In Situ Adaptive Tabulation for Nonlinear MPC

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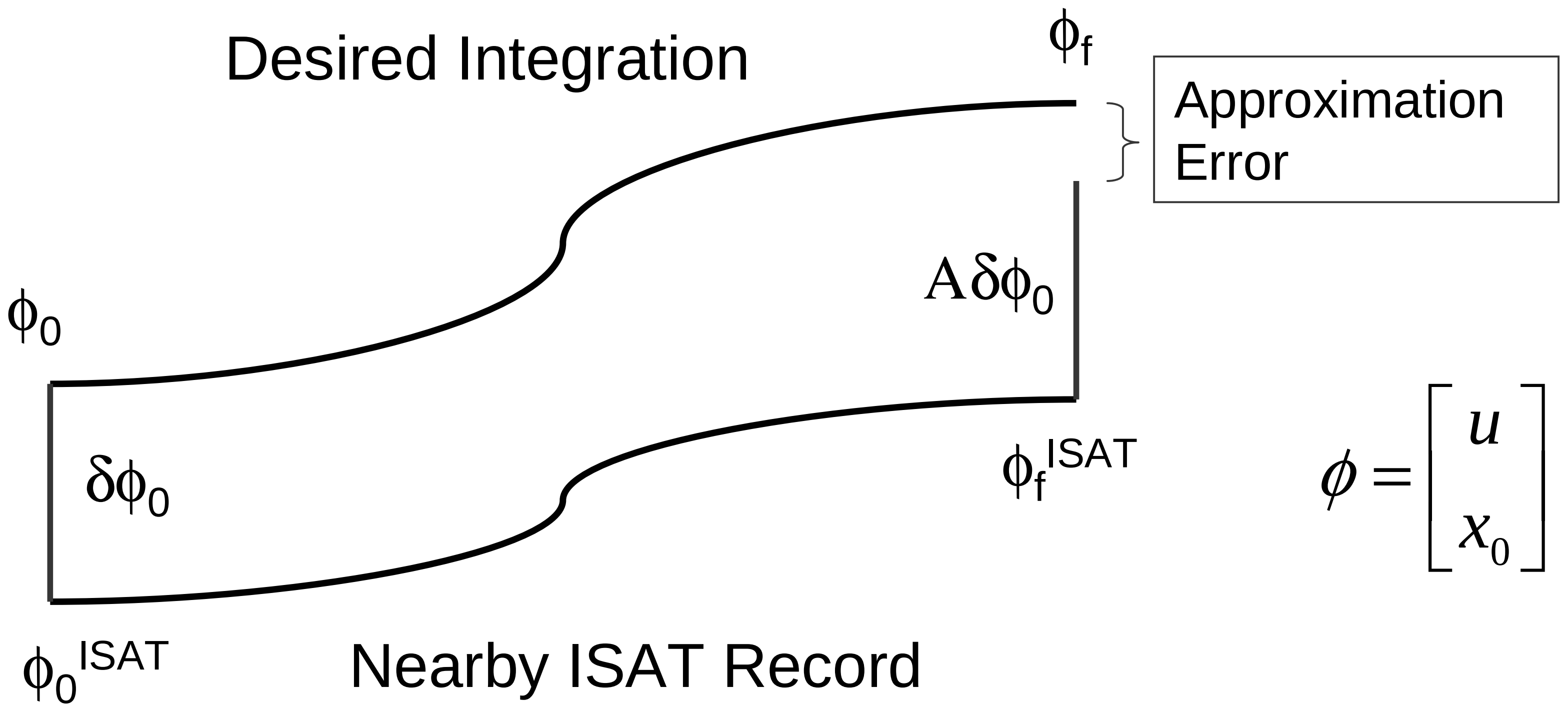
Outline

- Introduction to ISAT
- ISAT Theory
- NMPC with ISAT
- ISAT vs. Neural Nets
- Future Directions

In Situ Adaptive Tabulation (ISAT)

- Developed by Pope[1] in 1997 for turbulent combustion simulations.
- ASCI C-SAFE application[2] at the University of Utah in 2002.
- Integrated with FLUENT[3], popular computational fluid dynamics software.

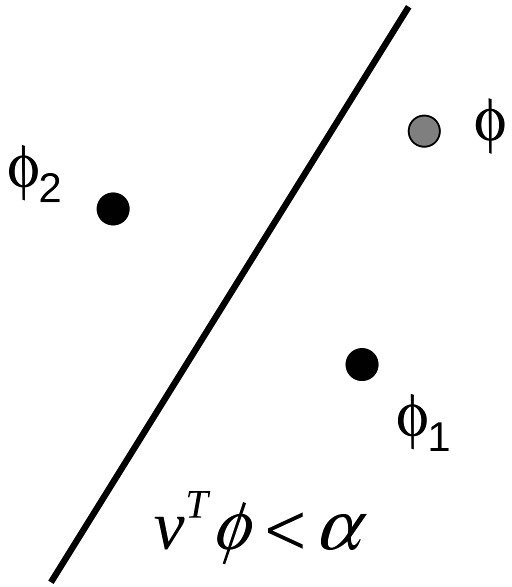
Computational Reduction Idea



In reacting flow simulations, the integration of the chemistry model can occur $>10^8$ times. ISAT is a storage and retrieval method for the integrations.

ISAT Search

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

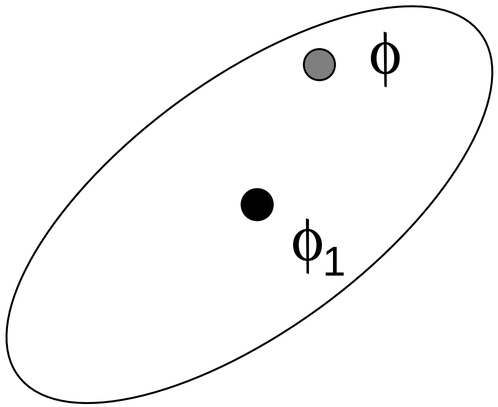


$$v = \phi_2 - \phi_1$$

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

ISAT Integration

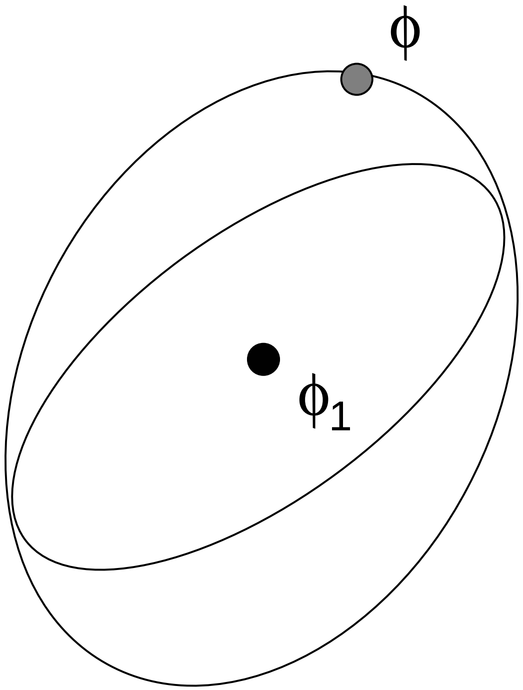
- Scenario #1: Inside the region of accuracy



$$\left(\phi - \phi_1\right)^T M \left(\phi - \phi_1\right) \le \varepsilon_{tol}$$

ISAT Integration

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

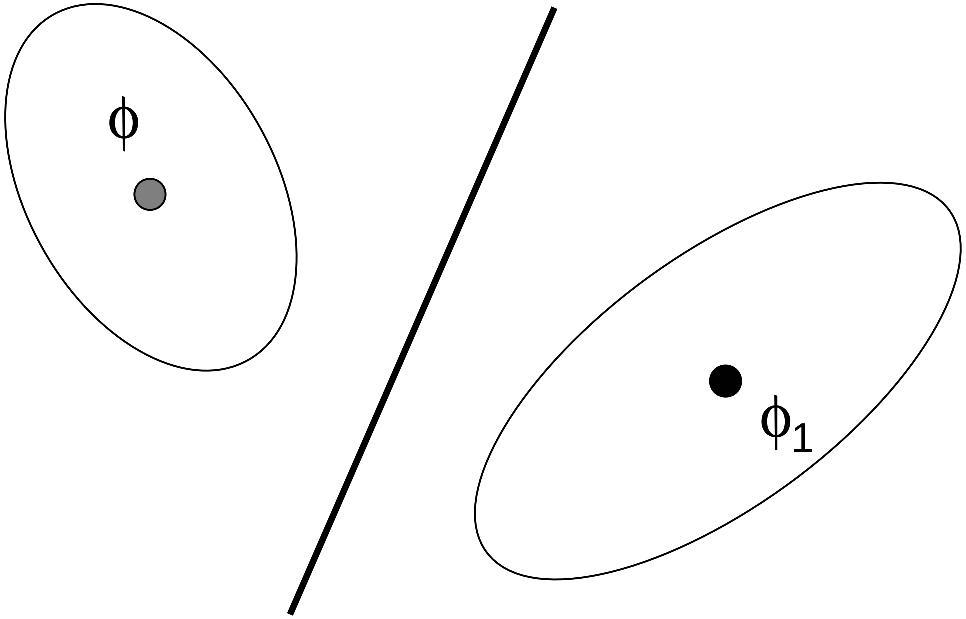


$$\left(\phi-\phi_1\right)^T M\left(\phi-\phi_1\right)>\varepsilon_{tol}$$

Compute M_{new} so that the new region is a symmetric, minimum volume ellipsoid that includes ϕ

ISAT Integration

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



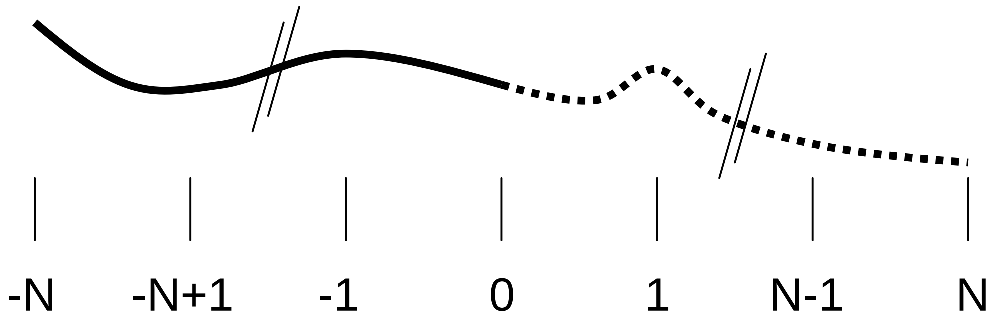
Define cutting plane

$$v = \phi - \phi_1$$

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

Find a conservative estimate for the region of accuracy around ϕ

Nonlinear MPC



Dynamic Data Reconciliation[4]

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

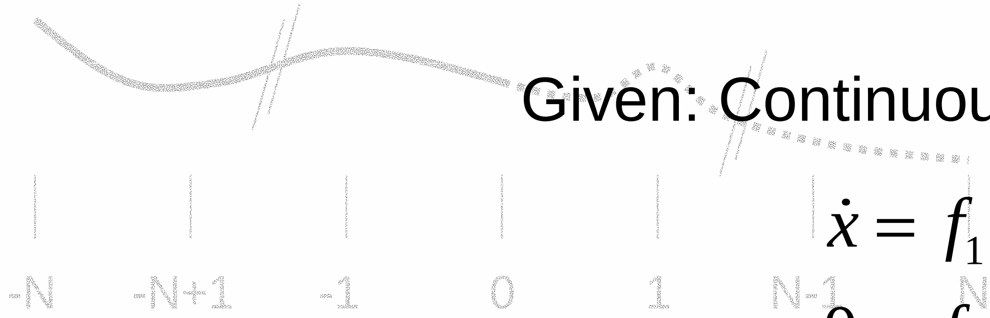
$$y \text{ given}, u \text{ given}, x_{k+1} = F(x_k, u_k), Gx_k - \eta_k \le g, \eta_k \ge 0$$

Dynamic Optimization[5]

$$\min_{x,u,\eta} \Phi(x,u,\eta) \quad s.t.$$

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

Nonlinear MPC



Given: Continuous DAE model

$$\dot{x} = f_1(x,u)$$
$$0 = f_2(x,u)$$

Dynamic Data Reconciliation[1]

Need: Discrete DAE model

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

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

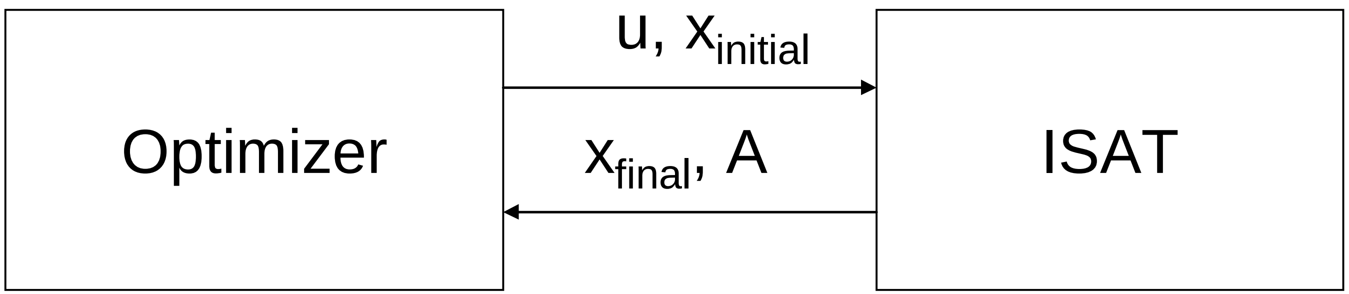
Dynamic Optimization[2]

$$\min_{x,u,\eta} \Phi(x,u,\eta) \quad s.t.$$

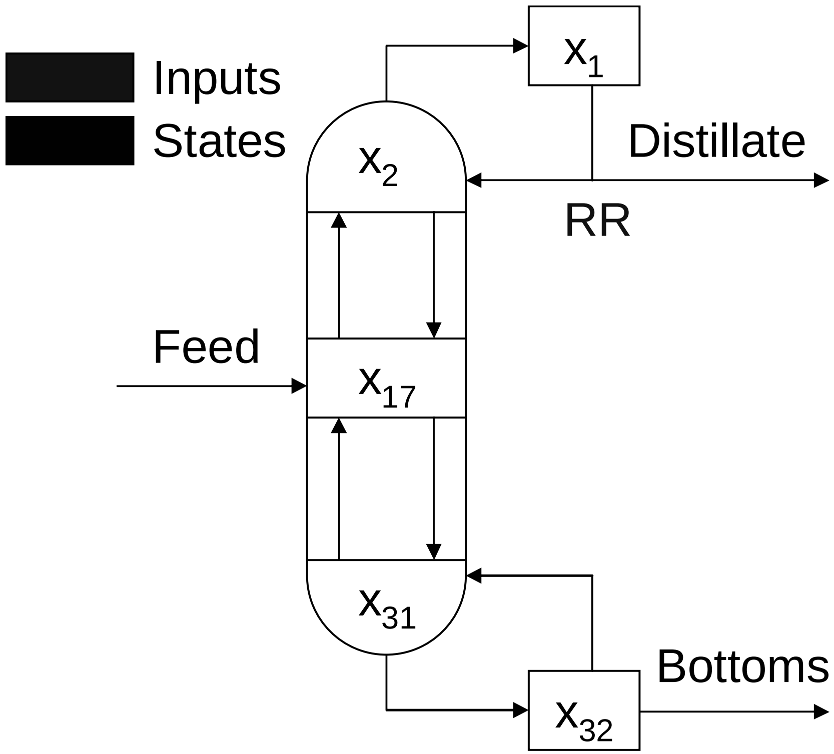
$$x_0\ given, \boxed{x_{k+1} = F(x_k, u_k)}, Du_k \le d, Gx_k - \eta_k \le g, \eta_k \ge 0$$

ISAT with NMPC

- ISAT replaces the DAE integrator and sensitivity calculator



NMPC Example with ISAT



32 state binary distillation column model

MV: reflux ratio

CV: distillate composition

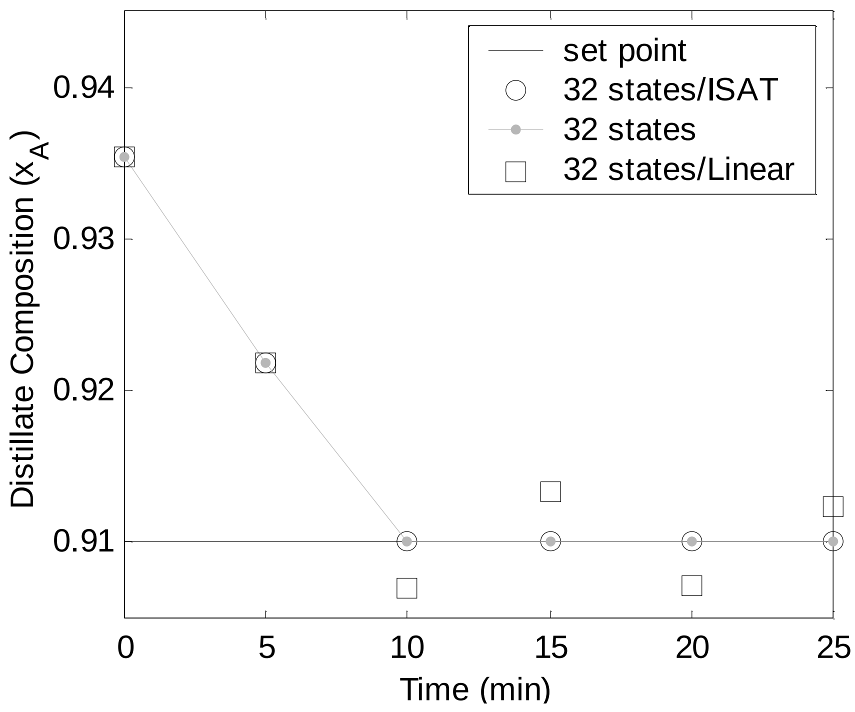
Simplex optimizer

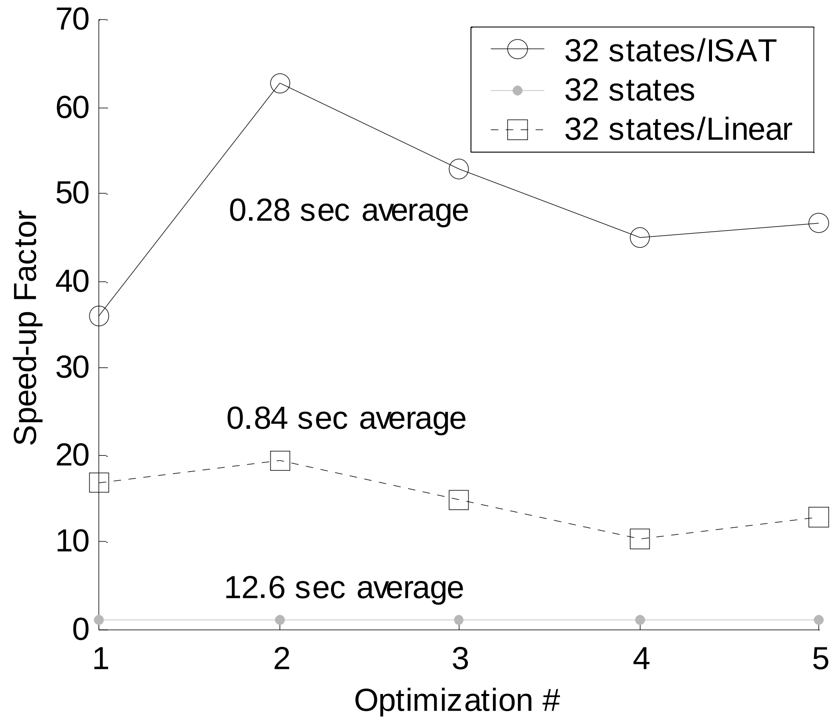
Soft constraint on the MV

Control Horizon = 10 min

Prediction Horizon = 15 min

Closed Loop Response

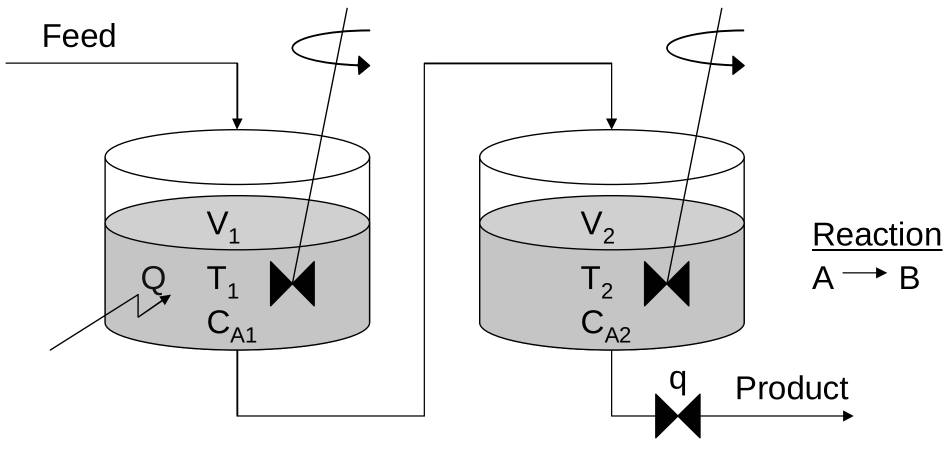


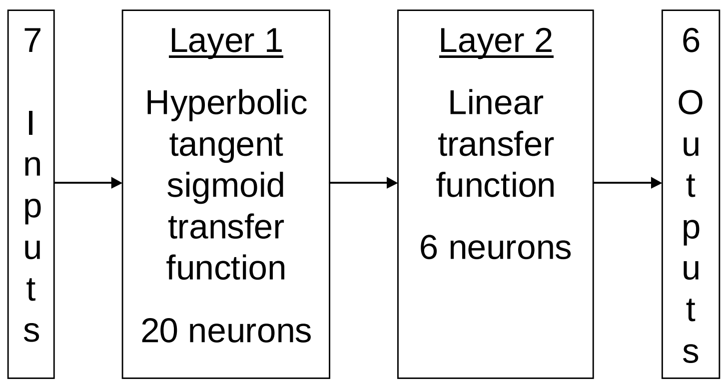


ISAT Performance

- Successful with ODE and DAE models
- Computational speedup 20 – 500 times
- Storage <100MB for 96 state DAE model with $\varepsilon_{tol} = 10^{-3}$

ISAT vs. Neural Nets





6 state dual CSTR model

MV: cooling rate of CSTR 1

CV: product temperature

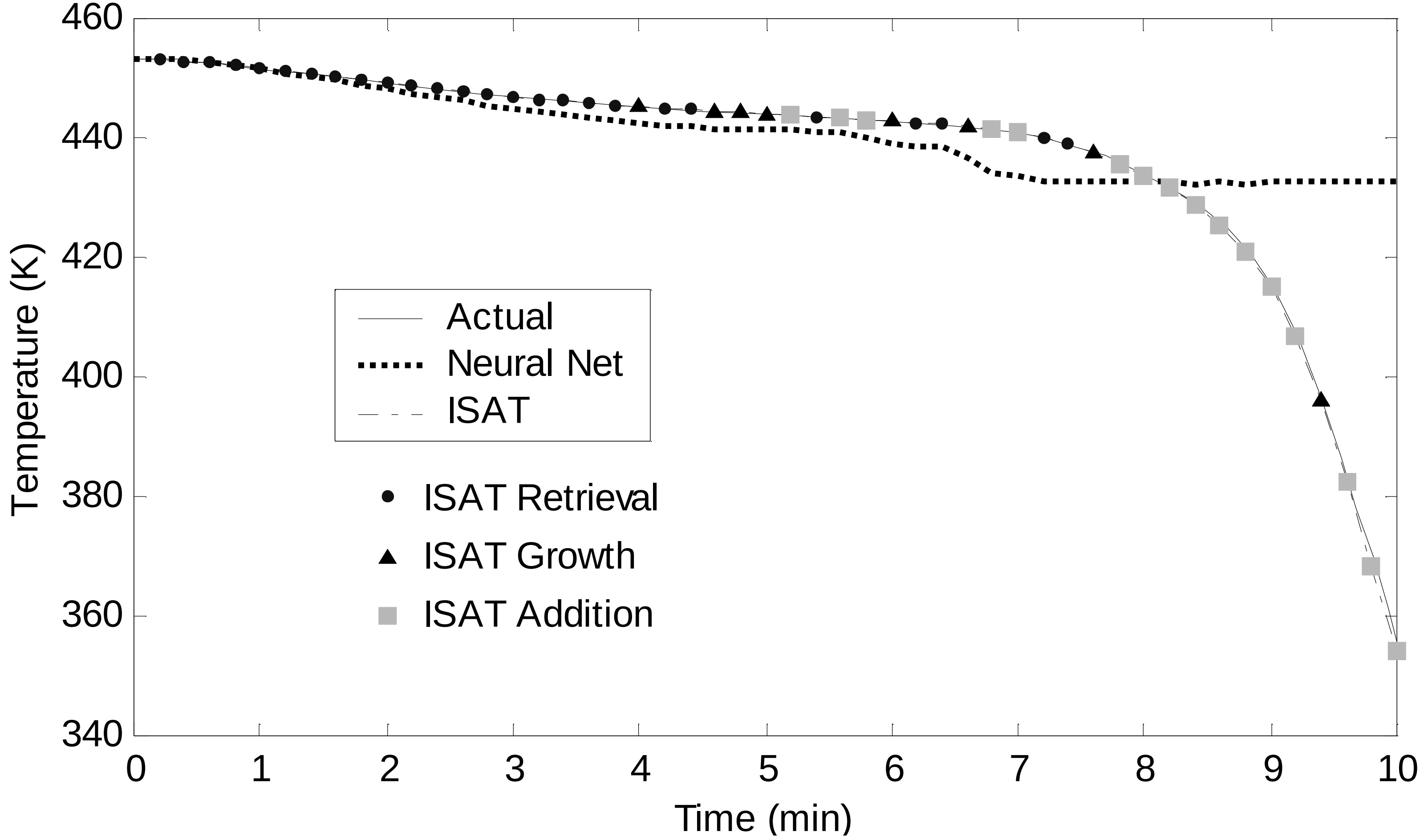
ISAT and Neural Net used the same training data

Compared in open loop and closed loop simulations

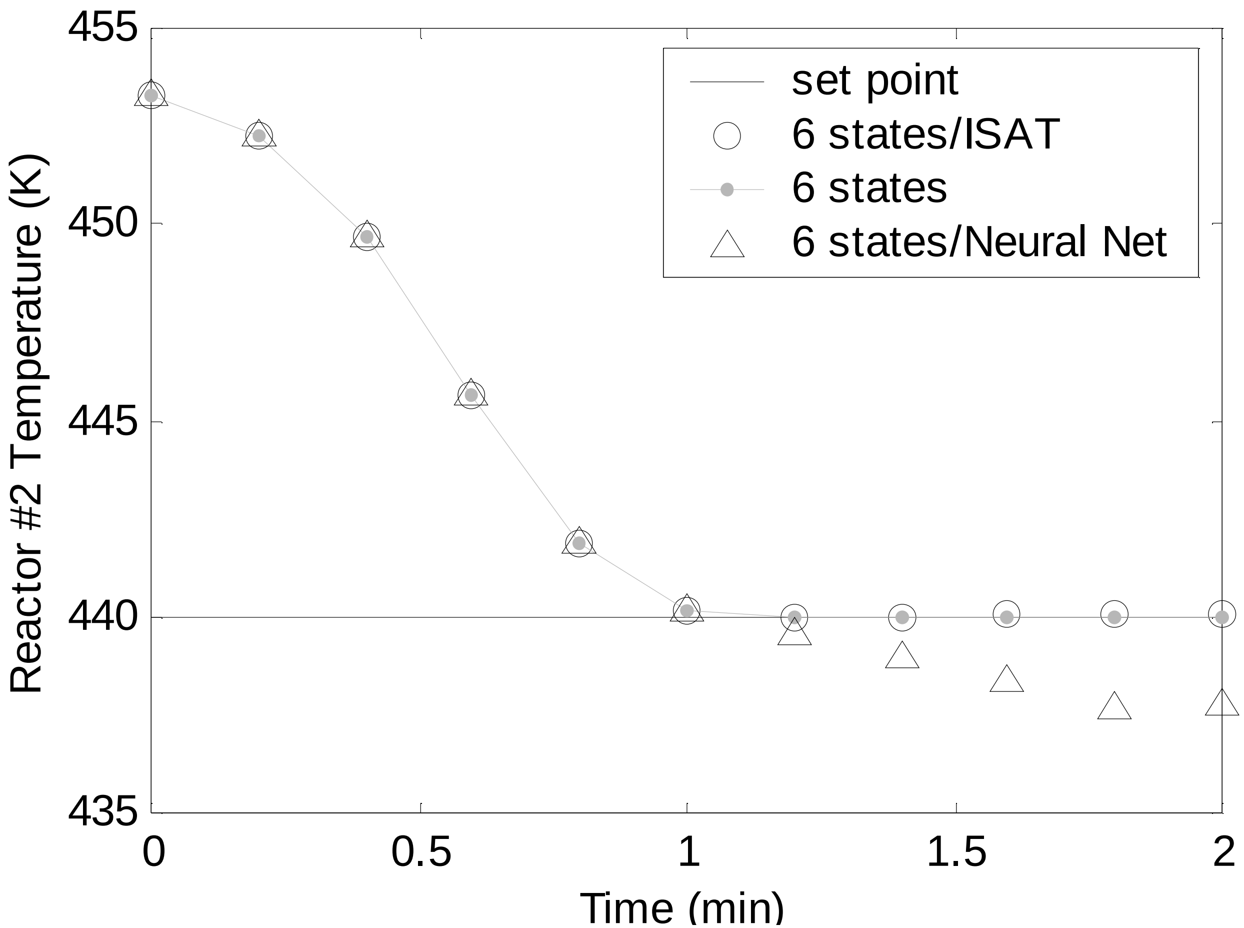
Control Horizon = 0.4 min

Prediction Horizon = 0.6 min

Open Loop (ISAT vs. Neural Net)



Closed Loop (ISAT vs. Neural Net)



Future Directions

- Develop ISAT in C++/Fortran (currently in MATLAB)
- Integrate ISAT with NMPC toolbox for Octave
- Control of Reactive Distillation
- Other applications?
- Questions?

References

[1] S. B. Pope, Pope, S. B. Computationally Efficient Implementation of Combustion Chemistry Using *In Situ* Adaptive Tabulation. *Combustion Theory Modeling* vol. 1, pp. 41-63, 1997.

[2] C-SAFE, Center for the Simulation of Accidental Fires and Explosions, URL: http://www.csafe.utah.edu/, Accessed Sept. 2003.

[3] FLUENT, Reacting Flows, URL: http://www.fluent.com/software/fluent/focus/reacting.htm, Accessed Sept. 2003.

[4] M. J. Liebman, T. F. Edgar, and L. S. Lasdon, Efficient data reconciliation and estimation for dynamic processes using nonlinear programming techniques, *Comp. Chem. Eng.*, 16:963-986, 1992.

[5] M. J. Tenny, S. J. Wright, and J. B. Rawlings, Nonlinear model predictive control via feasibility-perturbed sequential quadratic programming, Texas-Wisconsin Modeling and Control Consortium, Report TWMCC-2002-02, 2002.