC framework with the addition of adjustable parameters (p) in the nonlinear model.

$$\begin{aligned} \frac{dx}{dt} &= f(x(t), u(t), p) \\ 0 &= g(x(t), u(t), p) \end{aligned} \tag{5}$$

The adjustable parameters can be obtained from a first principles model of the disturbance or a least squares optimization of the model using plant historical data. The addition of adjustable parameters poses an interesting challenge for ISAT's error control strategy. Since ISAT is a storage and retrieval method, drastically changing the parameters can invalidate the stored data. Therefore, a strategy will be devised to gradually change the parameters and simultaneously filter out the unaccessed data. By controlling the parameter transition, ISAT will still show significant computational reduction over the original NMPC. Another advantage of gradual parameter transition is that it avoids possible instabilities that can occur by switching controllers on-line. Gradual parameter transition is a natural expression of the process dynamics when the system dynamics change slowly, such as for fouling or catalyst deactivation.

There may be some situations where the parameter transition should occur quickly (i.e. grade changes, large disturbances). In these situations, a gradual parameter transition is not appropriate. For a large change in the parameters, the ISAT database will provide a first order approximation to the nonlinear model integration while new sensitivities are computed. In this way the real-time controller requirements are automatically met with a simplified model. Once the ISAT database is rebuilt, the controller will improve according to the predictive capabilities of the full nonlinear model.

4.4 Reactive Distillation Modeling and Control

A challenging nonlinear control application is reactive distillation (RD) for the production of tert-amyl methyl ether (TAME). In RD both the conversion and product purity must be controlled. Manipulated variables include reflux ratio, reboiler duty, feed rate, pressure, and bottoms flow rate. First principles models of RD have been developed (Peng et. al., 2003) that include between 320 and 866 differential equations and 5596 and 24,522 algebraic equations. A final step for the modeling of RD will occur when experimental data become available. These experimental data will be used to select the appropriate assumptions that affect the model complexity. Another function of experimental data is to fit model parameters that were previously estimated. Fitting model parameters in a first principles model results in a hybrid model that should include excellent extrapolative properties. Once the reliable hybrid model is available, the control system can be developed.

A previous application of NMPC for distillation (Diehl, 2001) indicates that a divided control system reduces the sensitivity to time delays. Three processes (data acquisition, data reconciliation, and dynamic optimization) ran independently and communicated via input and output files. This idea will be extended to RD control with ISAT. Three processes (data acquisition, data reconciliation with dynamic optimization, and ISAT database building) will run on separate systems and communicate via input and output files. Data reconciliation and dynamic optimization will be run together because both occur successively when new measurements are received. ISAT database building will occur separately to eliminate the computational lag associated with computing the state, input, and parameter sensitivities. Updated versions of the ISAT database will be periodically transferred to the NMPC controller.

5 Summary of Contributions

This proposal outlines the application of ISAT for control. Modifications will be made to ISAT for real-time control and to interface with existing NMPC software. In addition to data reconciliation and dynamic optimization, other applications for ISAT in control will be explored. Nonlinear adaptive control with ISAT will be developed to design control systems that perform well under slow and fast changes in the process dynamics. The ability to adapt to changing process dynamics is an essential characteristic of a long-term control solution. In a comprehensive test of ISAT's effectiveness, real-time control of RD will be performed. With the size of the RD model, this control application will be the largest known application of real-time NMPC. This project also represents an effort to bridge the gap between modeling and control. Up to this point, models used for simulation were too large to be used for control. In this project, a complete simulation model will be used for RD control, thereby eliminating many of the deficiencies imposed by simplifying assumptions or model reduction.

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Appendix A

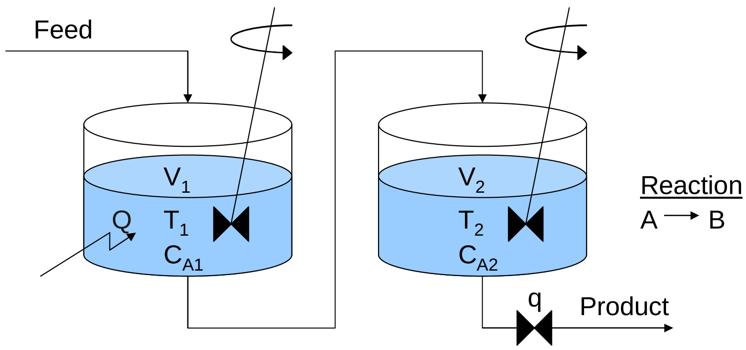
Description: Dual CSTR with an exothermic first-order reaction.

Inputs (2):
u Valve position at the outlet of reactor #2 (dimensionless)
Q Cooling heat flow from reactor #1 (J/sec)

States (6):
V_1 Volume of reactor #1 (m^3)
C_{A1} Concentration of A in reactor #1 (mol/m^3)
T_1 Temperature of reactor #1 (K)
V_2 Volume of reactor #2 (m^3)
C_{A2} Concentration of A in reactor #2 (mol/m^3)
T_2 Temperature of reactor #2 (K)

Other Parameters:
C_{AF} Concentration of A in the feed (mol/m^3)
T_F Feed temperature (K)
q_F Feed flow rate (mol/sec)
q_1 Flow rate out of reactor #1 (mol/sec)
q_2 Flow rate out of reactor #2 (mol/sec)
k_0 Pre-exponential factor (mol/m^3-sec)
E Activation energy (J/mol)
R Universal gas constant (8.31451 J/mol-K)
ρ Density of the liquid (kg/mol)
c_p Heat capacity of the liquid (J/kg-K)
ΔH Energy of reaction (J/mol)
c Constant relating valve position to flow rate (mol/sec-$m^{3/2}$)

Diagram:



Equations:

Flow rates

$$q_1 = c\sqrt{V_1 - V_2}$$

$$q_2 = c\sqrt{V_1}u$$

Reactor #1

Volume balance $$\frac{dV_1}{dt} = q_F - q_1$$

Component balance $$\frac{d(V_1 C_{A1})}{dt} = q_F C_{AF} - q_1 C_{A1} - k_0 C_{A1} V_1 \exp\left(-\frac{E}{RT_1}\right)$$

Energy balance $$\frac{d(V_1 T_1)}{dt} = q_F T_F - q_1 T_1 + \frac{\Delta H}{\rho c_p}\left(k_0 C_{A1} V_1 \exp\left(-\frac{E}{RT_1}\right)\right) - V_1 Q$$

Reactor #2

Volume balance $$\frac{dV_2}{dt} = q_1 - q_2$$

Component balance $$\frac{d(V_2 C_{A2})}{dt} = q_1 C_{A1} - q_2 C_{A2} - k_0 C_{A2} V_2 \exp\left(-\frac{E}{RT_2}\right)$$

Energy balance $$\frac{d(V_2 T_2)}{dt} = q_1 T_1 - q_2 T_2 + \frac{\Delta H}{\rho c_p}\left(k_0 C_{A2} V_2 \exp\left(-\frac{E}{RT_2}\right)\right)$$