



DYNAMIC OPTIMIZATION

Across Disciplines

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Overview

- PRISM Group Overview
- Dynamic Optimization for:
 - Unmanned Aerial Vehicles
 - Systems Biology
 - Solid Oxide Fuel Cells
 - Energy Storage and the Smart Grid
 - Oil and Gas Exploration and Production
 - Investment Planning Under Uncertainty
- Needs and resources for dynamic optimization

PRISM Group Overview

- PRISM: **P**rocess **R**esearch and **I**ntelligent **S**ystems **M**odeling
- Methods
 - Mixed Integer Nonlinear Programming (MINLP)
 - Dynamic Planning and Optimization
 - Uncertain, Forecasted, Complex Systems

- Fit Systems into Standard Problem Formulation

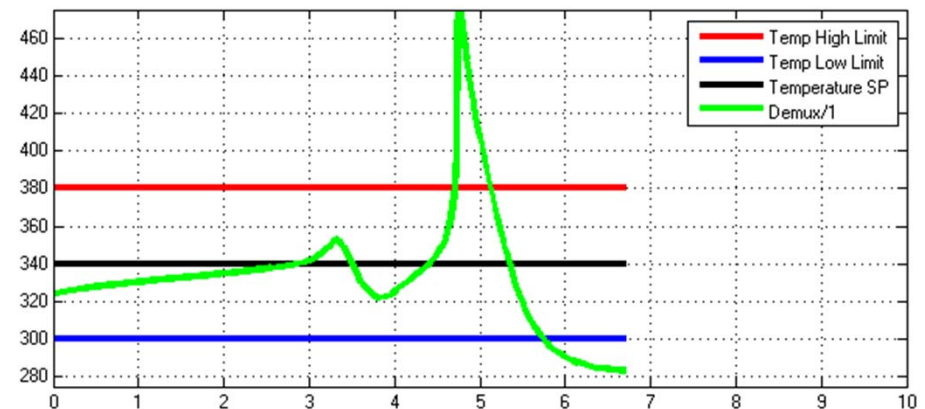
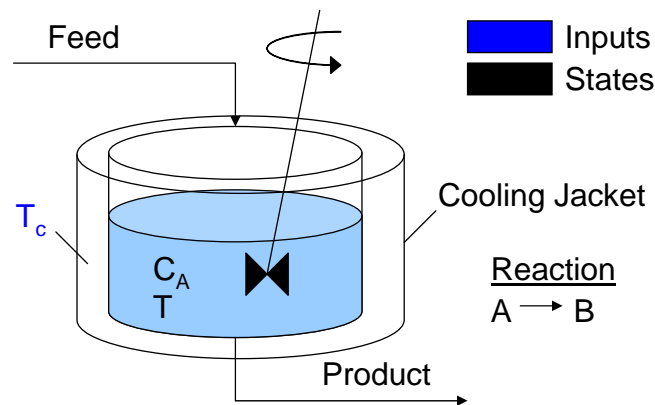
$$\begin{aligned} & \max f(x) \\ & \text{subject to } g\left(\frac{\partial x}{\partial t}, x, u, p\right) = 0 \\ & \quad h(x, u, p) \leq 0 \end{aligned}$$

- Solver development: Large-scale MINLP (100,000+ variables)



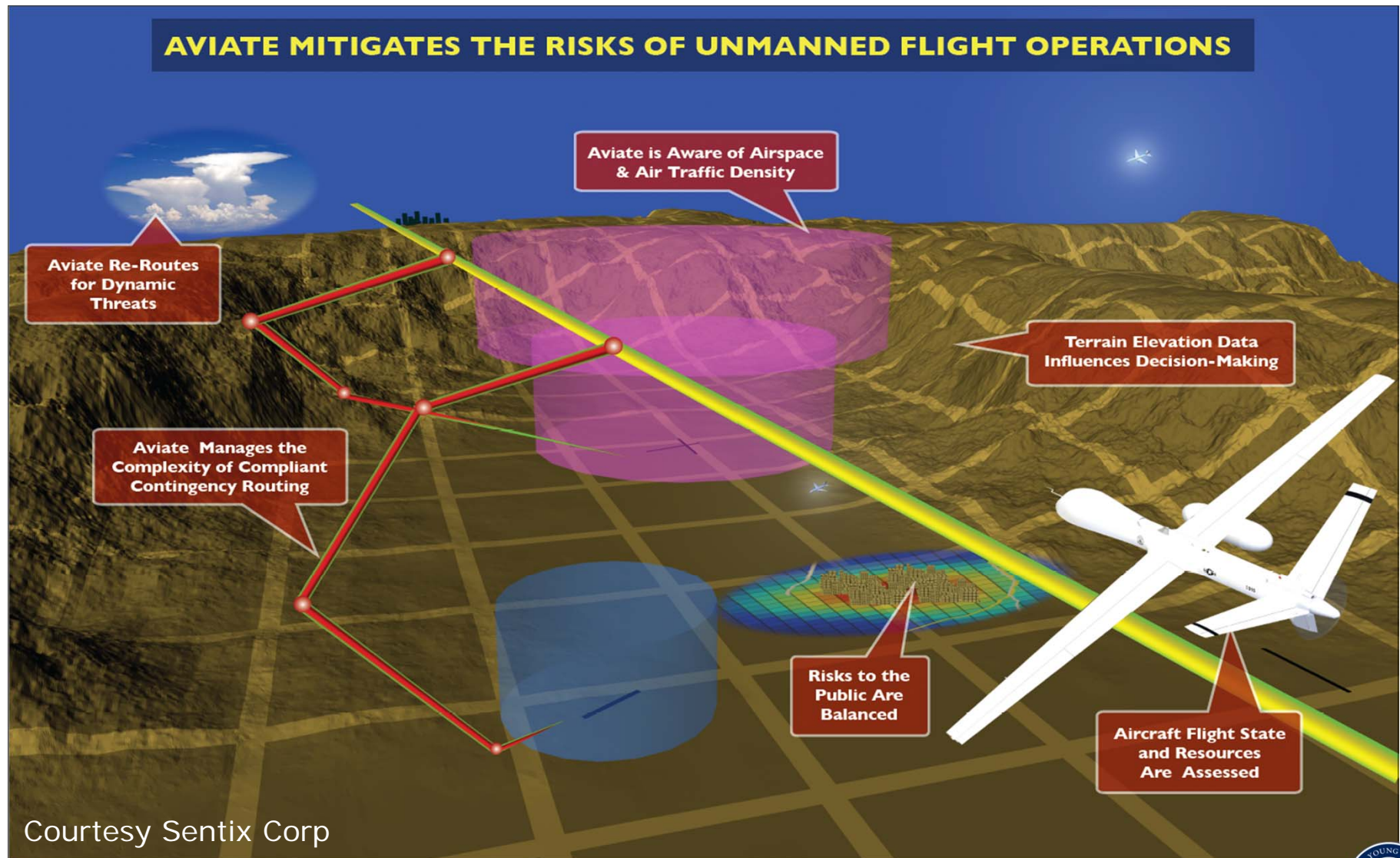
Reactor Control Exercise

- Manipulate the cooling jacket temperature (T_c)
- Reduce outlet concentration to $< 0.1 \text{ mol/m}^3$
- Keep exothermic reactor within temperature limits



Dynamic Optimization with UAVs

AVIATE MITIGATES THE RISKS OF UNMANNED FLIGHT OPERATIONS



Courtesy Sentix Corp

Information Sources

Multiple Sources of Information Can Be Utilized

Population Density



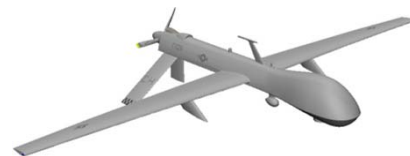
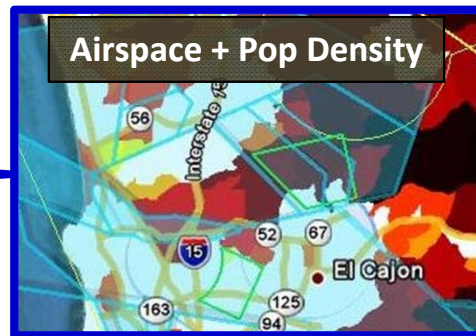
Controlled Airspace



**Safety
Thresholds**

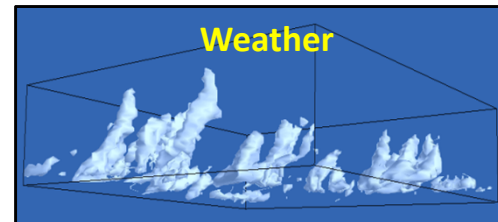
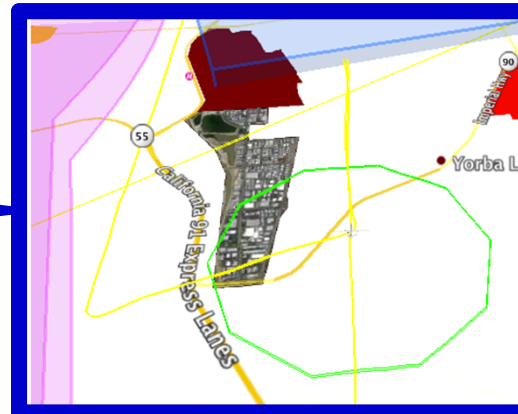
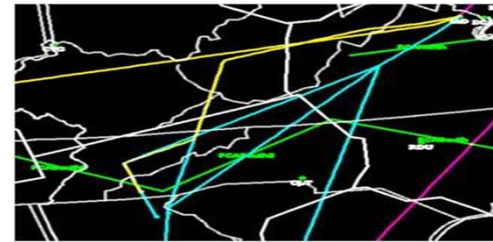
Courtesy Sentix Corp

Geospatial / Urban Dev



Aircraft Performance Model

Air Traffic Density



Weather

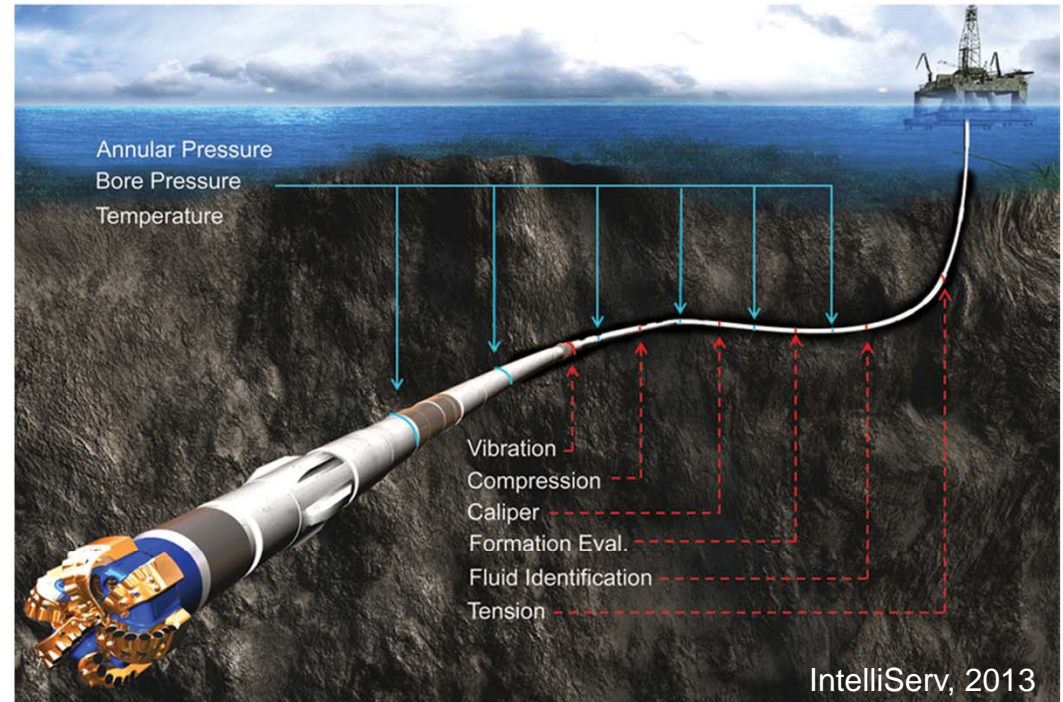
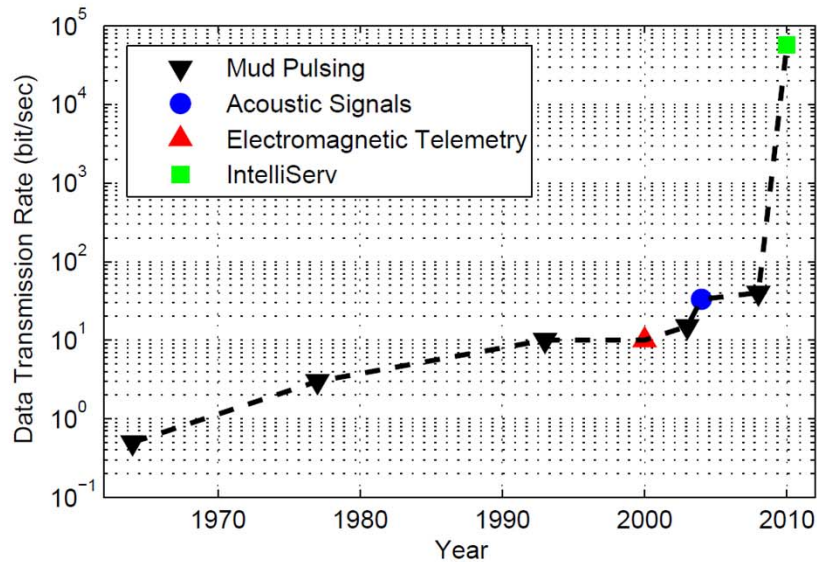
Functions

Define
Risk

Compute
Risk

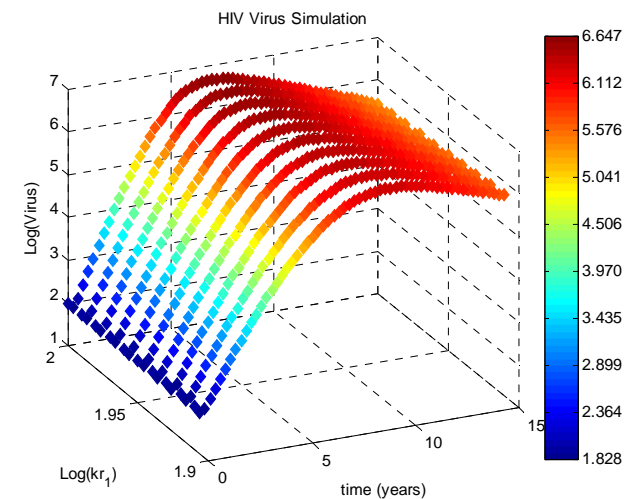
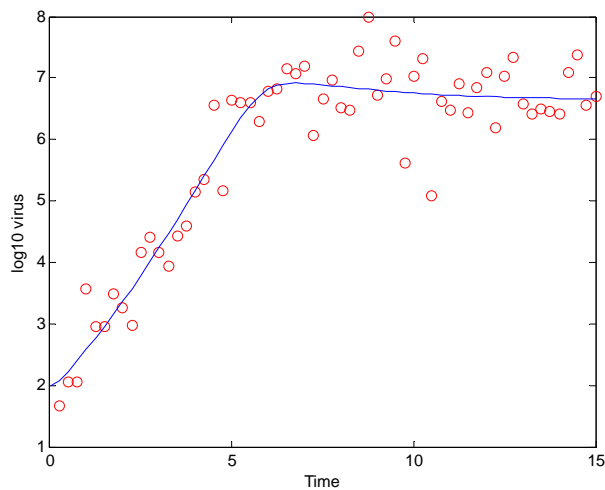
Minimize
Risk

Drilling and Production

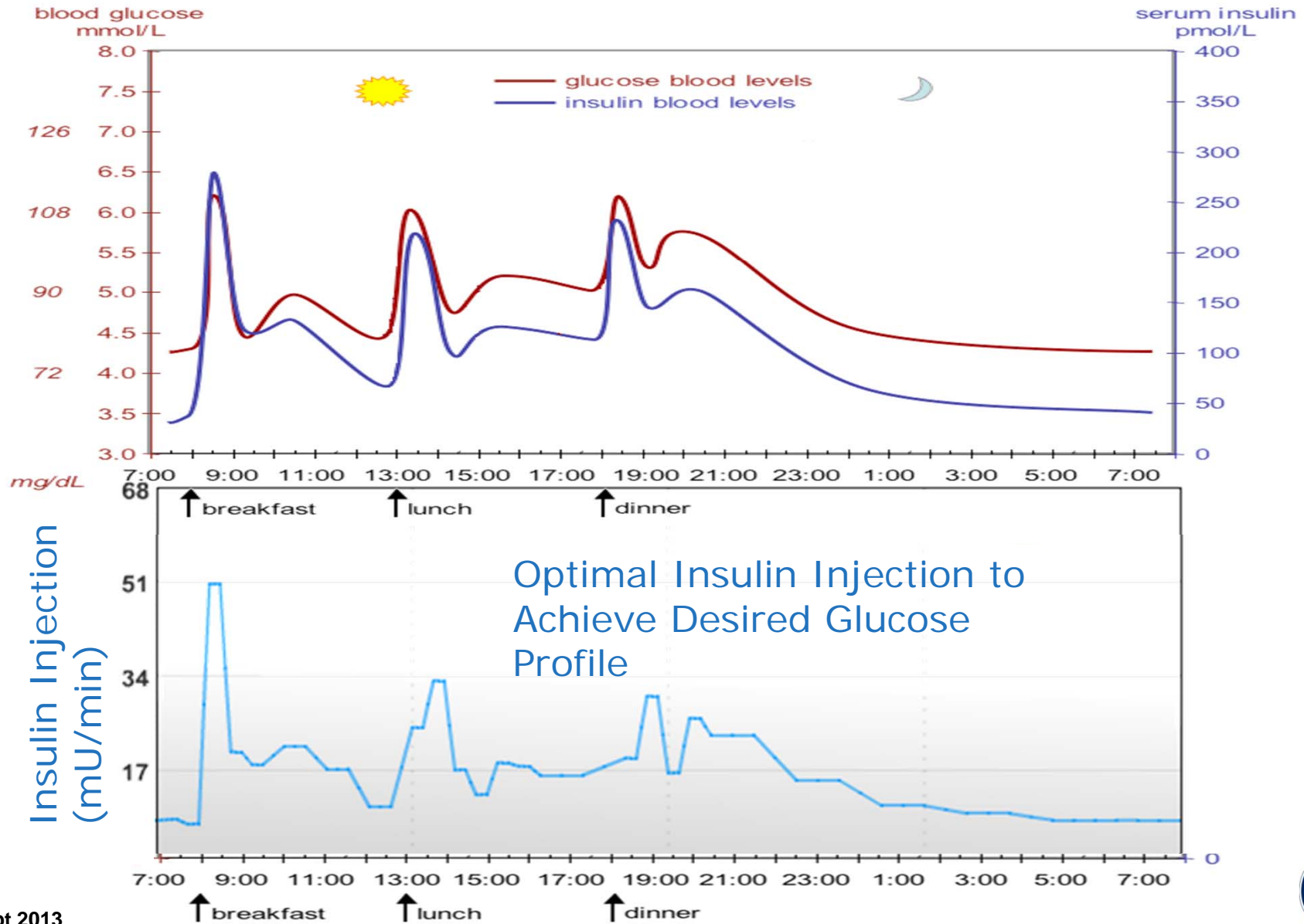


Systems Biology

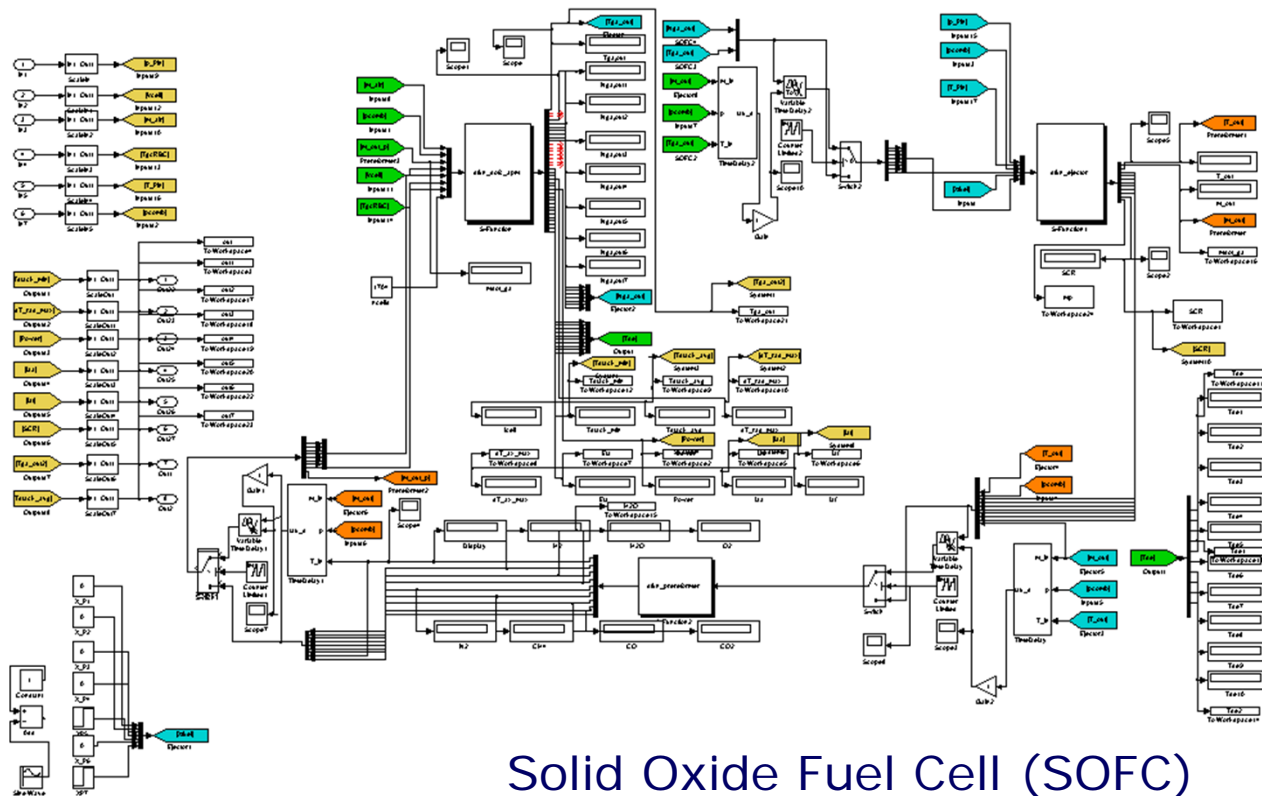
- Objective: Improve extraction of information from clinical trial data
- Dynamic data reconciliation
 - Dynamic pharmacokinetic models (large-scale)
 - Data sets over many patients (distributed)
 - Uncertain parameters (stochastic)



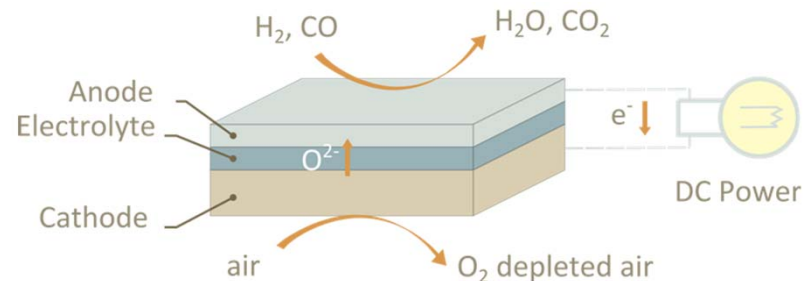
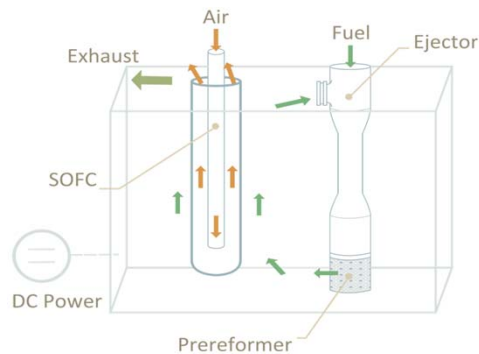
Artificial Pancreas Design



Dynamic Energy System Tools



Solid Oxide Fuel Cell (SOFC)

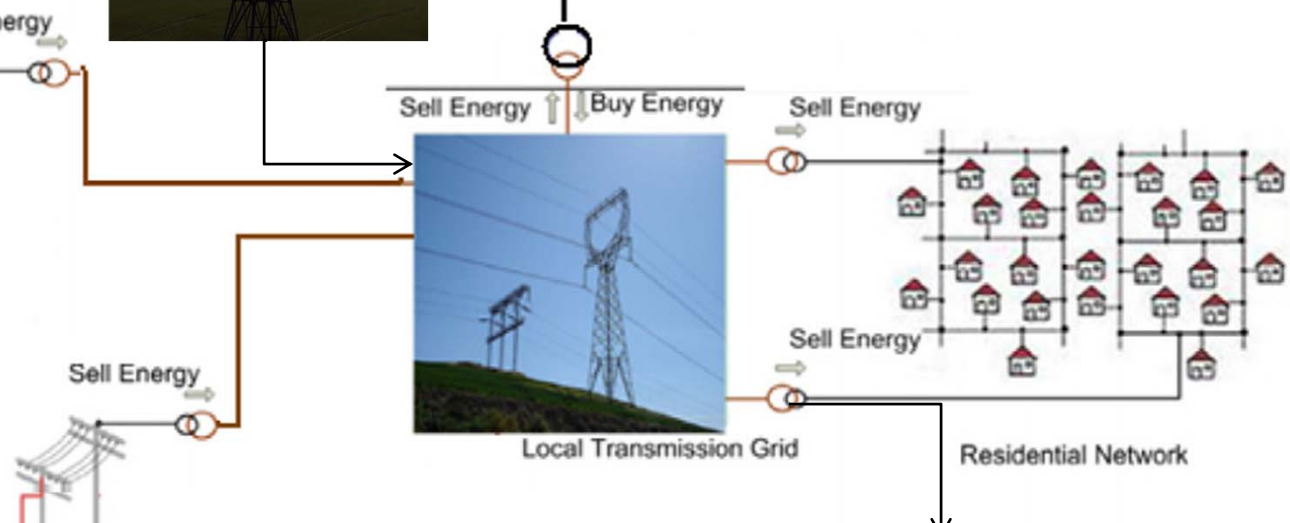
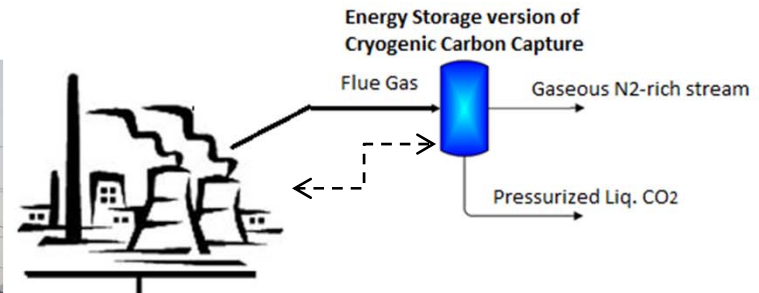
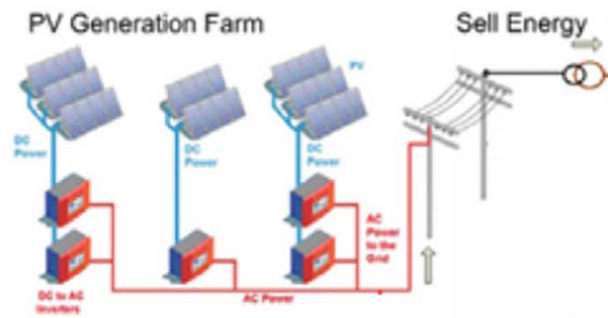


Toolbox for Object Oriented Modeling in MATLAB, Simulink, and Python

Advanced tools are required for collaborative modeling and high performance computing

Smart Grid Optimization

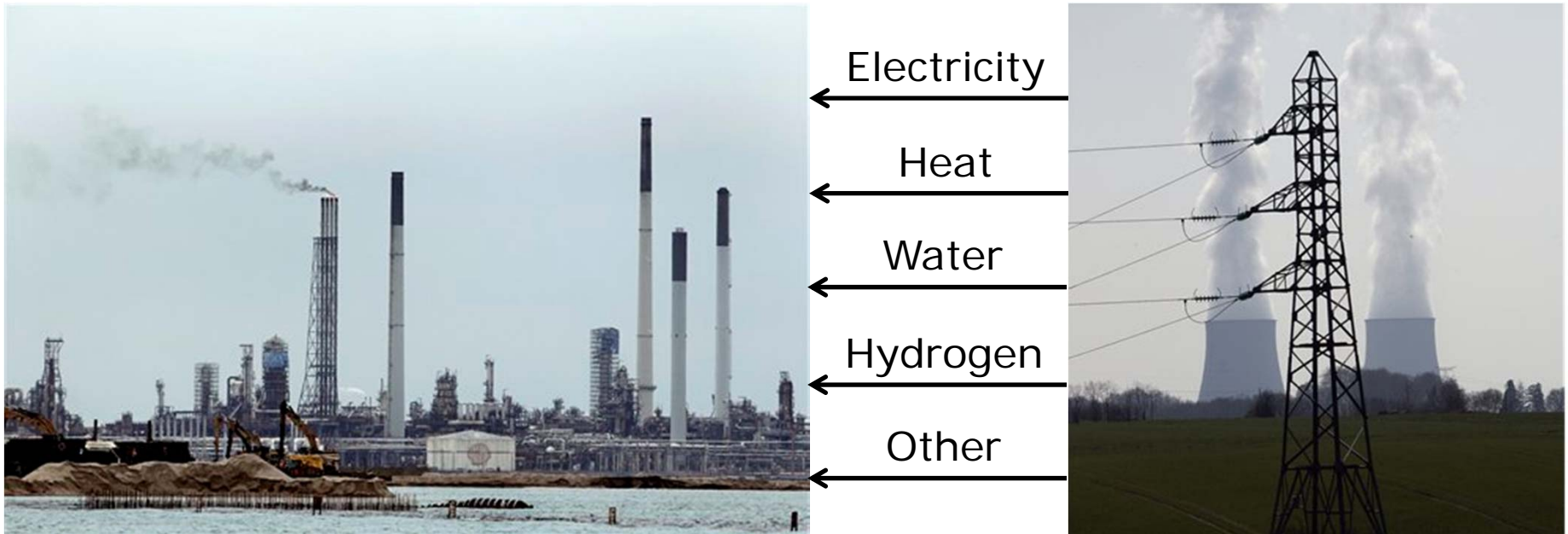
Smart grid integration with solar, wind, coal, biomass, natural gas, and energy storage



Nuclear integration with petrochemical production, processing, and distribution



SMRs with Petrochemical Industries



- 12% of total U.S. energy use from refining and chemicals
- \$57 billion annually on energy
- Potential refinery and nuclear integration with electricity, heat, hydrogen, and other production-consumption pairings
- Transportation fuels are 28% of U.S. energy total

Nuclear for Water Purification

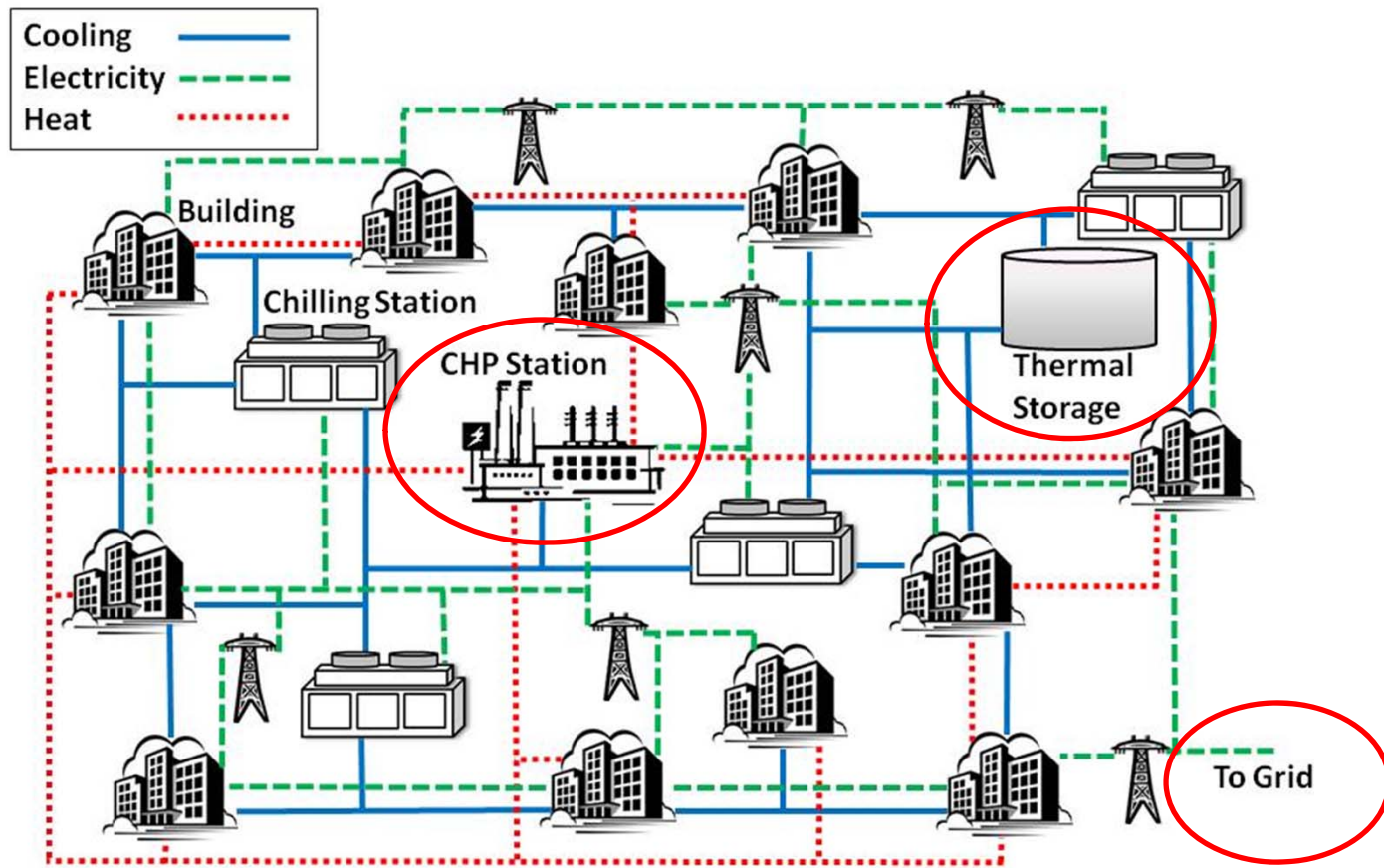
- Cooling towers purify and consume 1.05 gal/kW-hr
- Several nations have access to nuclear power, but limited amounts of renewable fresh water



World's largest desalination facility in Saudi Arabia to produce electricity and water (July 2013)

KSA desalination consumes 300,000 barrels of oil per day at \$3.20/m³ water

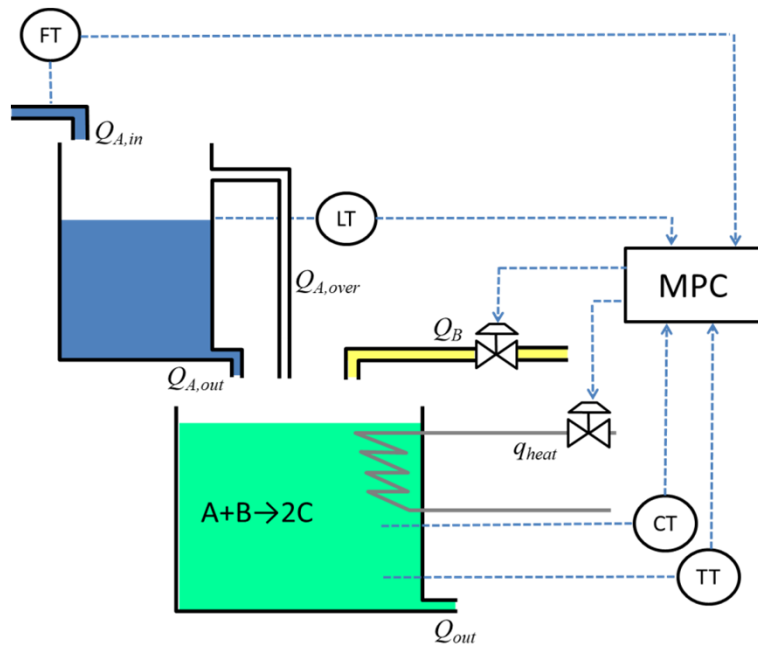
District Heating and Cooling



Simultaneous vs. Sequential

Table 1: Computational results from the sequential and simultaneous solution methods. Computations for each method are executed using an Intel® Core 2 Duo™ (2.54 GHz) processor with 4 GB RAM.

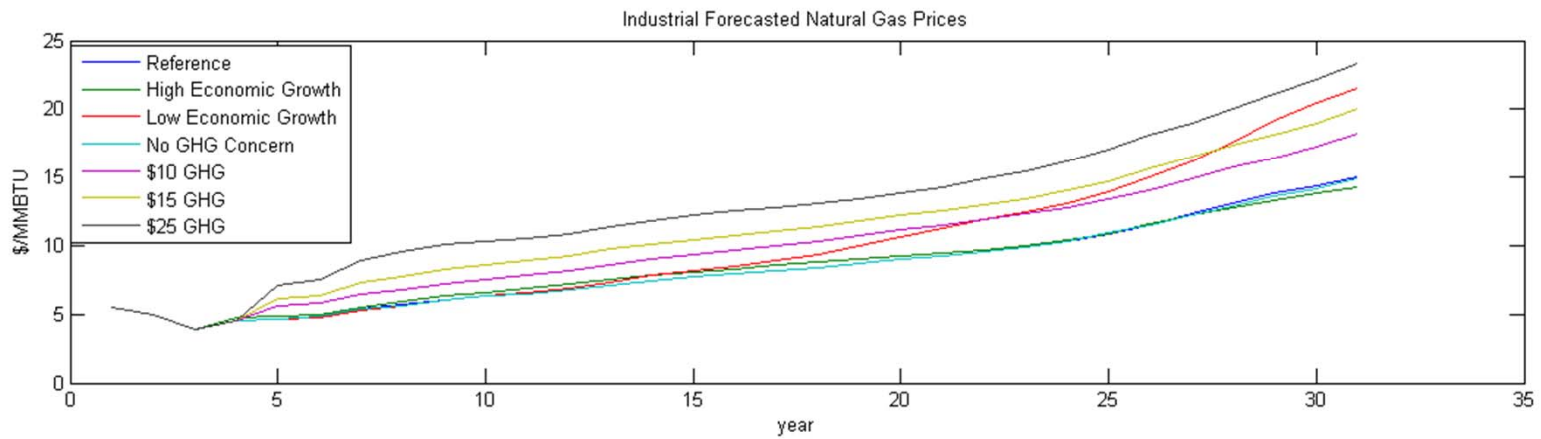
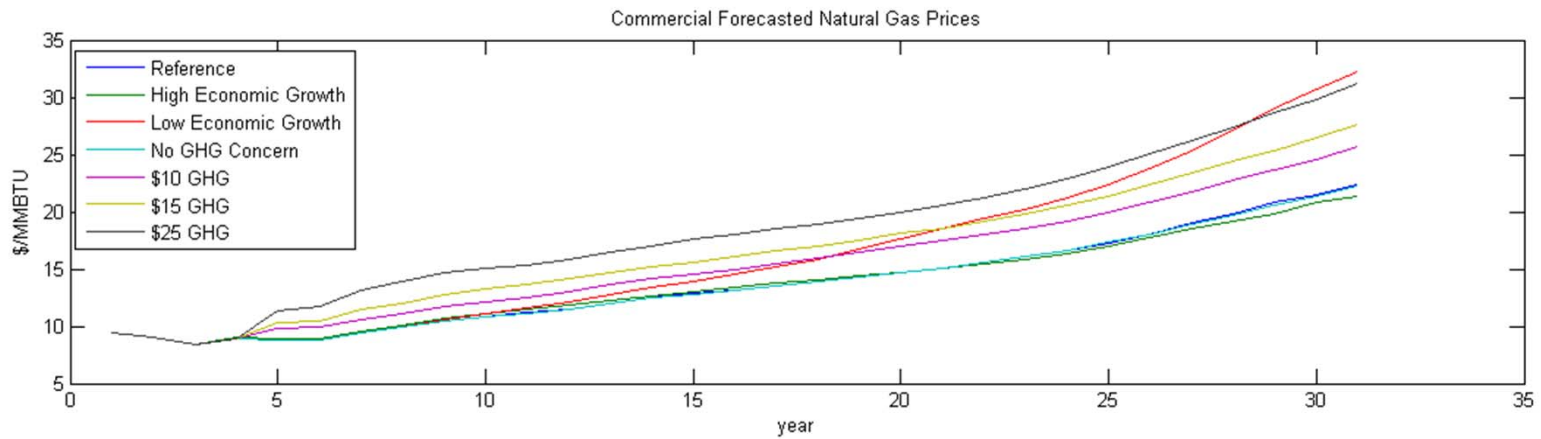
	Sequential	Simultaneous
Objective function value	0.0094	0.0108
System model evaluations	3,336	1
Computation time (s)	331.6	1.1



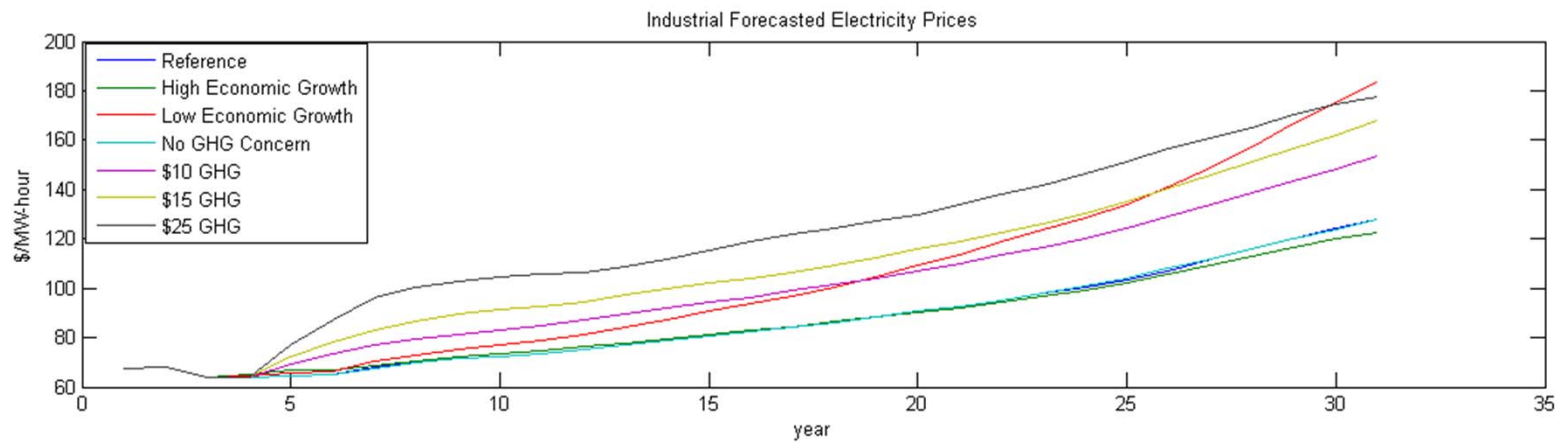
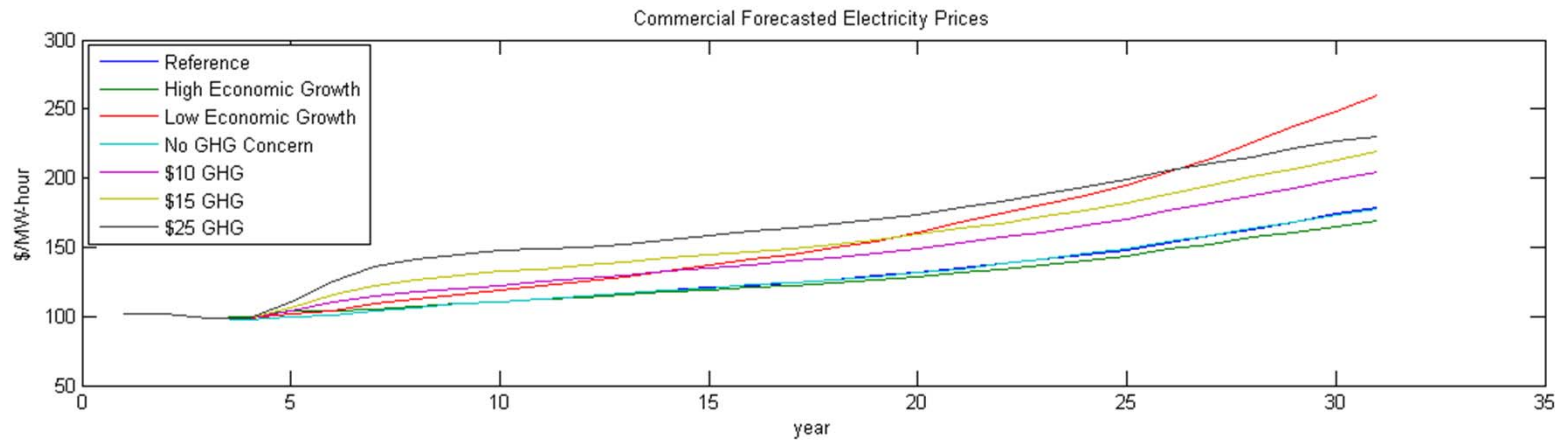
K.M. Powell, J.D. Hedengren, T.F. Edgar, A Continuous Formulation for Logical Decisions in Differential Algebraic Systems using Mathematical Programs of Equilibrium Constraints, Industrial and Engineering Chemistry Research, Submitted, 2013.



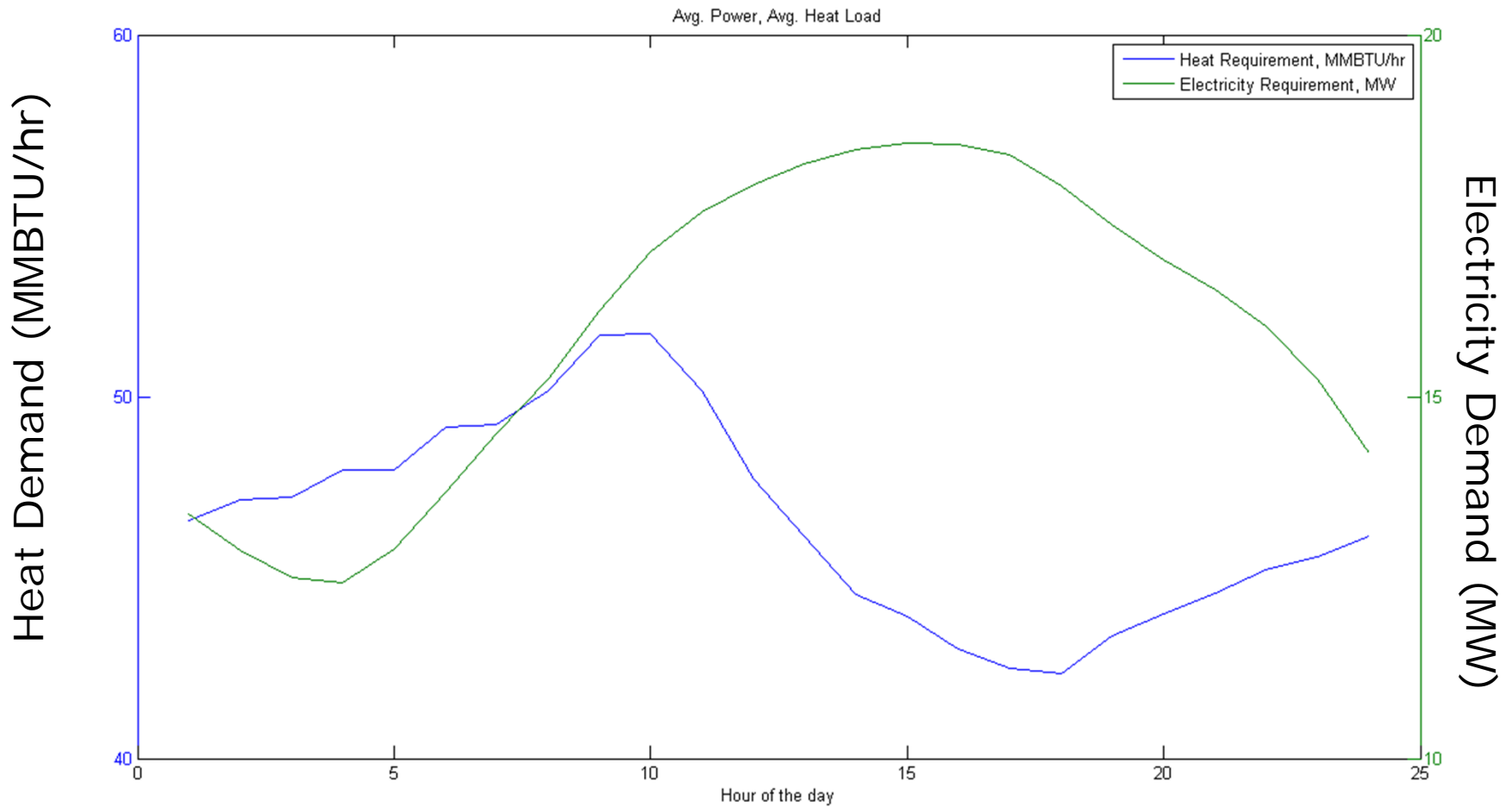
Uncertainty in Natural Gas Prices



Uncertainty in Electricity Prices

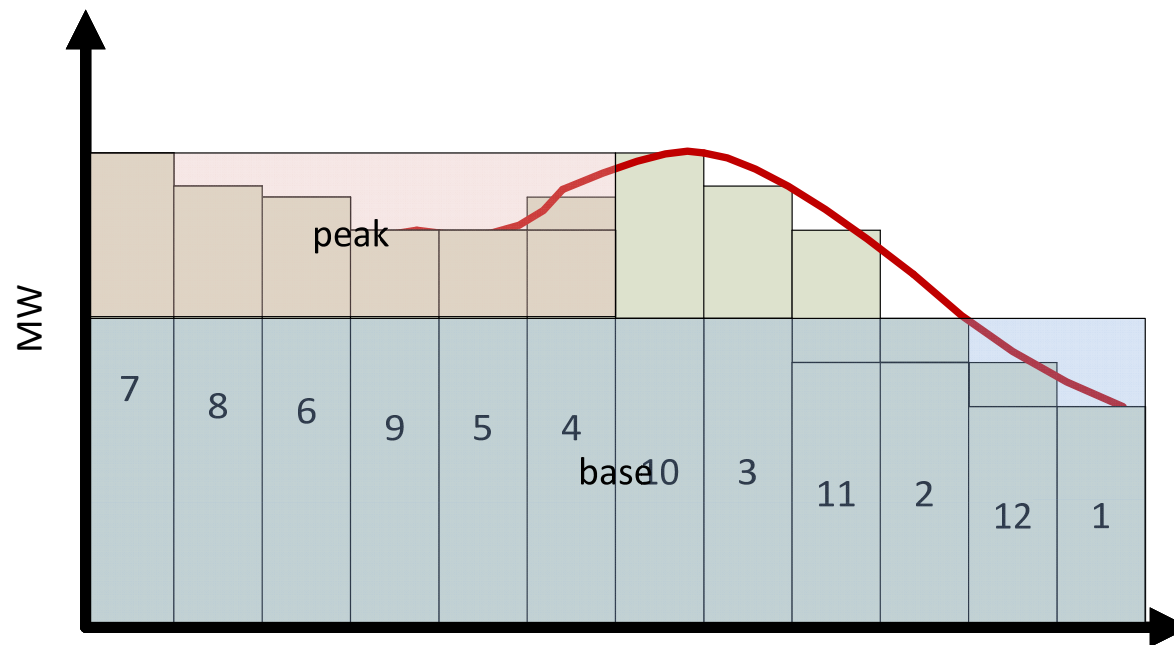


Dynamic Model for Dynamic System

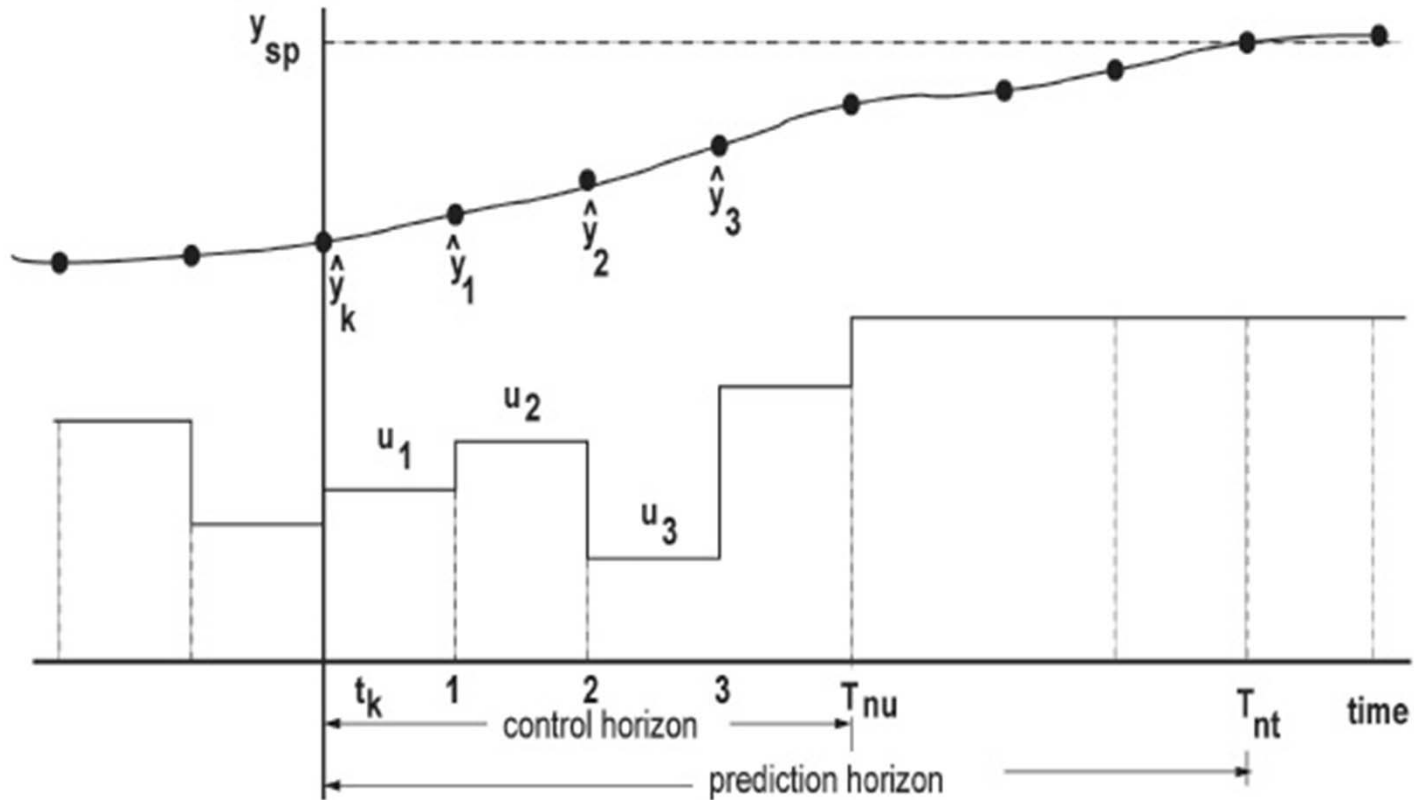


Simplifying System

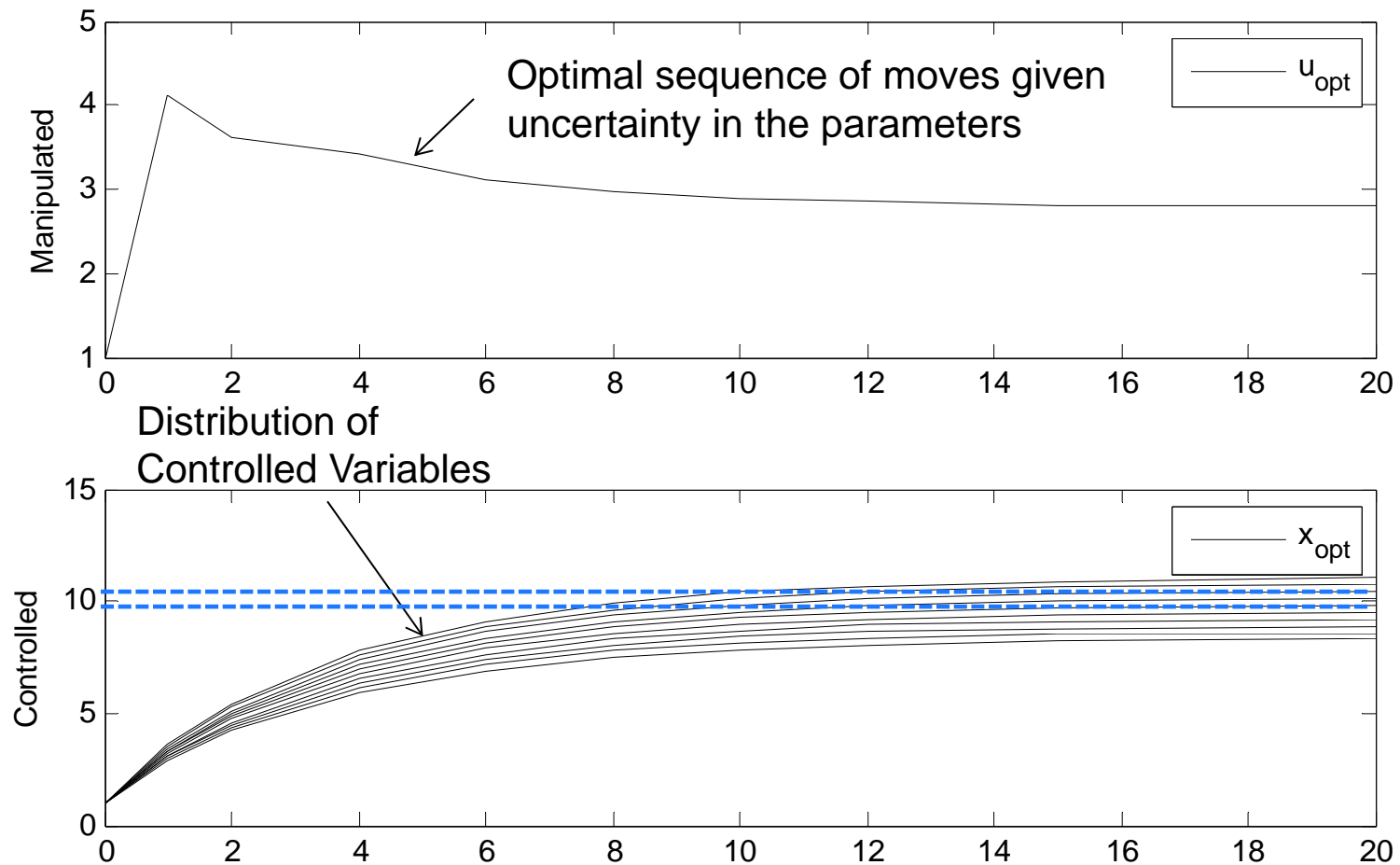
- Create Model:
- Electric and Heating Demand Model (winter and summer)



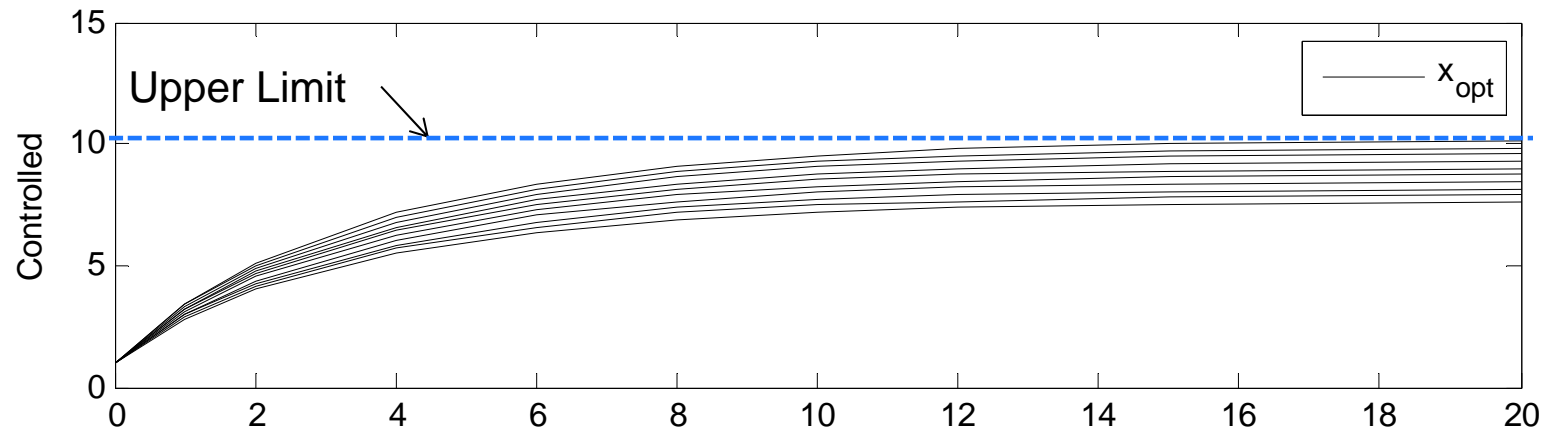
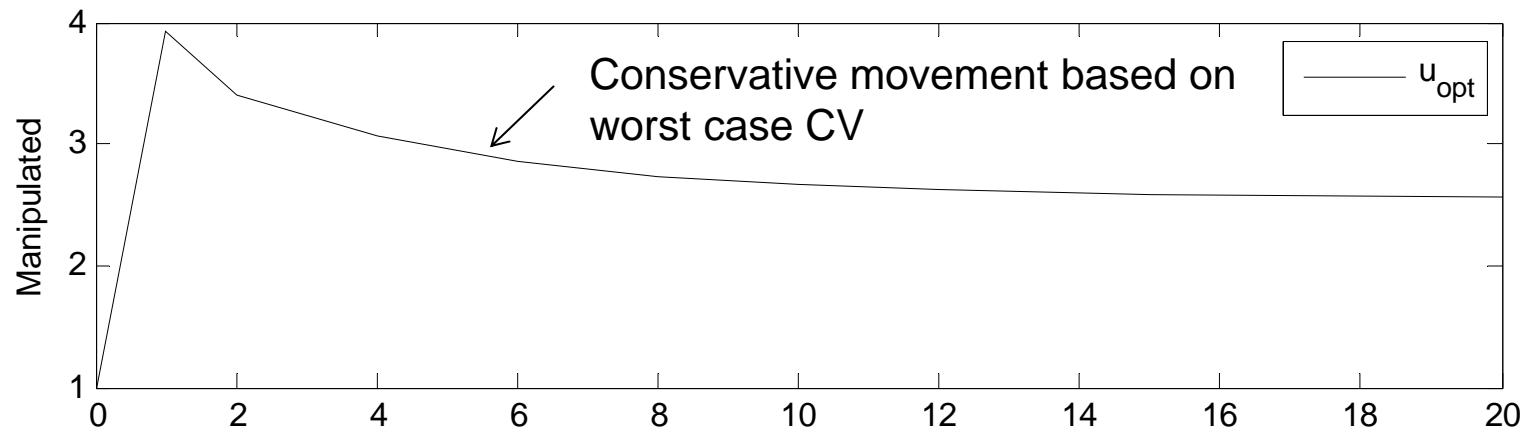
Model Predictive Control Approach



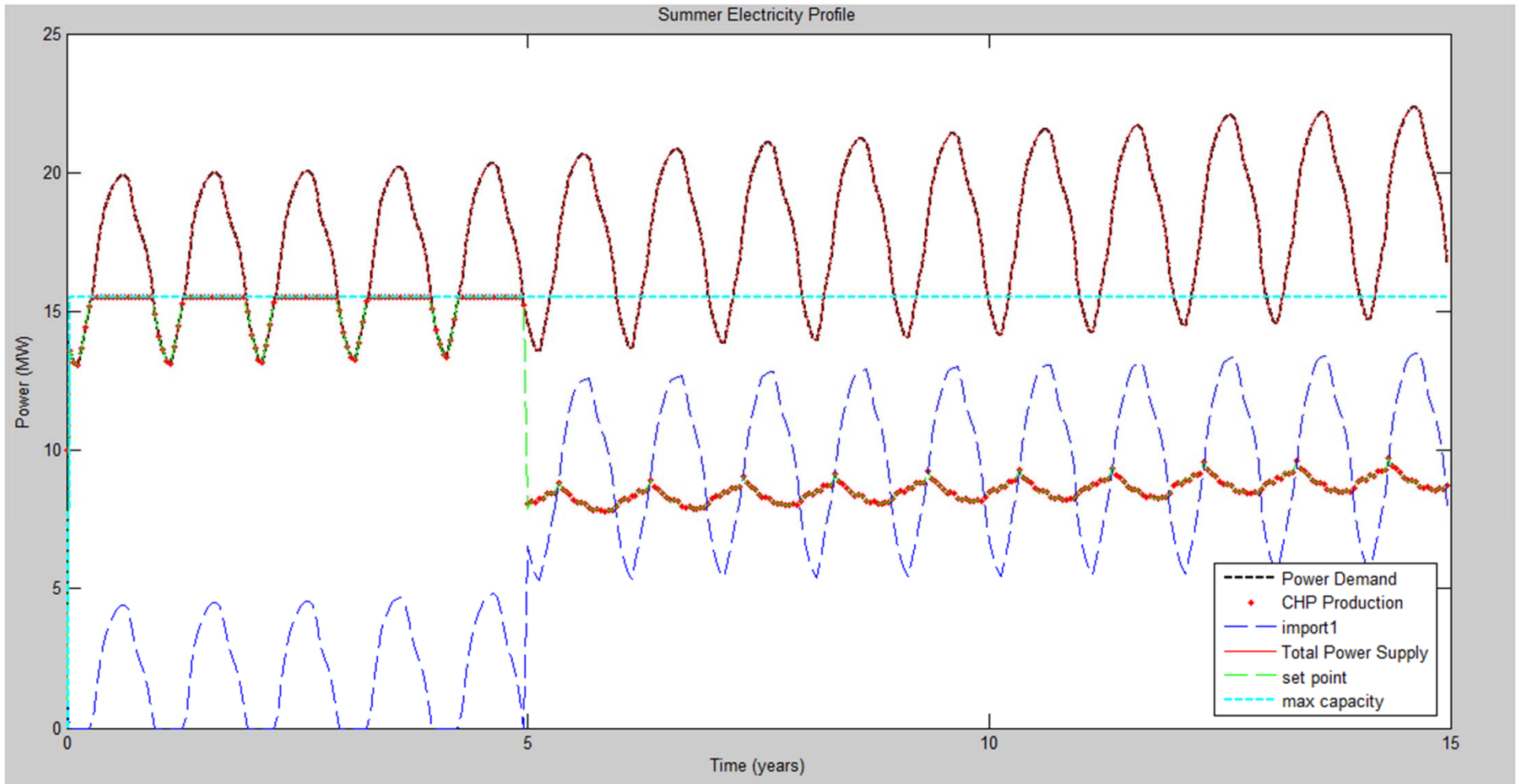
Optimize to a Target Range



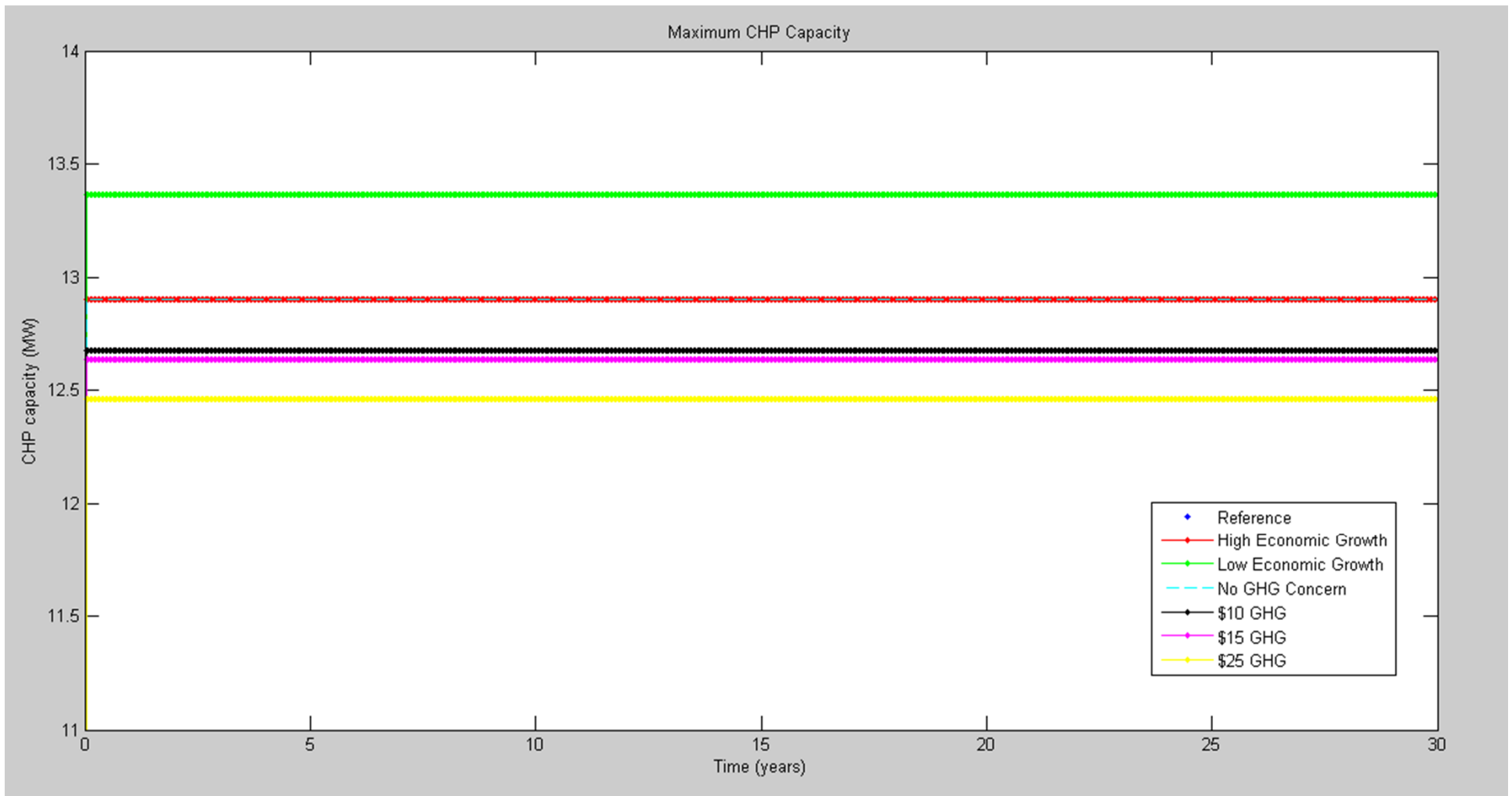
Optimize to a Limit



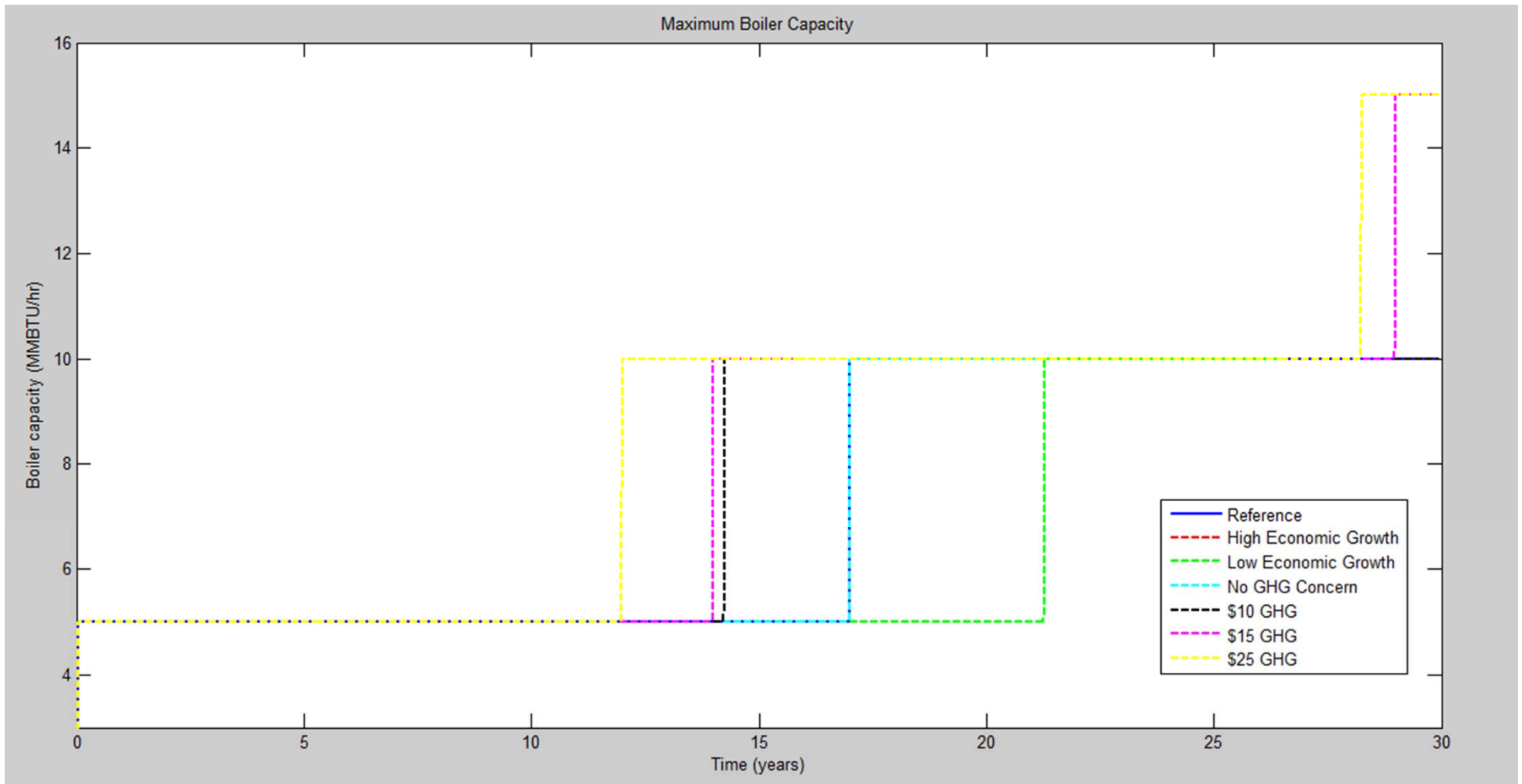
Dynamic Solution



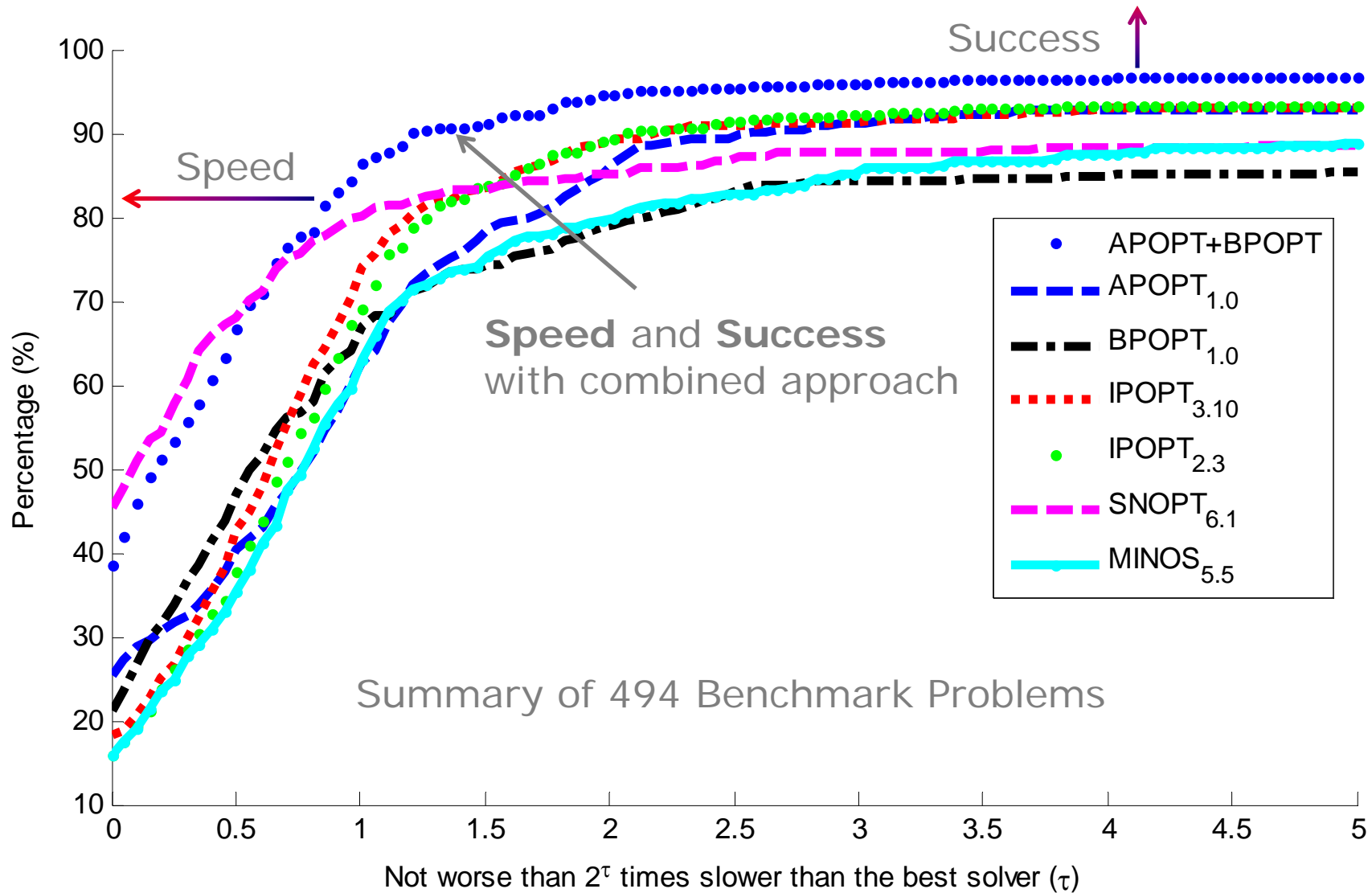
Turbine Max Capacity



Supplemental Boiler Firing Capacity



Optimization Benchmark



Survey of DAE Solvers

<u>Software Package</u>	<u>Max DAE Index</u>	<u>Form</u>	<u>Adaptive Time Step</u>	<u>Sparse</u>	<u>Partial-DAEs</u>	<u>Simultaneous Estimation / Optimization</u>
APMonitor	3+	Open	No	Yes	Yes	Yes
DASPK / CVODE / Jacobian	2	Open	Yes	No	No	No
gProms	1 (3+ with transforms)	Open	Yes	Yes	Yes	No
MATLAB	1	Semi-explicit	Yes	No	No	No
Modelica	1	Open	Yes	Yes	No	No

DAE = Differential and Algebraic Equation



Conclusions

- Powerful insights can be gained from modeling and data reconciliation over long periods of historical data
- When data, modeling, and optimization are combined, hidden savings are discovered through dynamic optimization
- Simulation and optimization can give realistic options to evaluate risks and rewards
- Simulation results can then be directly applied in practice to continuously monitor and optimize

Development Needs

- Library of high quality models that are open source and can be adapted to new problems
- Improvements to methods to simulate and optimize large-scale and complex systems
- Interface with operations and subject matter experts – need to know the process for effective modeling and optimizing

