In Situ Adaptive Tabulation for Real-time Control

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Candidacy Presentation

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Outline

- Previous work
- ISAT: *In situ* adaptive tabulation
- Preliminary results
- Proposed research
- Contributions

The Challenge

- Increase profit margin
  - reduce process variability
  - minimize costs from utilities, feed streams
  - reduce downtime
- Model predictive control (MPC)
  - incorporate fundamental knowledge of the process for tighter control
  - nonlinear model predictive control (NMPC)
  - “nonlinear” refers to the model form used in MPC

The Challenge

- Large scale models have been developed
- Implementing the large scale nonlinear models in MPC is often computationally prohibitive
- Attempts to make NMPC computationally feasible
  - Approximating the explicit solution
  - Dynamic programming
  - Artificial neural networks

Approximate Explicit Solution

- Linear model with constraints
- Piecewise linear approximation to the exact solution
- Pistikopoulos, Bemporad, Morari (2002)

Dynamic Programming

- Dynamic programming by Bellman (1962)
  - Optimal cost-to-go function
  - Works well for NMPC with few states
  - "Curse of dimensionality"
- Recent interest in this approach
  - Approximate cost-to-go function

Dynamic Programming

- Approximation of the cost-to-go function
  - Barto – reinforcement learning (1997)
  - Bertsekas – artificial neural nets (2001)
  - Lee – clustering of cost-to-go functions (2003)

Neural Networks

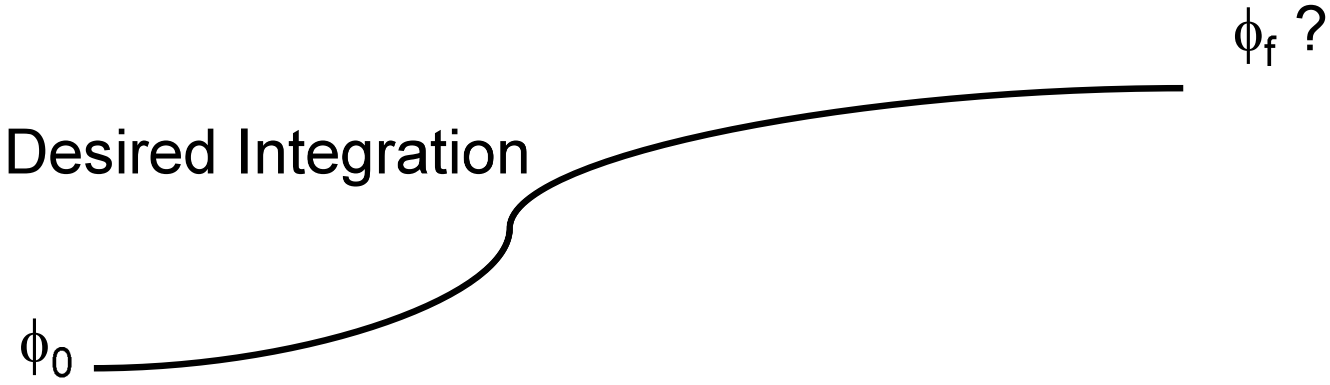
- Ideas have been around for ~50 years
- Increased interest in the last 15 years
- Applications in process control
  - Warwick (1995)
  - Qin (1997)

A New Approach

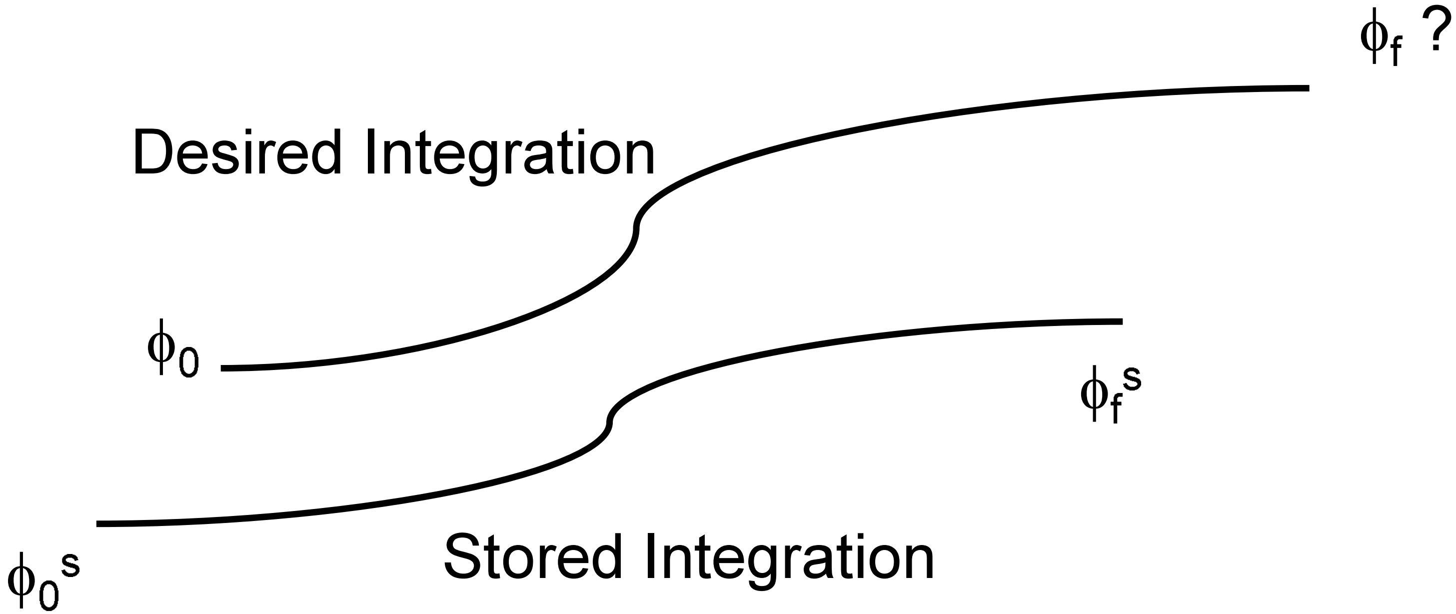
- Turbulent reacting flow simulations can take up to 6 years of CPU time
- Through storage and retrieval of chemistry integrations the simulation time was reduced by 1000x (Pope, 1997)
- Could the same approach work for NMPC?
- Is it applicable to large scale NMPC?

In Situ Adaptive Tabulation (ISAT)

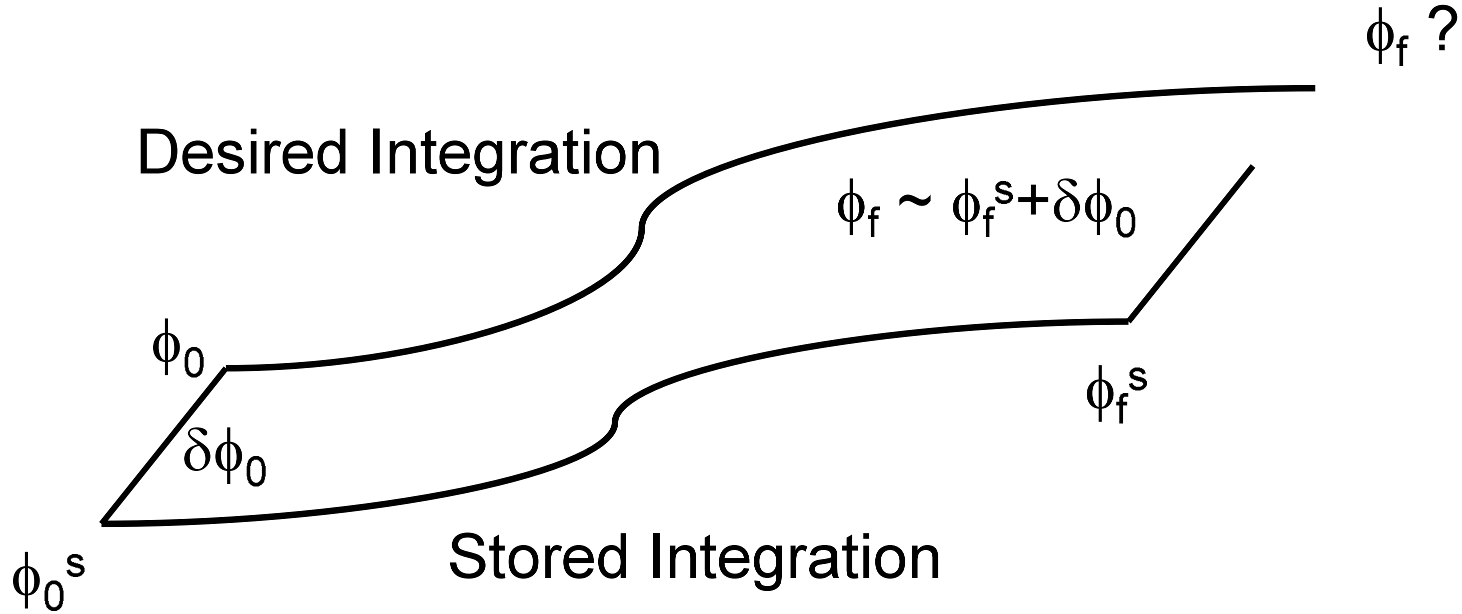
- Developed by Pope for turbulent combustion simulations (1997)
- Integrated with Fluent™



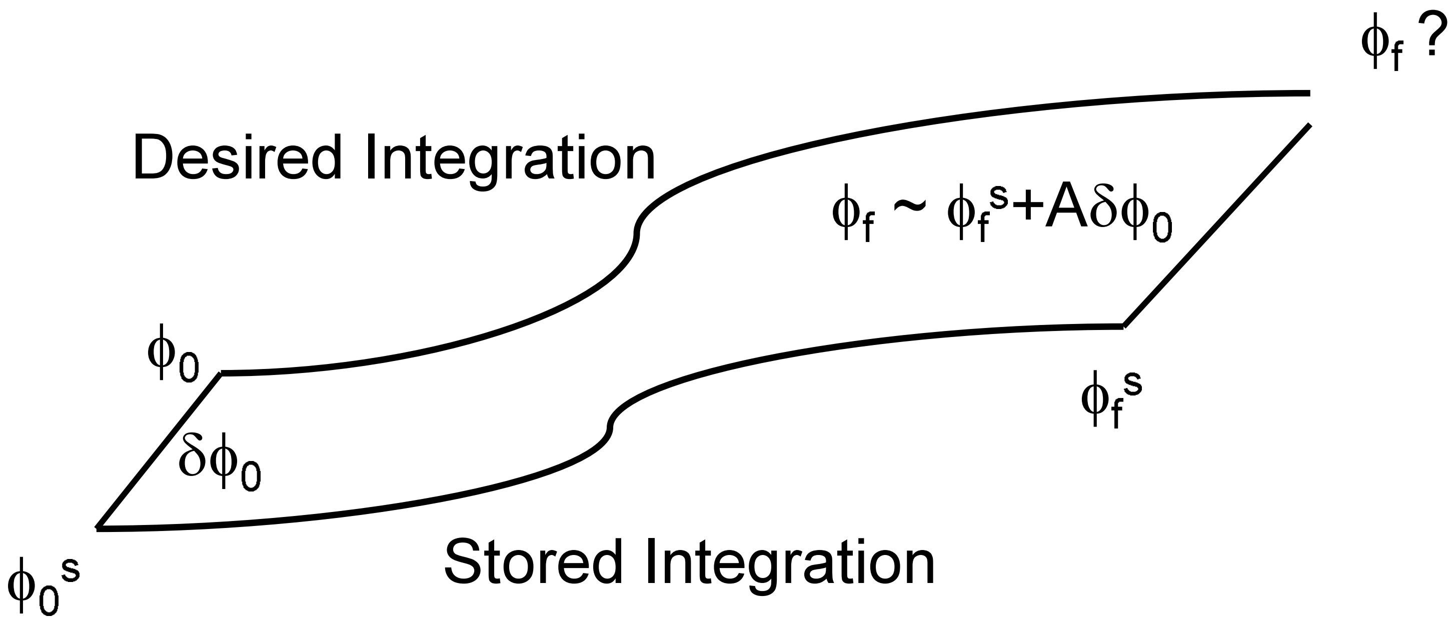
$$\phi = \begin{bmatrix} u \\ x \\ \alpha \end{bmatrix} = \begin{bmatrix} \text{Inputs} \\ \text{States} \\ \text{Parameters} \end{bmatrix}$$



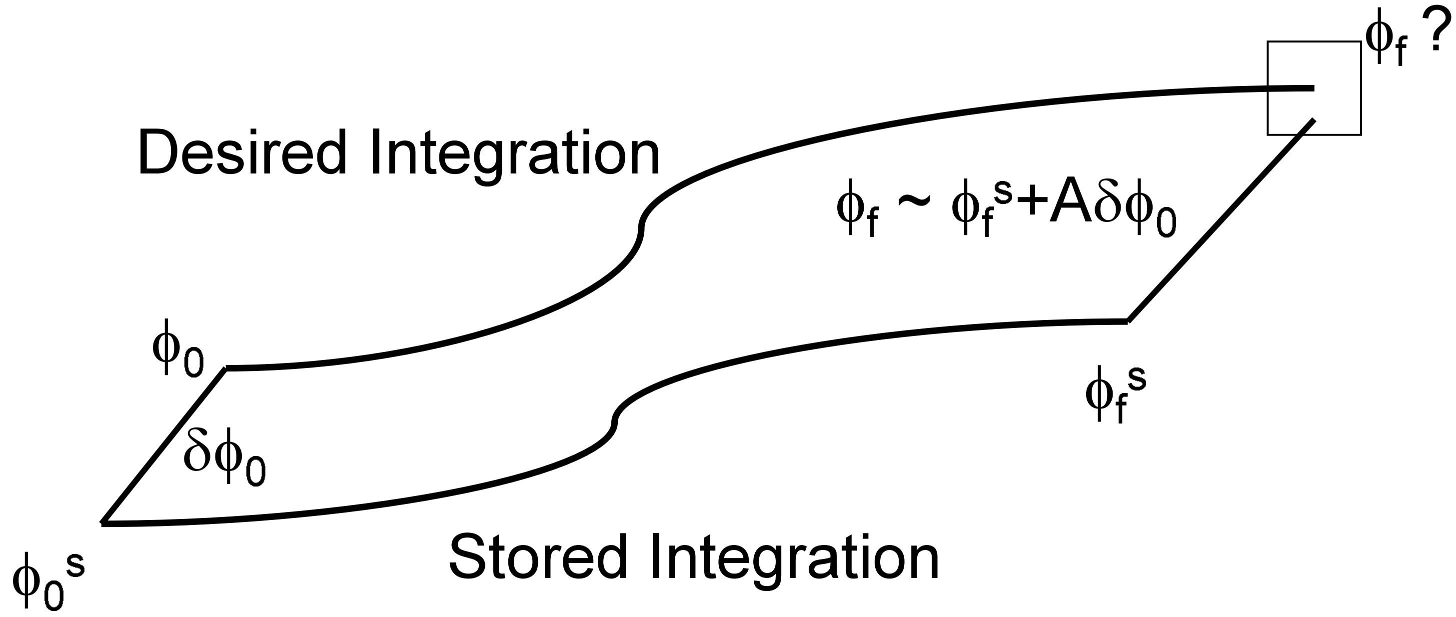
ϕ_f ?
Desired Integration
ϕ_0
ϕ_f^s
ϕ_0^s
Stored Integration



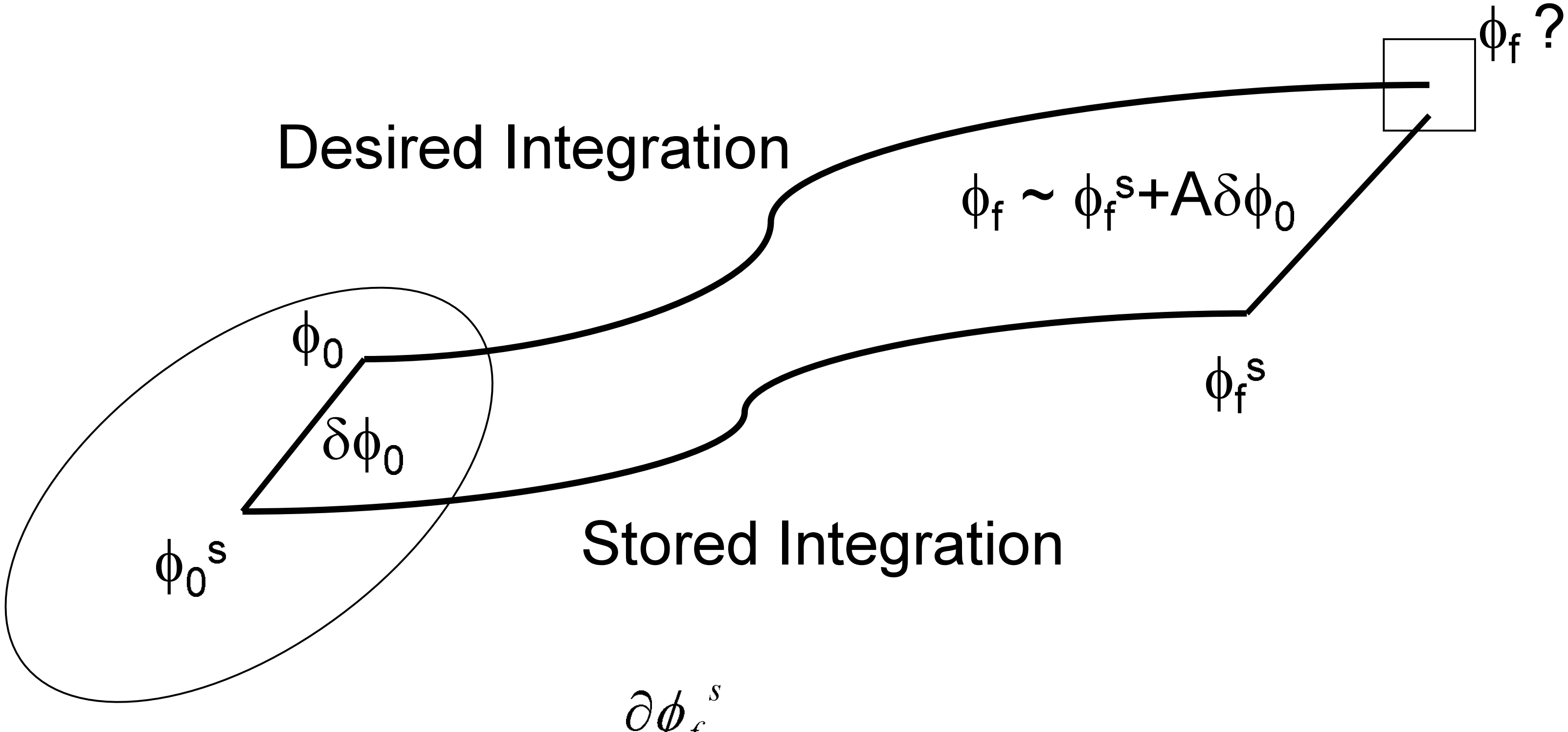
ϕ_f ?
Desired Integration
$\phi_f \sim \phi_f^s + \delta\phi_0$
ϕ_0
ϕ_f^s
$\delta\phi_0$
ϕ_0^s
Stored Integration



$$A = \frac{\partial \phi_f^{\ s}}{\partial \phi_0^{\ s}}$$ First Order Sensitivities



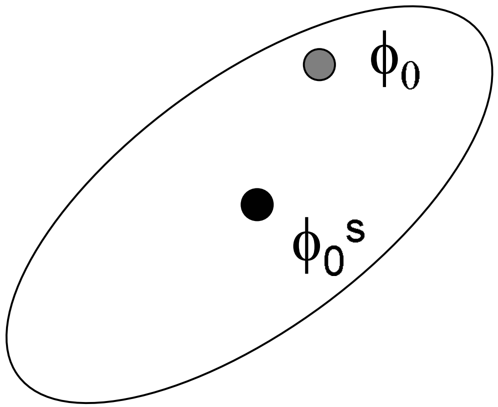
$$A = \frac{\partial \phi_f^{\ s}}{\partial \phi_0^{\ s}}$$ First Order Sensitivities



$$A = \frac{\partial \phi_f^{\ s}}{\partial \phi_0^{\ s}}$$ First Order Sensitivities

ISAT Integration

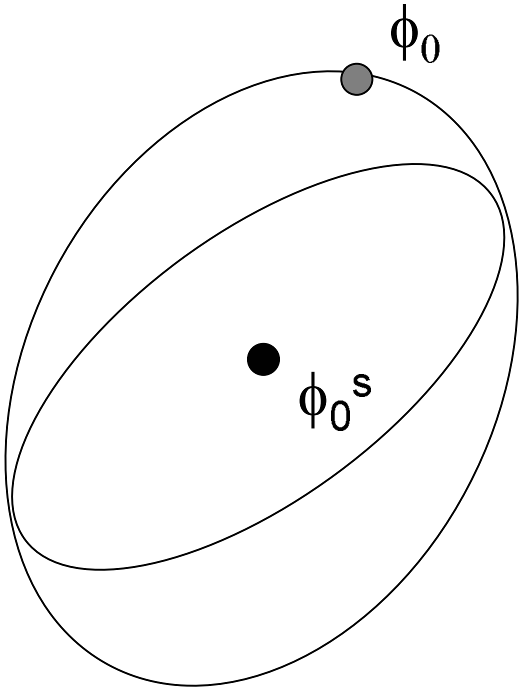
- Scenario #1: Inside the region of accuracy



$$\left(\phi_0 - \phi_0{}^s\right)^T M\left(\phi_0 - \phi_0{}^s\right) \le \varepsilon_{\mathrm{tol}}{}^2$$

ISAT Integration

- Scenario #2: Outside the region of accuracy but within the error tolerance

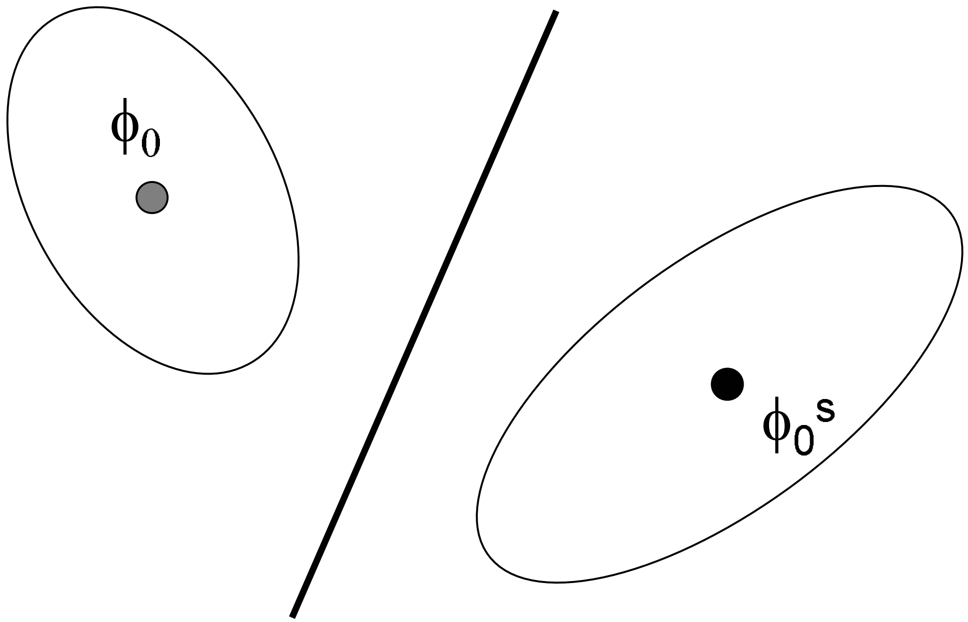


$$\left(\phi_0 - \phi_0{}^s\right)^T M \left(\phi_0 - \phi_0{}^s\right) > \varepsilon_{\text{tol}}{}^2$$

$$\left(\phi_0 - \phi_0{}^s\right)^T M_{\text{expanded}} \left(\phi_0 - \phi_0{}^s\right) = \varepsilon_{\text{tol}}{}^2$$

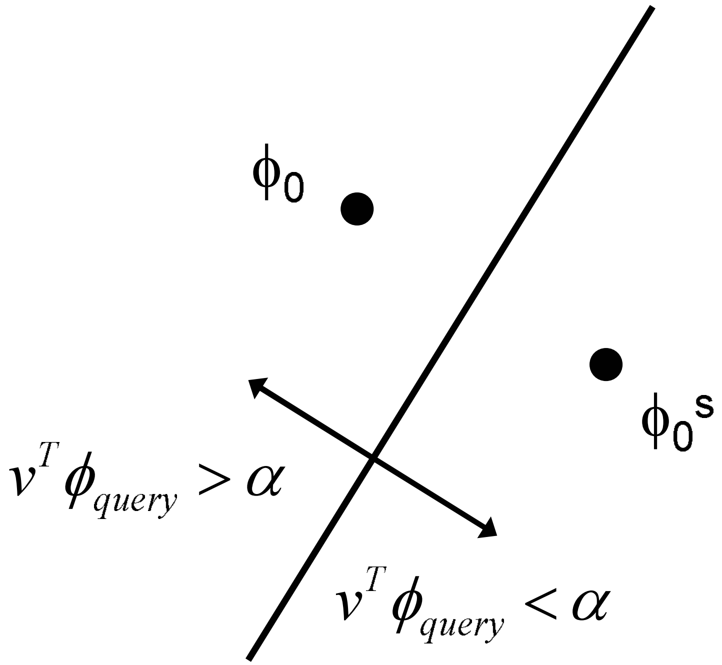
ISAT Integration

- Scenario #3: Outside the region of accuracy and outside the error tolerance



ISAT Search

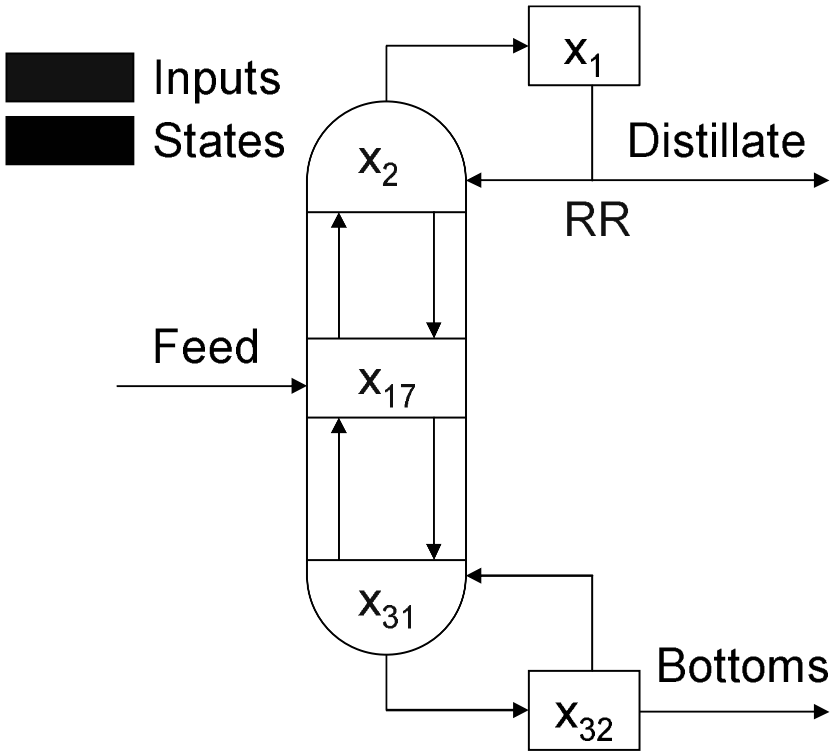
- Binary Tree Architecture
  - Search times are $O(\log_2(N))$ compared with $O(N)$ for a sequential search



$$v = \phi_0 - \phi_0^{\ s}$$

$$\alpha = v^T \left(\frac{\phi_0 + \phi_0^{\ s}}{2} \right)$$

Can ISAT make NMPC computationally feasible?



<u>Test Case</u>

32 state binary distillation column model

MV: reflux ratio

CV: distillate composition

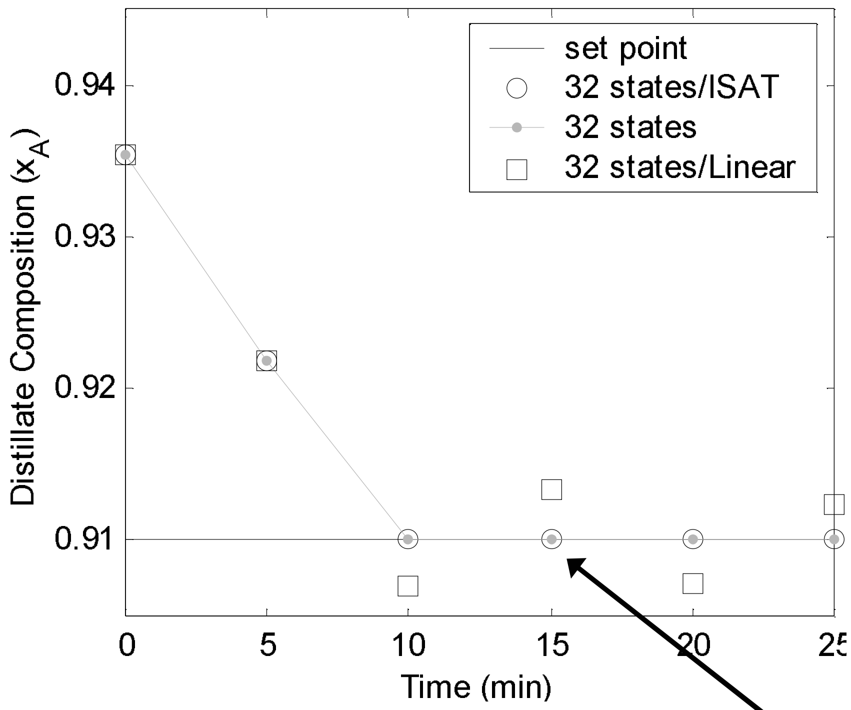
Simplex optimizer

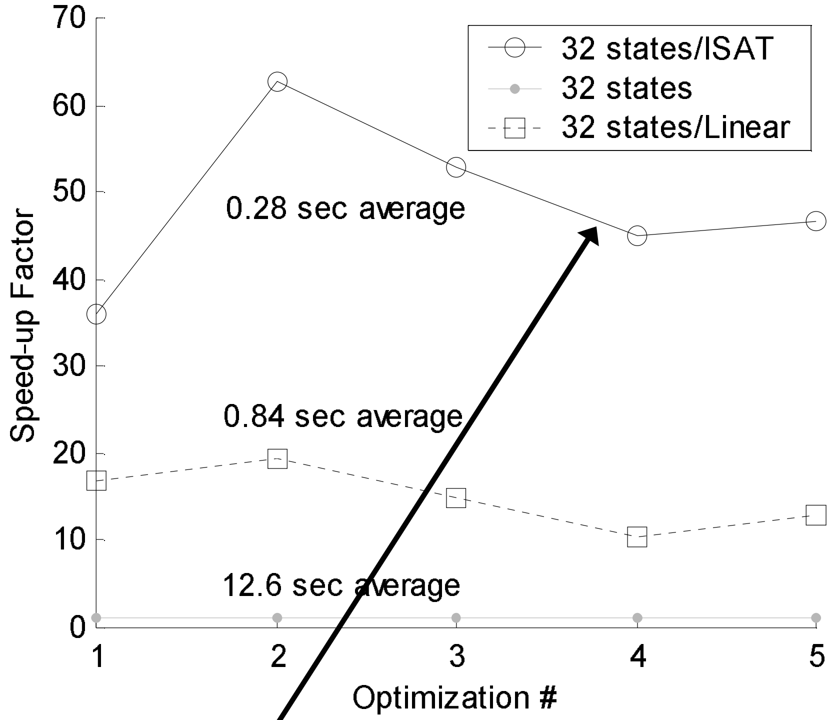
Soft constraint on the MV

Control Horizon = 10 min

Prediction Horizon = 15 min

Closed Loop Response





NMPC with ISAT maintains the accuracy

of NMPC while achieving the computational time of linear MPC

ISAT Preliminary Conclusions

- Successful with ODE and DAE models
- Computational speedup 20 – 500 times
- Storage requirements are under 100 MB
- Performs well for small scale NMPC
  - 96 state DAE model (500x speedup)
- What about large scale NMPC?

Proposed Research

- State and parameter estimation
- Optimal input calculation

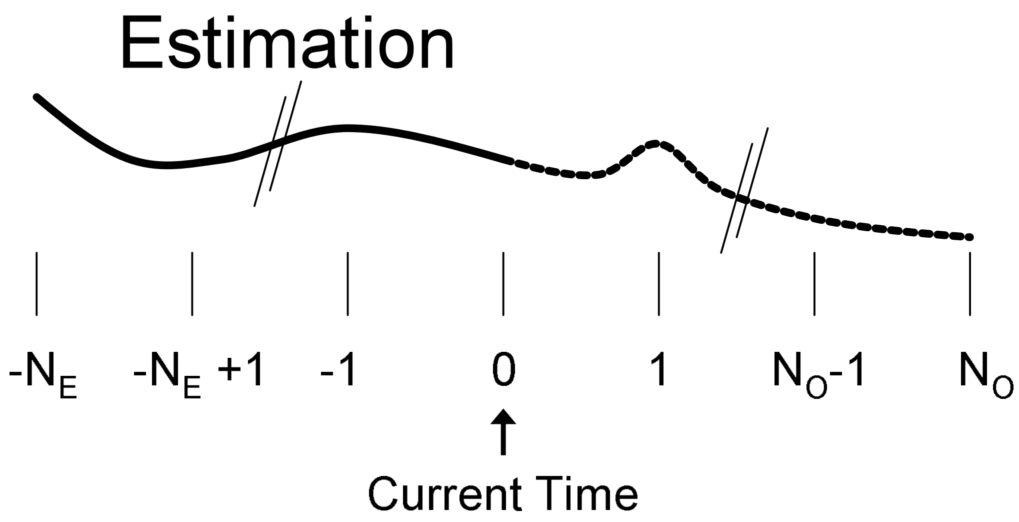
(State and parameter estimation and Optimal input calculation: NMPC)

- Reactive distillation model reduction
- Real-time control of reactive distillation

State and Parameter Estimation

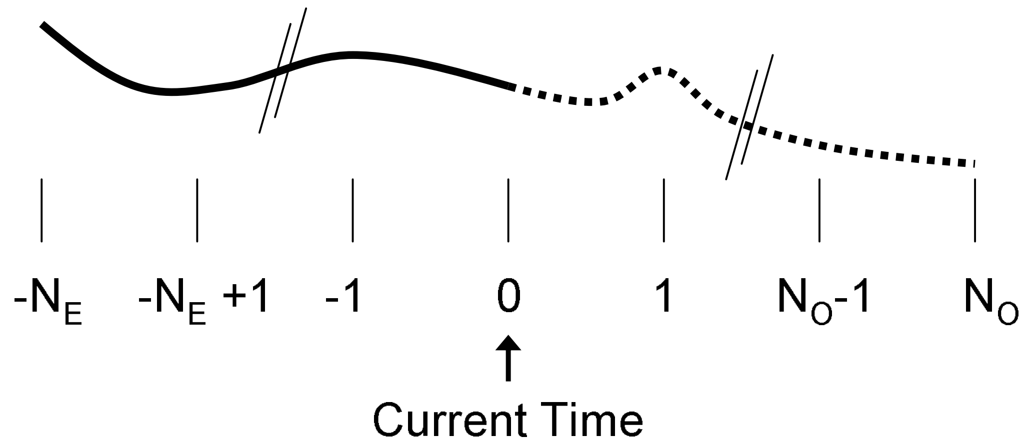
$$\min_{x,\alpha} J(x,y) \stackrel{def}{=} \sum_{k=-N_E}^{0} A(x_k, y_k) \quad s.t.$$

$$y \; given, u \; given, x_{k+1} = F(x_k, u_k), H\alpha \le h$$



State and Parameter Estimation

- Estimation of x,α during real-time control
  - Estimate x before every optimization
  - Frequency of α update is variable
  - New approach to nonlinear model identification



Proposed Research

- State and parameter estimation
- Optimal input calculation

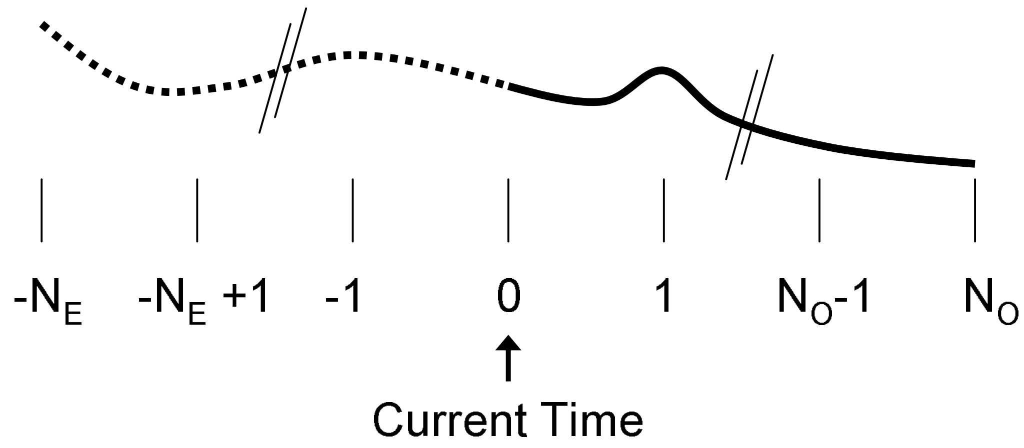
} NMPC

- Reactive distillation model reduction
- Real-time control of reactive distillation

Optimal Inputs

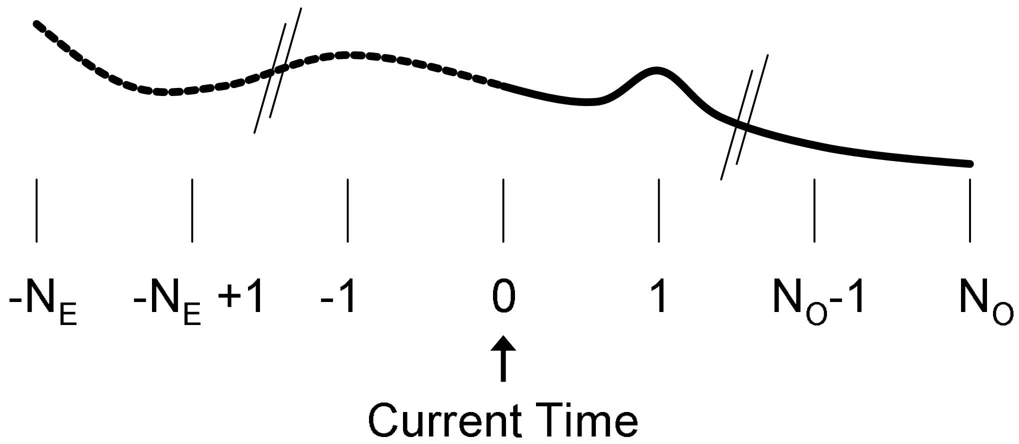
$$\min_{x,u,\eta} J(x,u,\eta) \overset{def}{=} \sum_{k=0}^{N_O} \left[B(x_k,u_k) + E(\eta_k) \right] \quad s.t.$$

$$x_0 \text{ given}, x_{k+1} = F(x_k,u_k), Du_k \le d, Gx_k - \eta_k \le g, \eta_k \ge 0$$



Optimal Inputs

- Calculate optimal path of states by adjusting the inputs
  - Success depends on the state and parameter estimation



Application of ISAT

- Powell's SQP requires 4 results at a given ϕ

Cost Function

$$J(\phi) \quad \text{Integrate with ISAT}$$

$$\frac{dJ(\phi)}{d\phi} \quad \text{Compute sensitivities with ISAT}$$

Constraints

$$C(\phi)$$

$$\frac{dC(\phi)}{d\phi}$$

Proposed Research

- State and parameter estimation
- Optimal input calculation

} NMPC

- Reactive distillation model reduction
- Real-time control of reactive distillation

Reactive Distillation Model Reduction

- Develop model for control
  - Synthesize work by Lextrait, Peng, Hahn, and Rueda
  - Current models (Lextrait and Peng)
    - 320 to 866 differential equations
    - 5596 to 24,522 algebraic equations
  - Optimally reduce the model (Hahn)
  - Experimental verification with Rueda's work on the SRP pilot plant

Reactive Distillation Model Reduction

- Reactive distillation model form

$$\dot{x} = f(\phi)$$
$$0 = g(\phi)$$

$$\phi_{Lower} < \phi < \phi_{Upper}$$

$$\phi = \begin{bmatrix} u \\ x \\ \alpha \end{bmatrix} = \begin{bmatrix} \text{Inputs} \\ \text{States} \\ \text{Parameters} \end{bmatrix}$$

Kinetic parameters, diffusion coefficients, and other uncertain parameters that can be used to fit the model with experimental data

Modeling Conclusions

- Implementing current models in Fortran
- Develop heuristics for the selection of adjustable parameters
  - Long term validity of the model
  - Examples:
    - Catalyst deactivation
    - Fouling of a heat exchanger

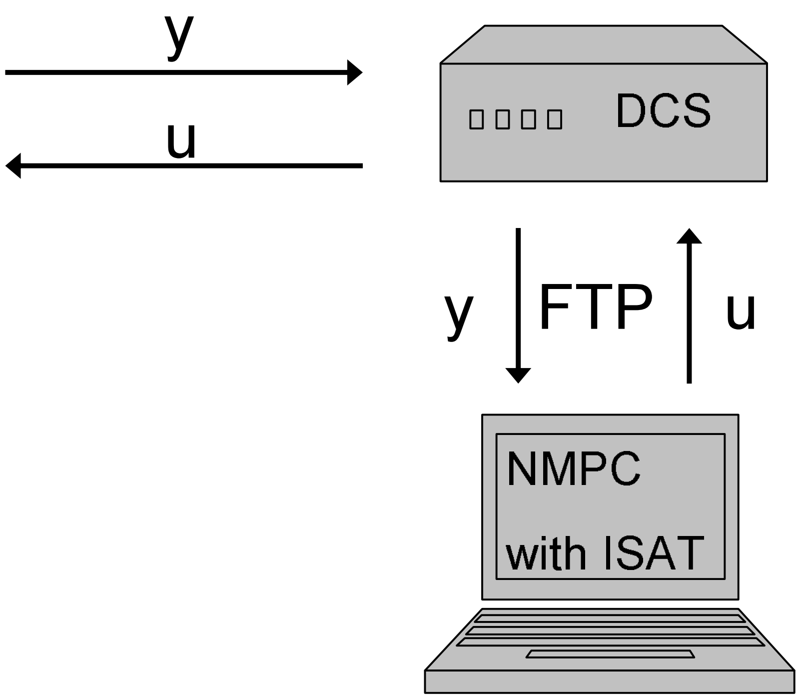
Proposed Research

- State and parameter estimation
- Optimal input calculation

} NMPC

- Reactive distillation model reduction
- Real-time control of reactive distillation

Real time control



Contributions So Far

- Developed 1st ISAT application in process control
- Extended ISAT to DAE systems
- Augmented ISAT with stepwise constant inputs/parameters - allows hybrid systems
- Developed ISAT in MATLAB, Octave, and Fortran
- Compared ISAT to neural networks for open-loop and closed loop simulations
- Conducted preliminary tests of ISAT with NMPC

Contributions So Far

- Developed regulator and state estimator in Fortran
  - SQP code by Powell (HSL VF13)
  - “Watchdog” approach for constraints

Summary of Future Contributions

- Nonlinear model identification heuristics
- Real-time control software package
- Largest model application of ISAT (>5000 states)
- Real-time NMPC of reactive distillation

Publications and Presentations

Presented

Hedengren, J. D. and T. F. Edgar, "*In situ* adaptive tabulation for nonlinear MPC," Texas-Wisconsin Modeling and Control Consortium (TWMCC), Madison, WI, 22 Sept. 2003.

Published

Hedengren, J. D. and T. F. Edgar, "Nonlinear MPC computational reduction for real-time control applications," AIChE 2003 National Meeting, presented at Systems and Process Control Poster Session, 19 Nov. 2003.

Submitted

Hedengren, J. D. and T. F. Edgar, "In situ adaptive tabulation for real-time control," American Control Conference (ACC) 2004, Boston, MA.

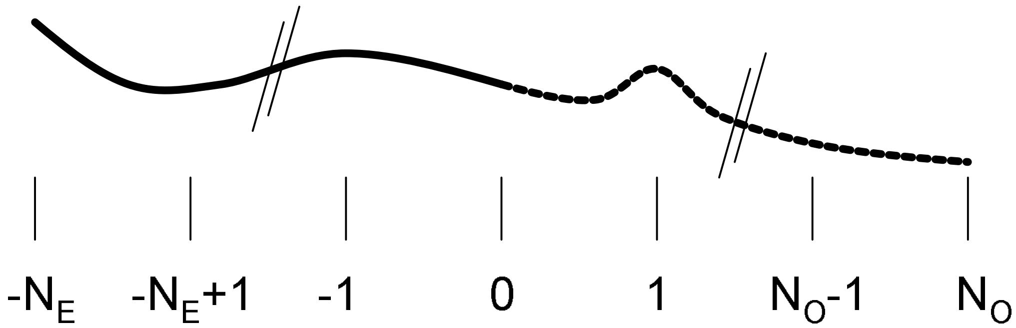
Thank you

Supplemental Slides

- <u>NMPC multiple shooting formulation</u>
- <u>Replacing the Integrator and SSA</u>
- <u>ISAT vs. Neural nets</u>
- <u>Thoughts on cost functions</u>
- <u>NMPC Formulations</u>
- <u>Committee members</u>

NMPC Multiple Shooting Formulation

Nonlinear MPC



Dynamic state and parameter estimation

$$\min_{x,\alpha} J(x,y) \stackrel{def}{=} \sum_{k=-N_E}^{0} \left[A(x_k, y_k) \right] \quad s.t.$$

$$y \; given, u \; given, x_{k+1} = F(x_k, u_k), H\alpha \le h$$

Dynamic optimization

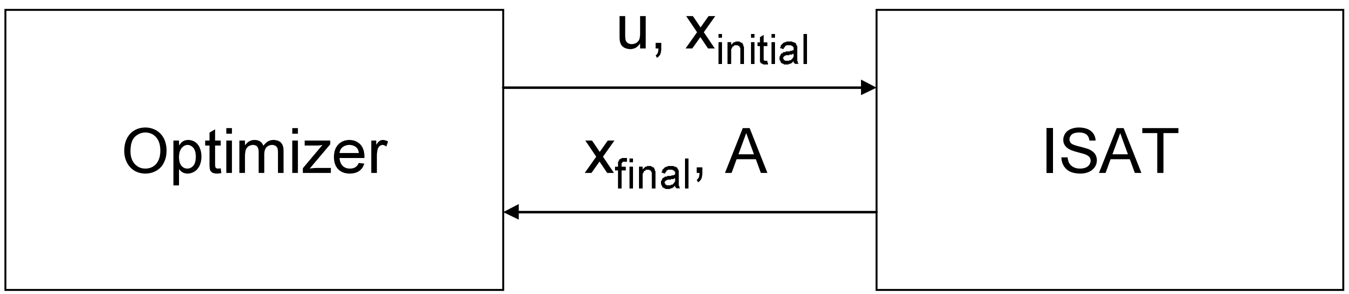
$$\min_{x,u,\eta} J(x,u,\eta) \stackrel{def}{=} \sum_{k=0}^{N_O} \left[D(x_k, u_k) + E(\eta_k) \right] \quad s.t.$$

$$x_0 \; given, x_{k+1} = F(x_k, u_k), Du_k \le d, Gx_k - \eta_k \le g, \eta_k \ge 0$$

Replacing the Integrator and SSA

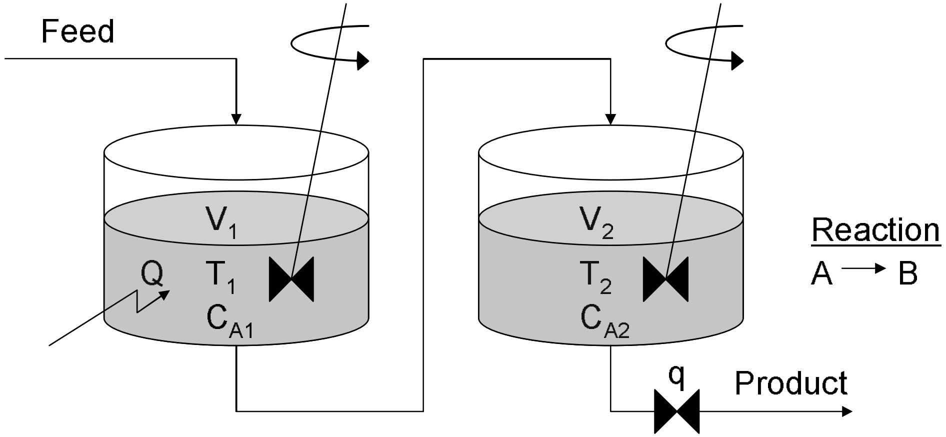
ISAT with NMPC

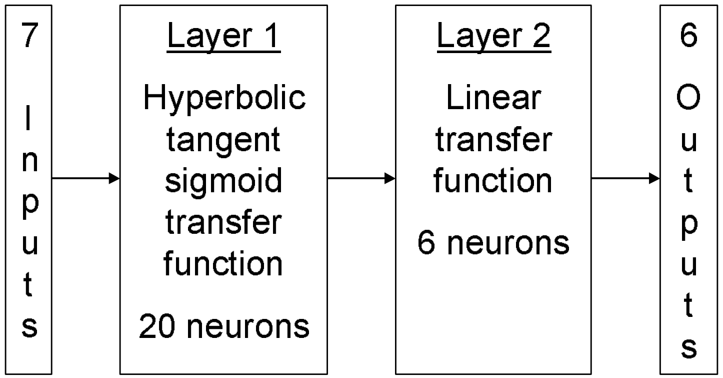
- ISAT replaces the DAE integrator and sensitivity calculator



ISAT vs Neural Nets

ISAT vs. Neural Nets





6 state dual CSTR model

MV: cooling rate of CSTR 1

CV: product temperature

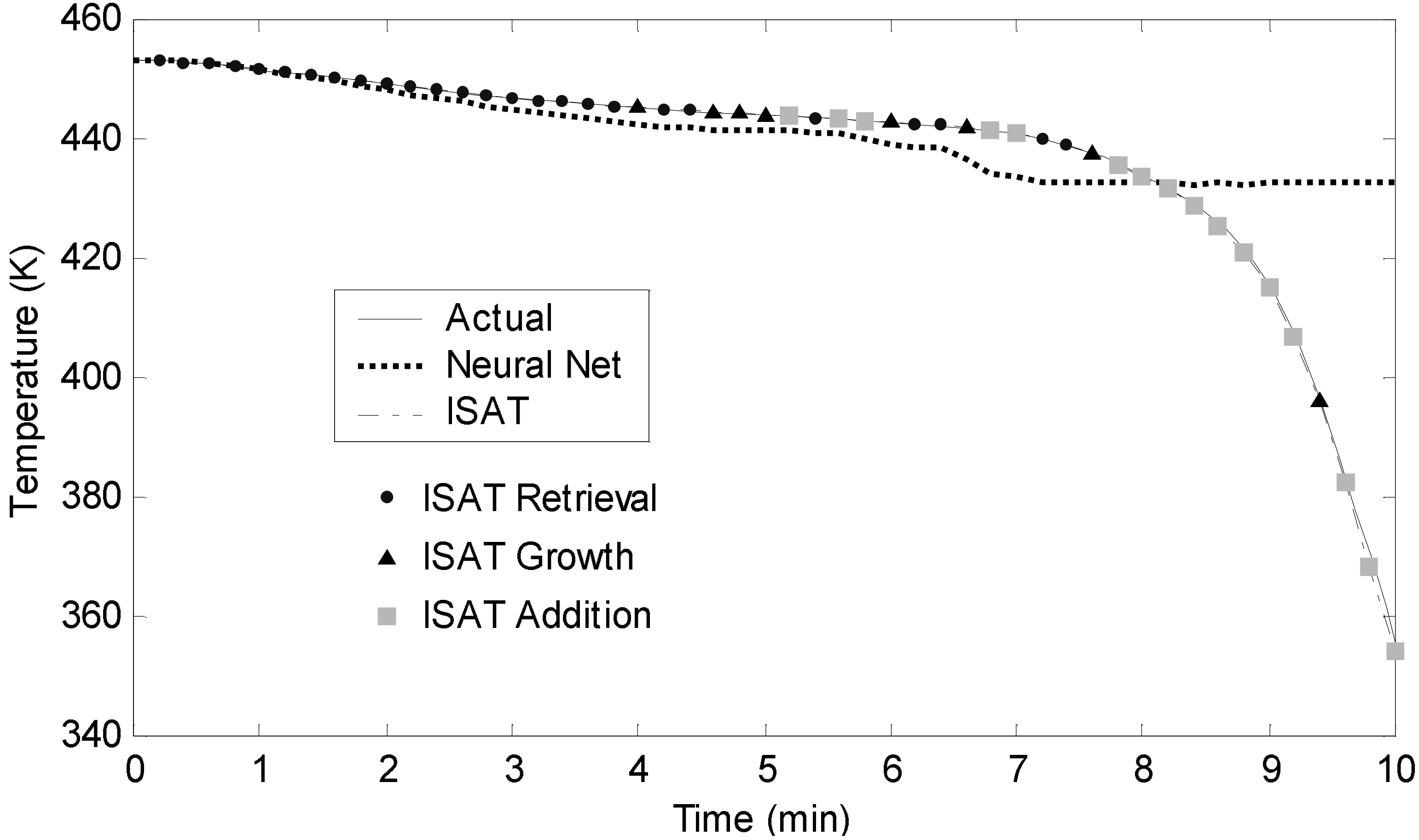
ISAT and Neural Net used the same training data

Compared in open loop and closed loop simulations

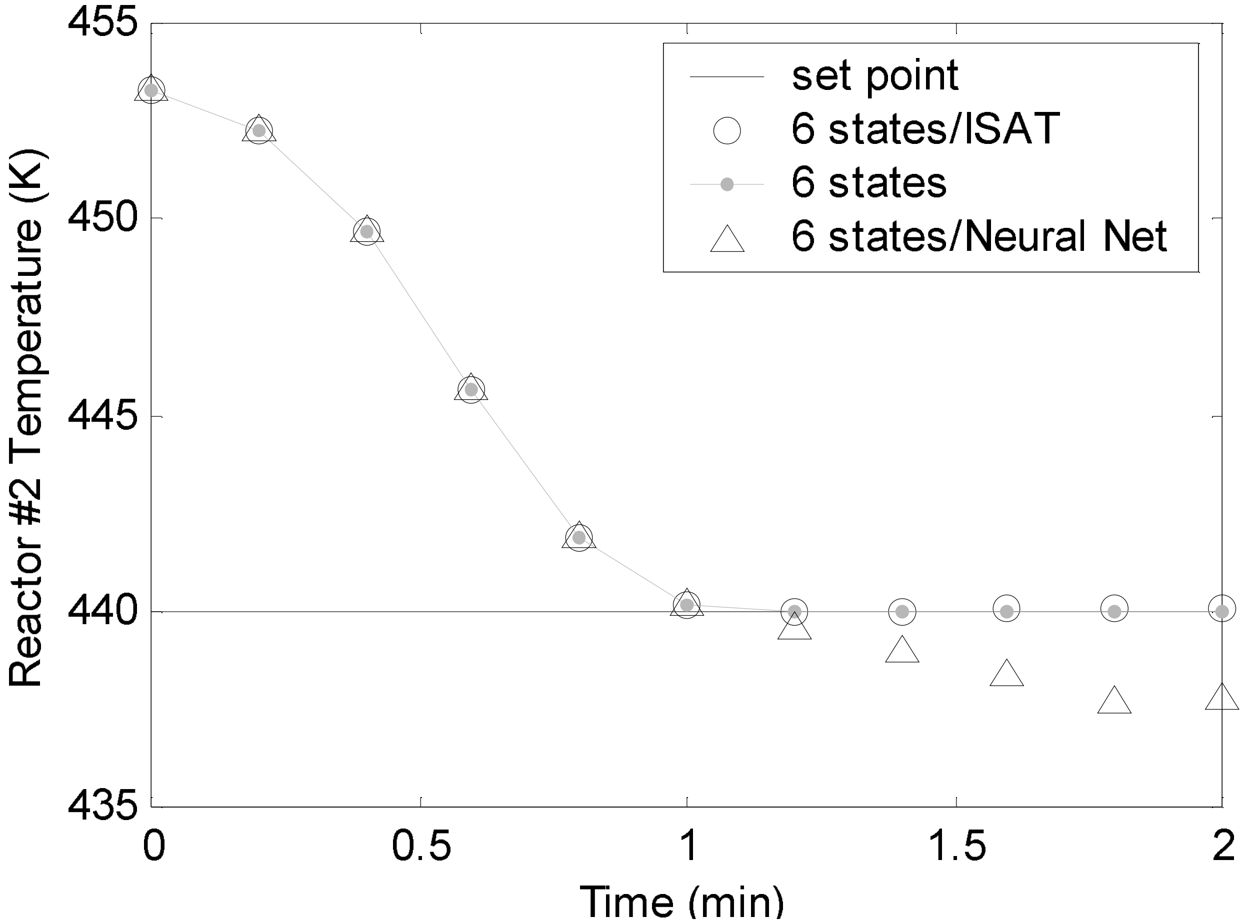
Control Horizon = 0.4 min

Prediction Horizon = 0.6 min

Open Loop (ISAT vs. Neural Net)



Closed Loop (ISAT vs. Neural Net)



Some thoughts on cost functions

Some thoughts on cost functions

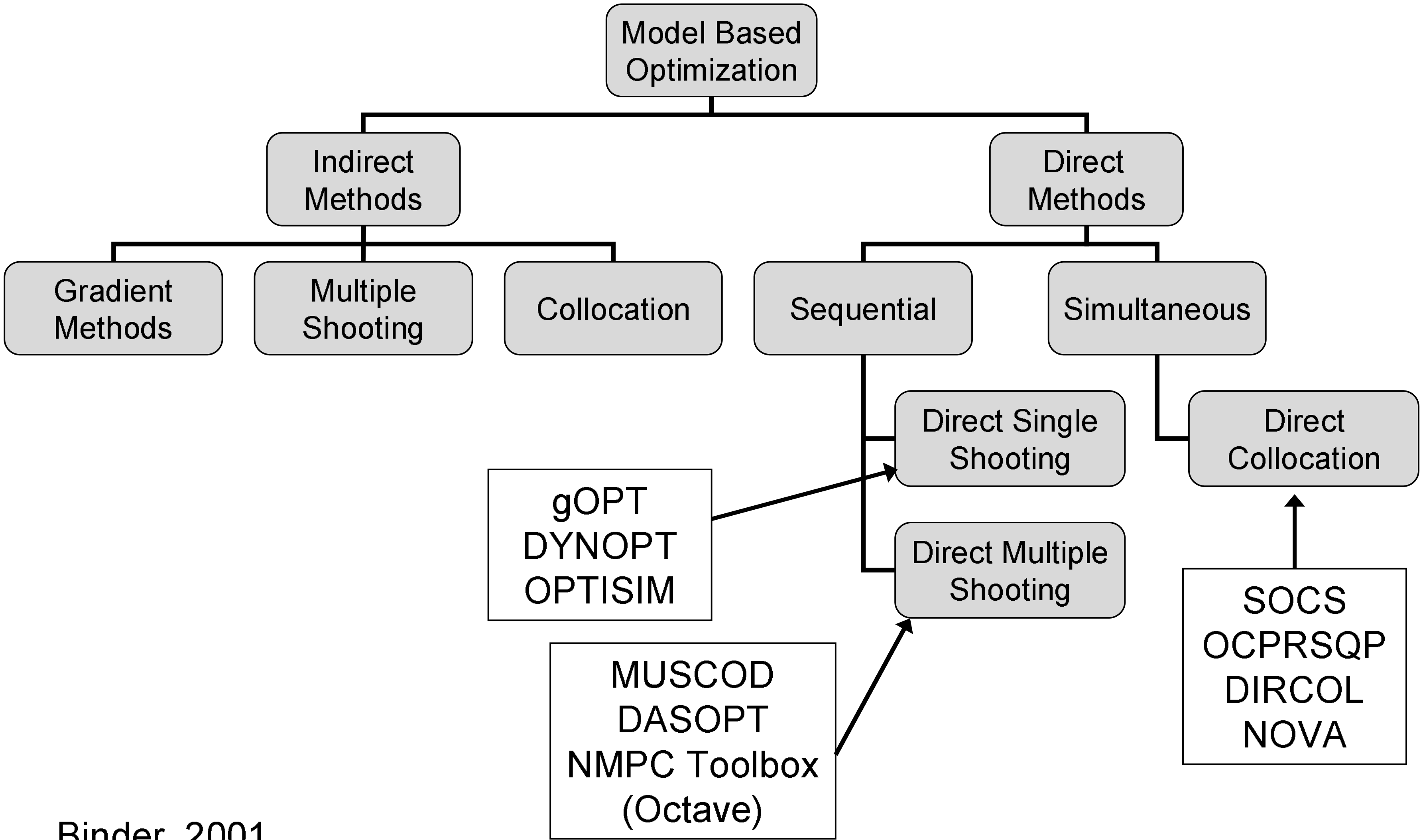
- Quadratic cost functions
  - Advantages
    - Preserve convexity of NLP
    - Explicit cost function derivatives
  - Disadvantages
    - Does not accurately reflect the true process costs
    - Maximizing a function with a solution that is not necessarily optimal

Some thoughts on cost functions

- Generalized cost functions
  - Advantages
    - Flexibility to reflect real dollar amounts
    - Explicit tie to real costs
      - Incorporate changing utility costs for time of day pricing
      - Changing feed costs or product
    - Global solution will maximize profits
    - Incorporate plant-wide optimization results (use Lagrange multipliers, etc.)
  - Disadvantages
    - Numerical cost function derivatives
    - Convexity not guaranteed
    - Need a global optimizer

NMPC Formulations

NMPC Formulations



Binder, 2001

Comparison of Direct Methods

	Direct Single Shooting	Direct Multiple Shooting	Direct Collocation
general solution approach	sequential	hybrid	simultaneous
use of (state of the art) DAE solvers	yes	yes	no
number of variables / size of NLP	small	intermediate	large
initial guess for system states	initial state	all node values	all node values
applicable to highly unstable systems	no	yes	yes
DAE model fulfilled in each iteration step	yes	partially	no

Binder, 2001

Committee Members, Course Work, and Comments

Suggestions and Comments

- Jim Rawlings (ChE, Wisc)
  - Storage and retrieval of the optimal solution is more efficient than storage and retrieval of the states
  - Look at the work on explicit LQR solutions
- Melba Crawford (ME, UT)
  - The current EOA expansion scheme is too aggressive
- Robert Young (ExxonMobil)
  - We solve optimization problems with thousands of variables with no problem – why not use collocation?
- Keenan Thompson (Control Engineer)
  - I’m going to stick with my PID loops
- Joe Qin (ChE, UT)
  - You need more rigor in your presentation, not that it works or doesn’t work but *why* it works or doesn’t
  - You need to account for unmeasured disturbances

I am currently investigating these ideas – please let me know if you have others.

Courses

- Master’s degree from BYU (7 courses)
- ASE 381P 3-Optimal control
- ORI 391Q Nonlinear programming
- ASE 381P 2-Multivariable control systems
- CHE 391 Modern control theory
- ORI 390R Multivariate statistical analysis
- TA CHE 360 Process control

Committee Members

- Advisor: Tom Edgar
- UT Professors
  - Joe Qin
  - Bruce Eldridge
- UWisc Professor
  - Jim Rawlings
- Cornell Professor
  - Stephen Pope