APOPT and BPOPT: New NLP and MINLP Solvers for Differential Algebraic Systems with Benchmark Testing

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Presentation Overview

- Overview of Benchmarking Testing.
  - NLP Benchmarking
    - Hock-Schittkowski
    - Dynamic optimization
    - Biological models
  - MINLP Benchmarking
    - MacMINLP
- Case studies
  - Gravity Drained tank (MIDAE control problem)
  - Energy Storage for smart grid
- Future Developments

Overview of Benchmark Testing

- NLP Benchmark Testing
  - APOPT[1], BPOPT[1], IPOPT[2], SNOPT[3], MINOS[3]
  - Problem characteristics:
    - Hock Schittkowski, Dynamic Opt, SBML
    - Nonlinear Programming (NLP)
    - Differential Algebraic Equations (DAEs)
    - APMonitor Modeling Language

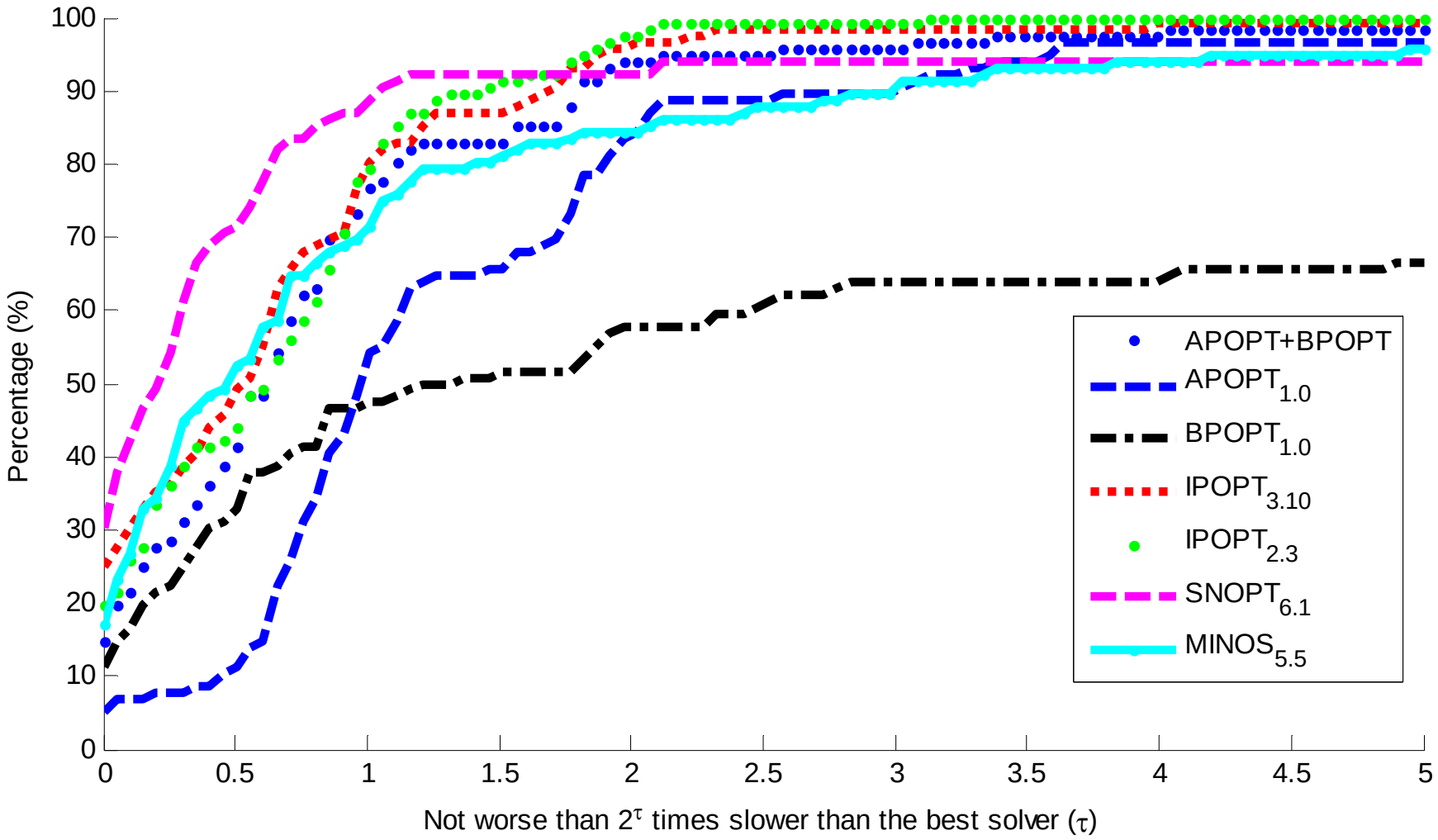
$$\begin{aligned}
&\min J(x,y,u)\\
&s.t.\ 0 = f\left(\frac{\partial x}{\partial t}, x, y, u\right)\\
&\quad 0 = g(x,y,u)\\
&\quad 0 < h(x,y,u)\\
&\quad x, y \in \Re^n\ u \in \Re^m
\end{aligned}$$

- MINLP Benchmark Testing
  - APOPT[1], BPOPT[1], BONMIN[2], DICOPT[4]
  - Problem characteristics:
    - MacMINLP, Industrial Test Set
    - Mixed Integer Nonlinear Programming (MINLP)
    - Mixed Integer Differential Algebraic Equations (MIDAEs)
    - APMonitor & AMPL Modeling Language

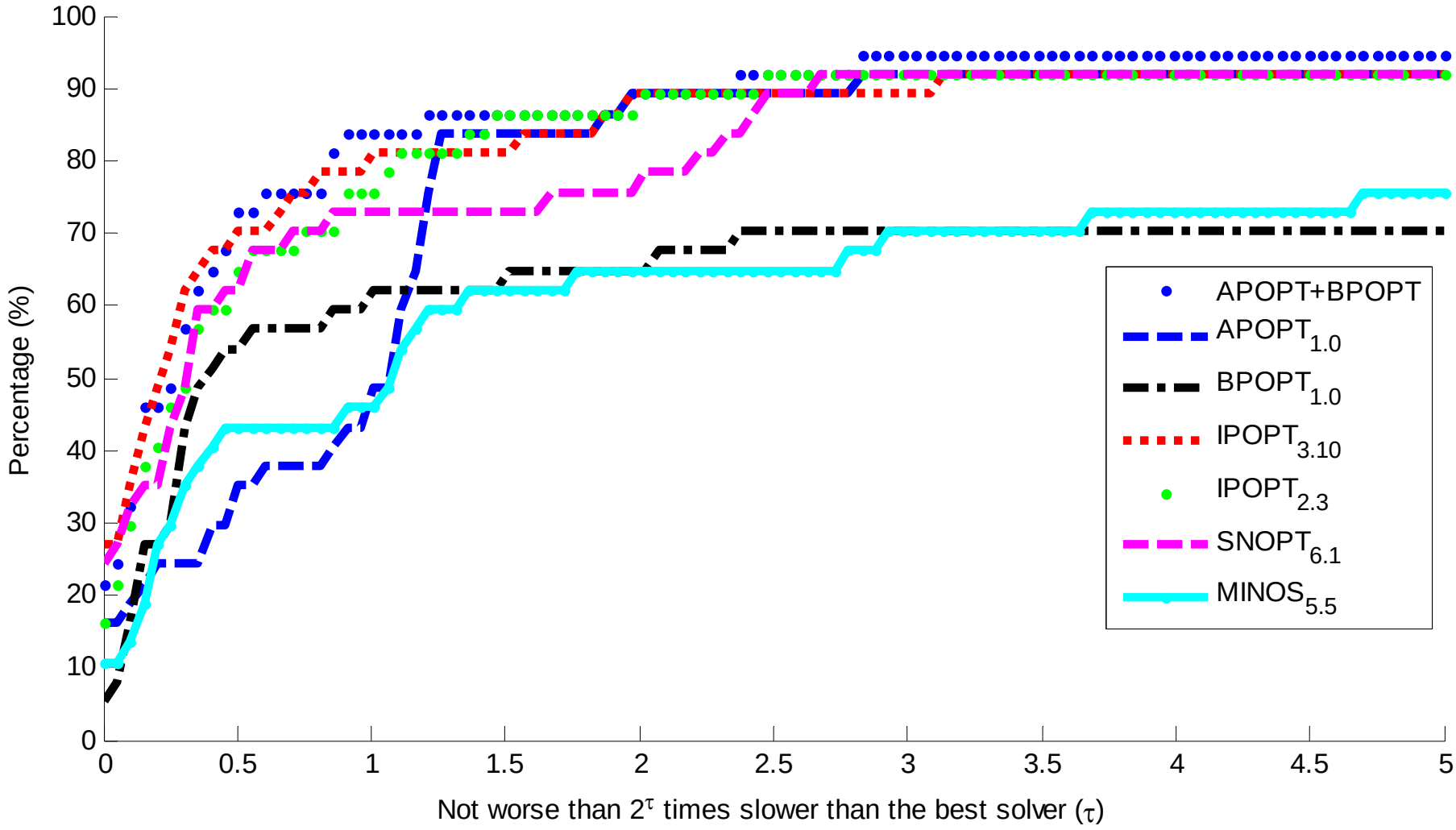
$$\begin{aligned}
&\min J(x,y,u,z)\\
&s.t.\ 0 = f\left(\frac{\partial x}{\partial t}, x, y, u, z\right)\\
&\quad 0 = g(x,y,u,z)\\
&\quad 0 < h(x,y,u,z)\\
&\quad x, y \in \Re^n\ u \in \Re^m\ z \in \mathrm{I}^m
\end{aligned}$$

1–APS, LLC 2–EPL, 3–SBS, Inc., 4-CMU

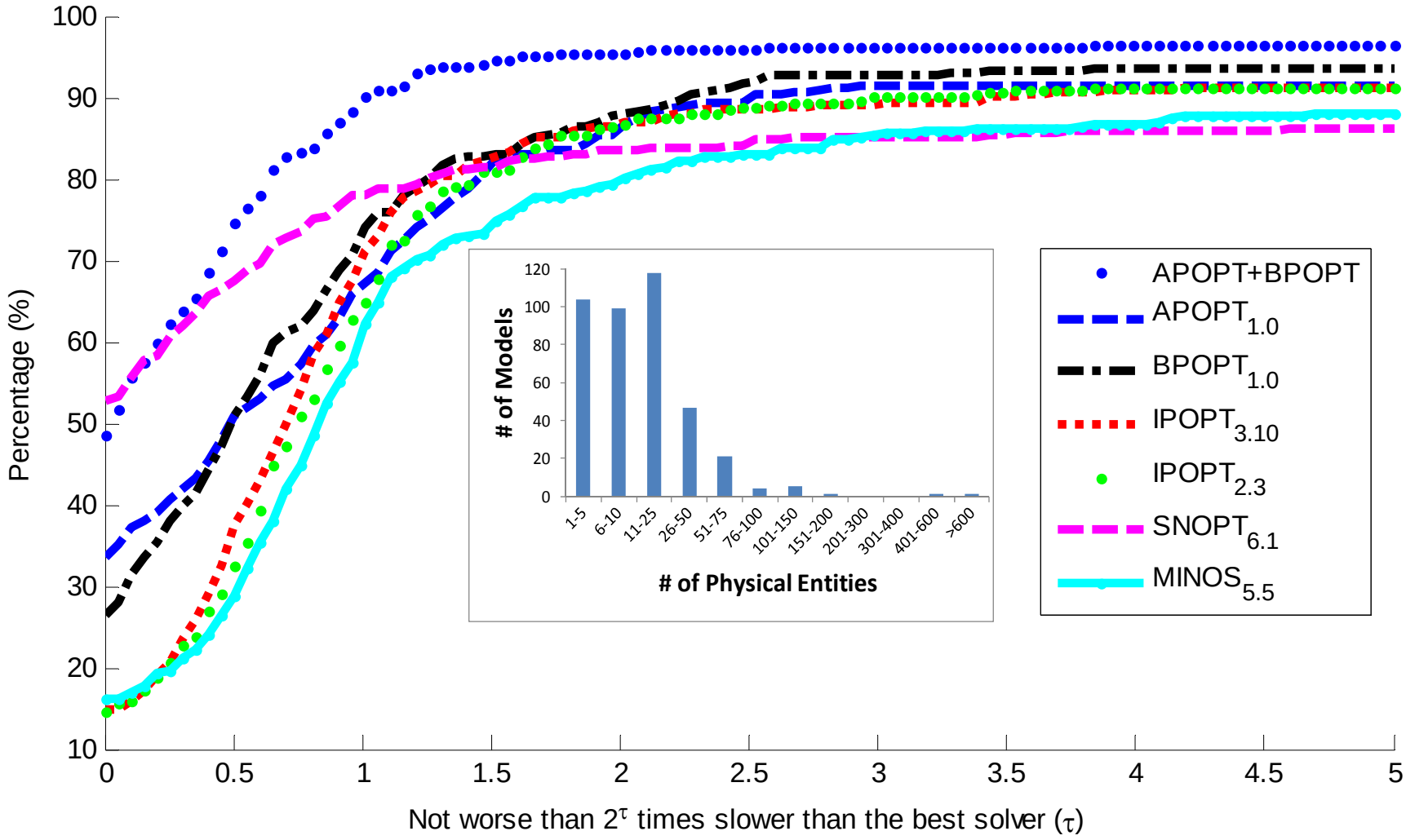
NLP Benchmark – Hock-Schittkowski (116)



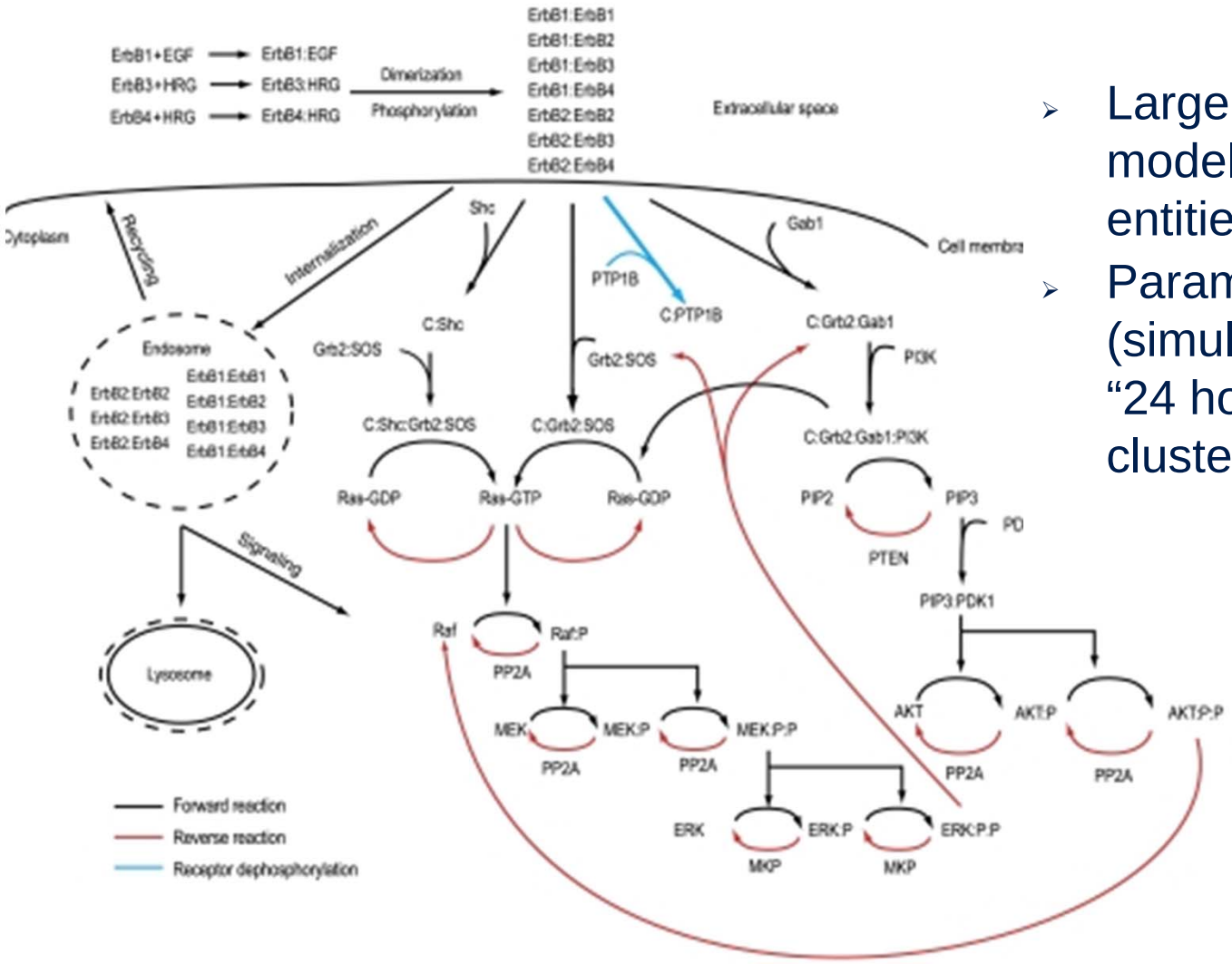
NLP Benchmark - Dynamic Optimization (37)



NLP Benchmarking – SBML (341)



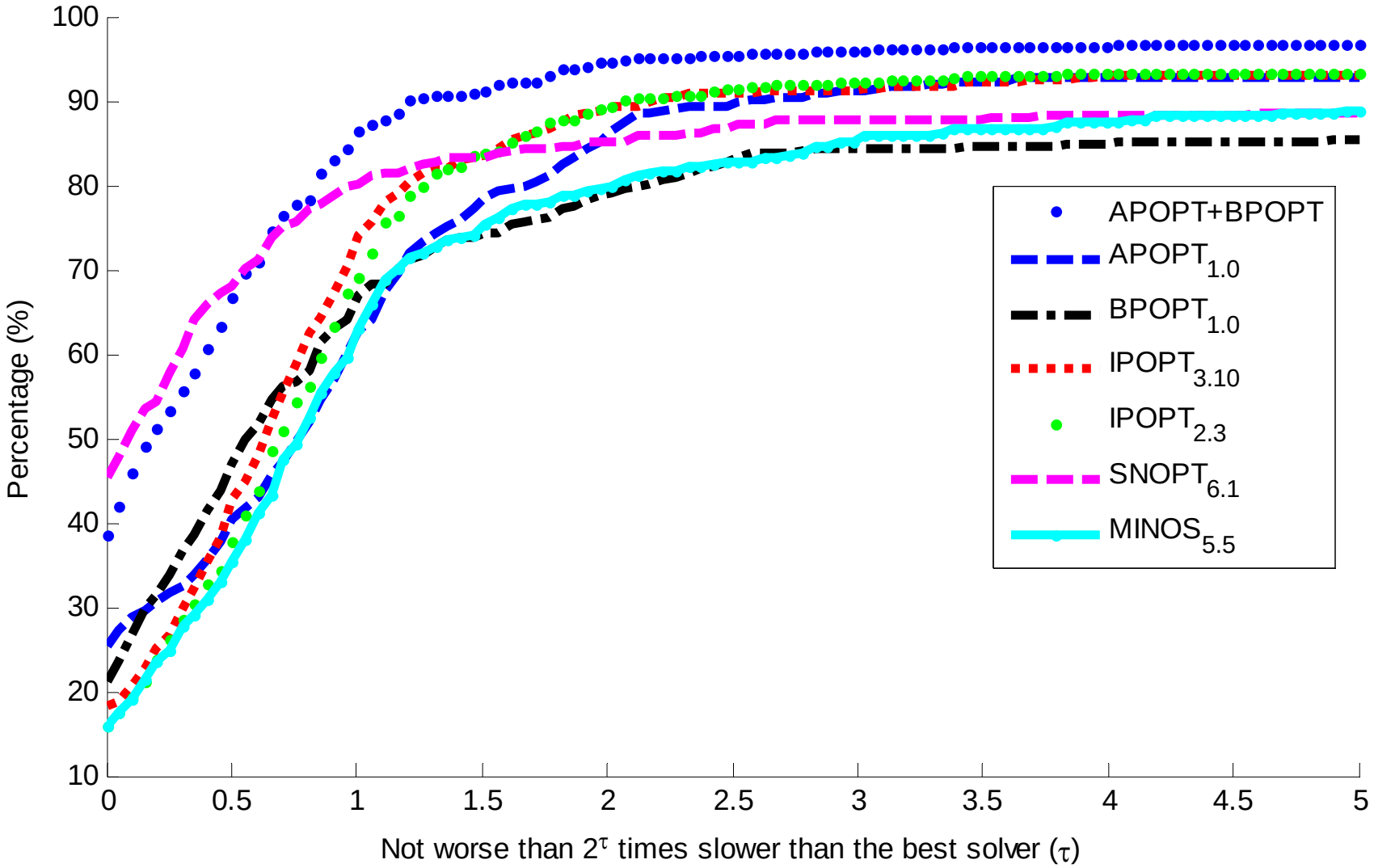
Example: ErbB Signal Transduction Cascade



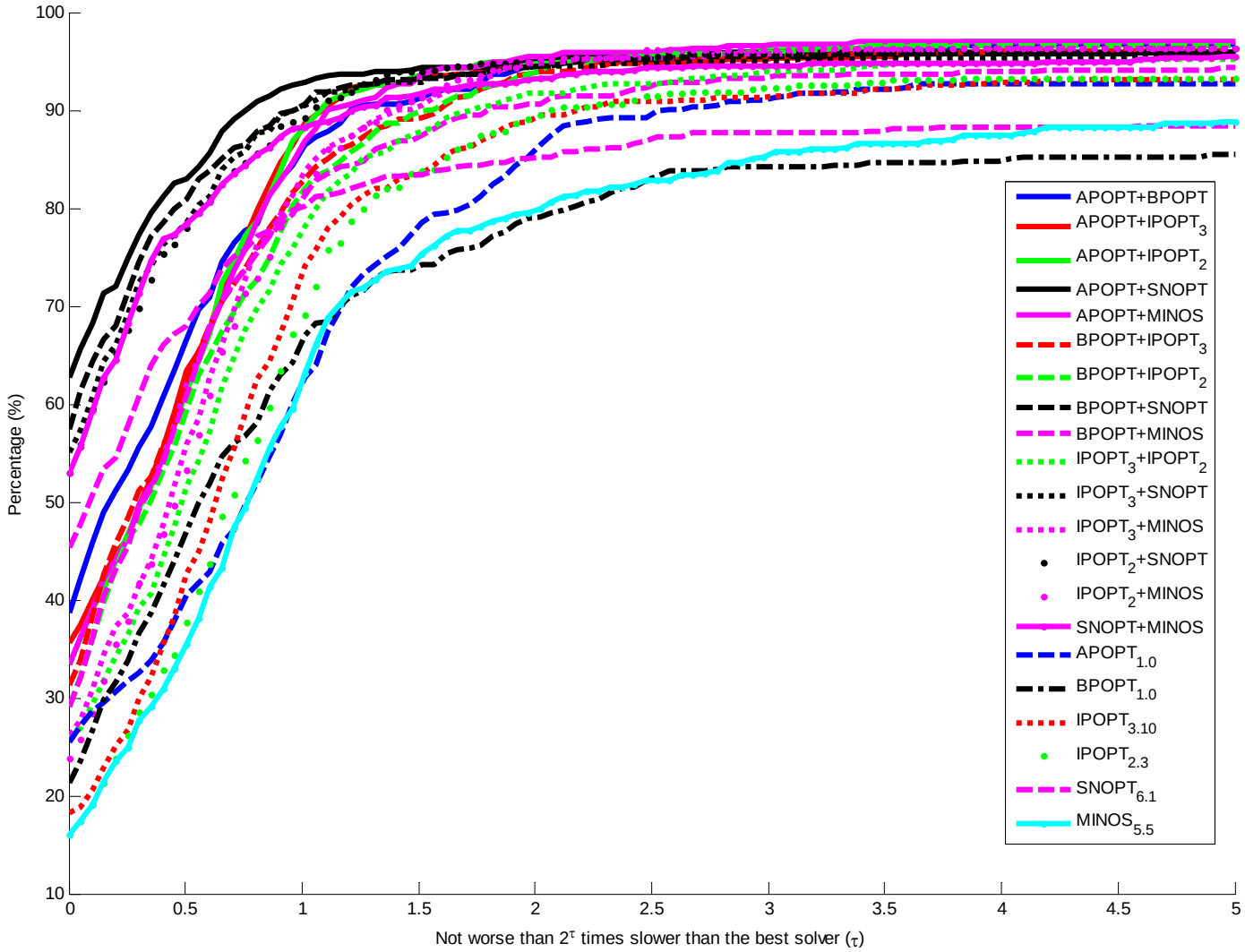
- Large ErbB signalling model (~504 physical entities)*
- Parameter estimation (simulated annealing) took “24 hours on a 100-node cluster computer”

*Chen et al. Mol Syst Biol. 2009;5:239 .

NLP Benchmark – Summary (494)



NLP Benchmark – Combo Solvers (494)



MacMINLP Benchmark Summary Results

Variables	Integers	Equations	NLP Obj	MINLP Obj	Solution Time	Status	
10	4	4	1.55E+02	1.74E+02	0.031	Success	an_integer_test
107	24	73	2.59E+05	2.86E+05	0.25	Success	batch
4	4	0	6.30E-13	7.78E-07	0.016	Success	geartrain1
27	16	7	5.02E+00	1.30E+01	0.094	Success	mittelman
12	3	6	7.59E-01	6.01E+00	0.031	Success	synthes1
23	5	14	4.18E+00	7.30E+01	0.047	Success	synthes2
38	8	24	1.65E+01	7.57E+01	0.062	Success	synthes3
6	3	5	1.18E-01	2.54E-01	0.031	Success	wind-fac
510	168	308	-1.01E+00	-1.01E+00	8.865	Success	c-reload-14a
510	168	308	-1.02E+00	-1.02E+00	13.728	Success	c-reload-14b
510	168	308	-9.91E-01	-9.56E-01	48.344	Failure	c-reload-14c
510	168	308	-1.03E+00	-1.03E+00	6.724	Success	c-reload-14d
510	168	308	-1.03E+00	-1.03E+00	4.852	Success	c-reload-14e
510	168	308	-1.01E+00	-1.01E+00	6.614	Success	c-reload-14f

Case Study- MPC with MINLP

- PCT40 is a basic process control unit produced by Armfield
- Main Devices: Large Process Vessel, CSTR, Hot water Tank
- Sensors: temperature, pressure, and level sensors
- Devices: valves, heating coils, and pumps

How does this work for MINLP Problems?

Objective: Keep the tank level at 100 mm

Continuous: Proportional Solenoid Valve (PSV)

Discrete: On/Off Valve (SOL1)

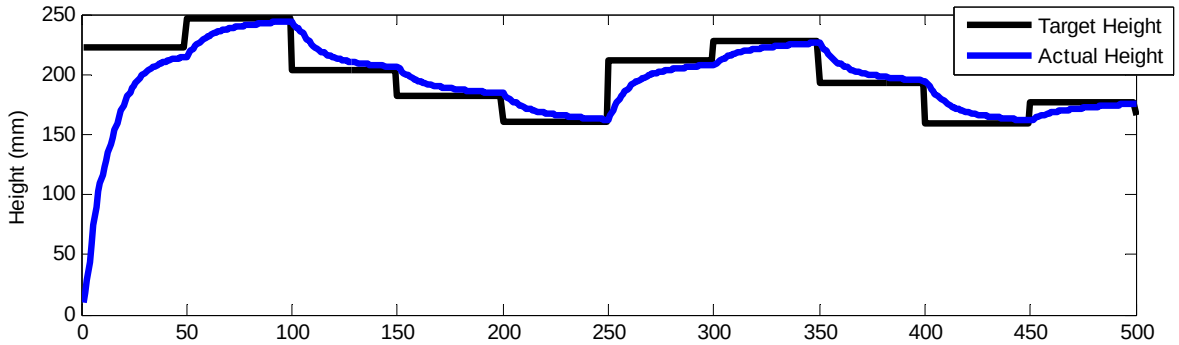
MINLP Model Predictive Control

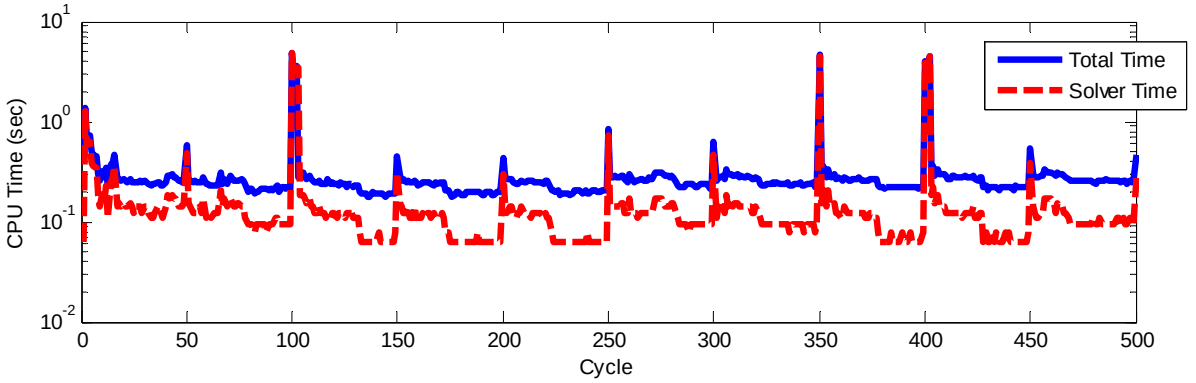
MIDAE System
Variables: 576
Integers: 16
Equations: 544

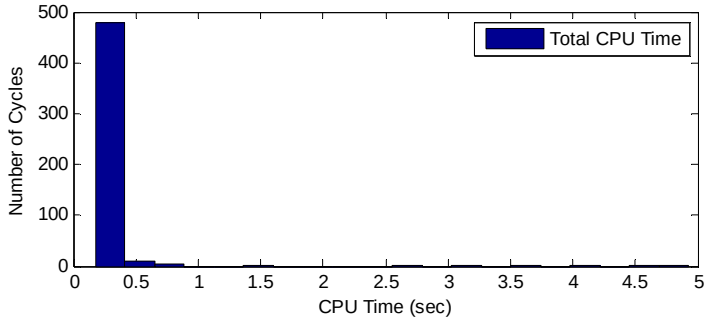
Features
Warm Start Solutions

Discrete (16) and Continuous (16) Decisions

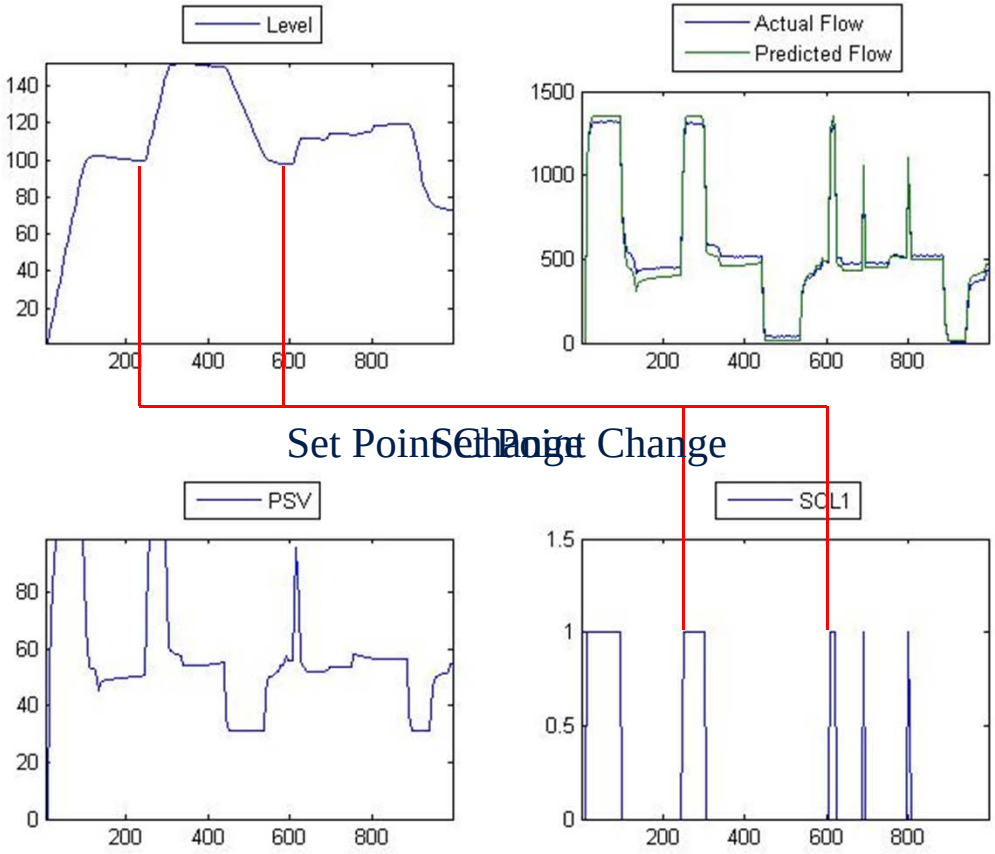
CPU Increases with Setpoint Changes







Results –set point changes

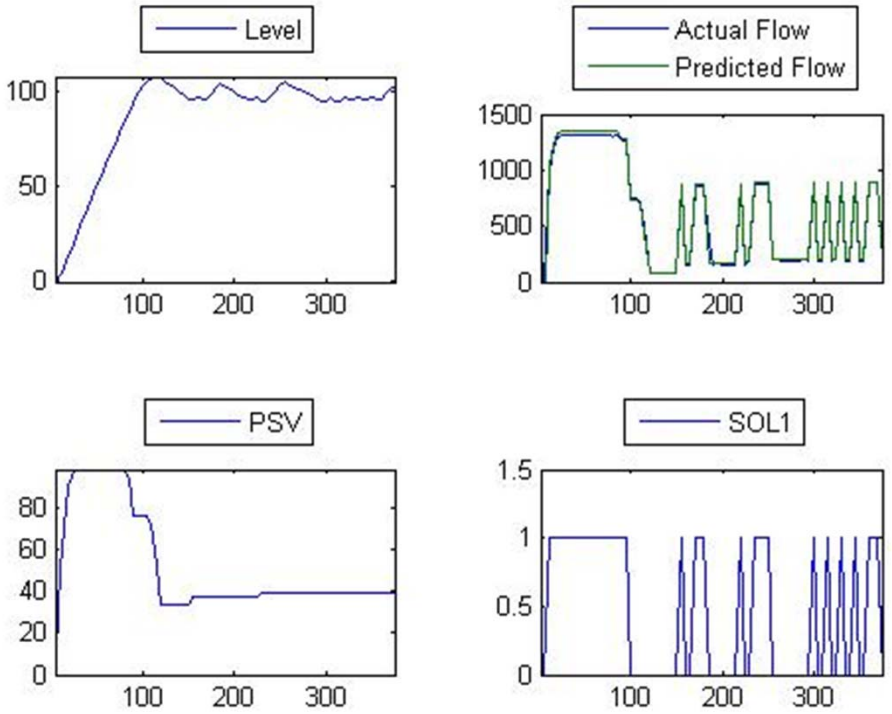


Set Point Changes

- Large (50) – ON
- Medium(20) – ON
- Small (5) – ON
- Very Small – OFF

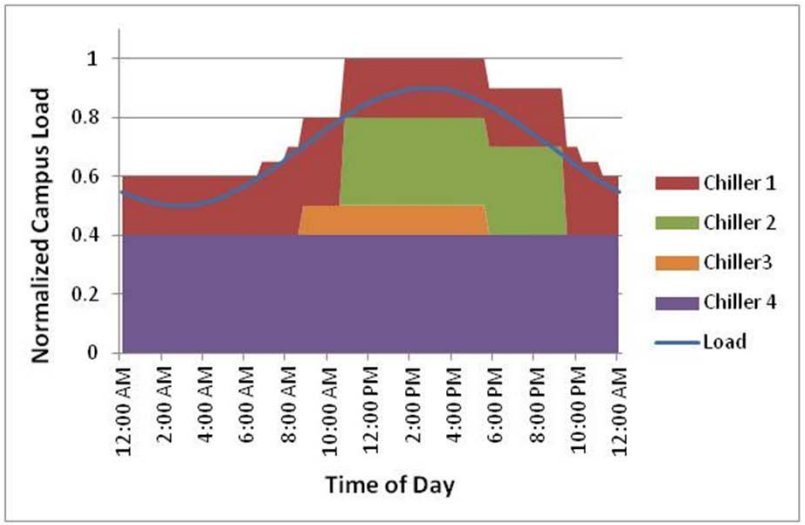
Needs another constraint to limit SOL1 use.

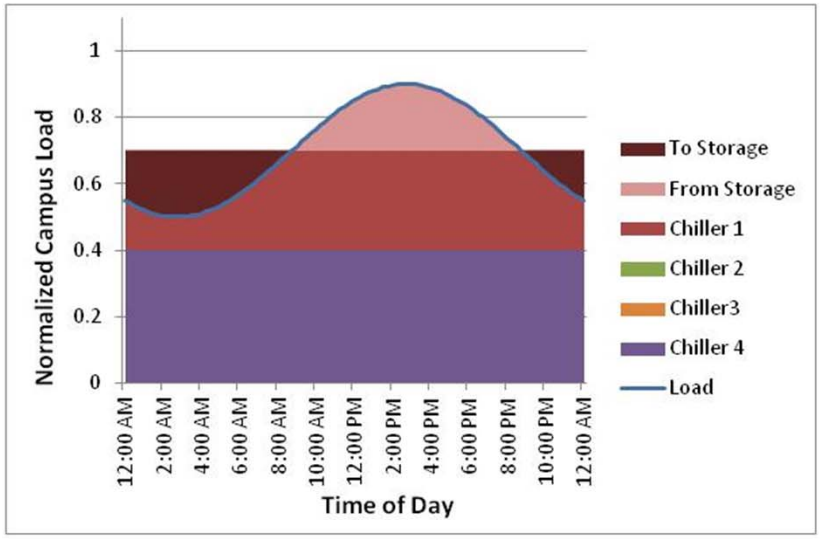
Results-disturbances

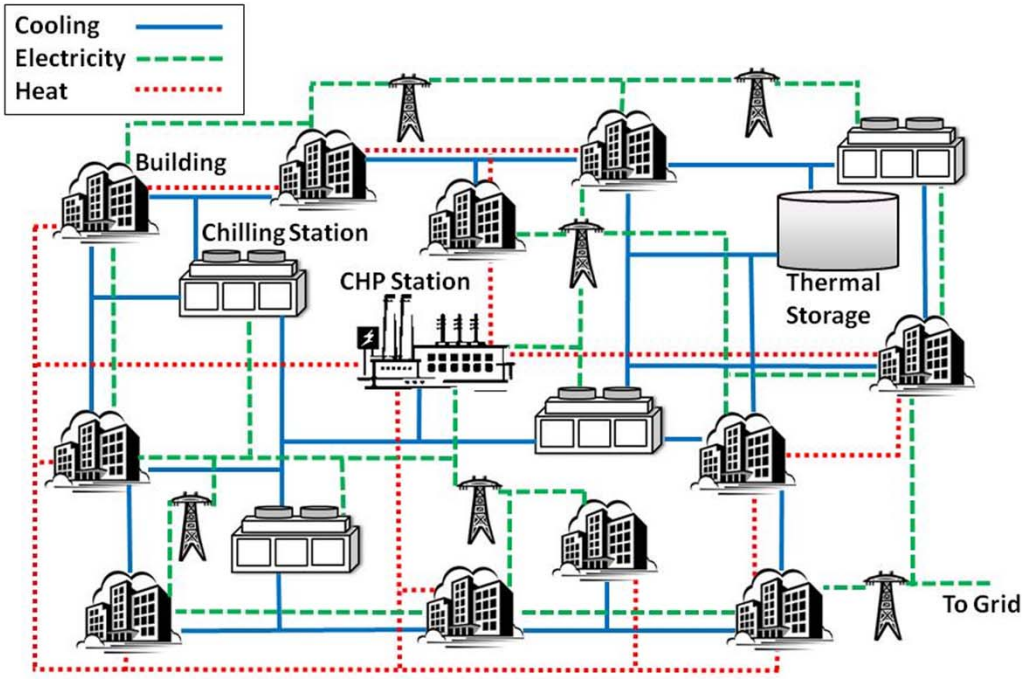


- Disturbance – Opened up an exit valve which is not part of the model
- Reduced Solenoid fluctuations, but still a problem, add cost to opening SOL 1

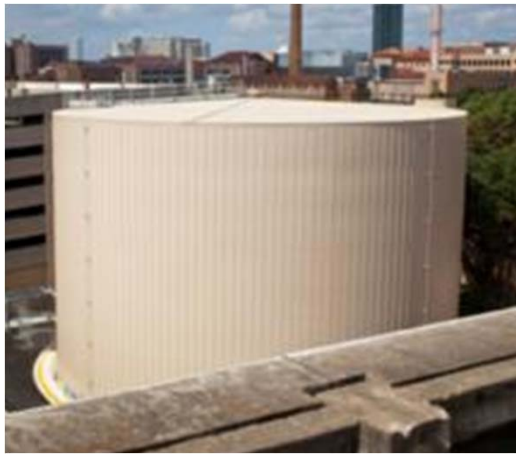
Smart Grid Energy Systems

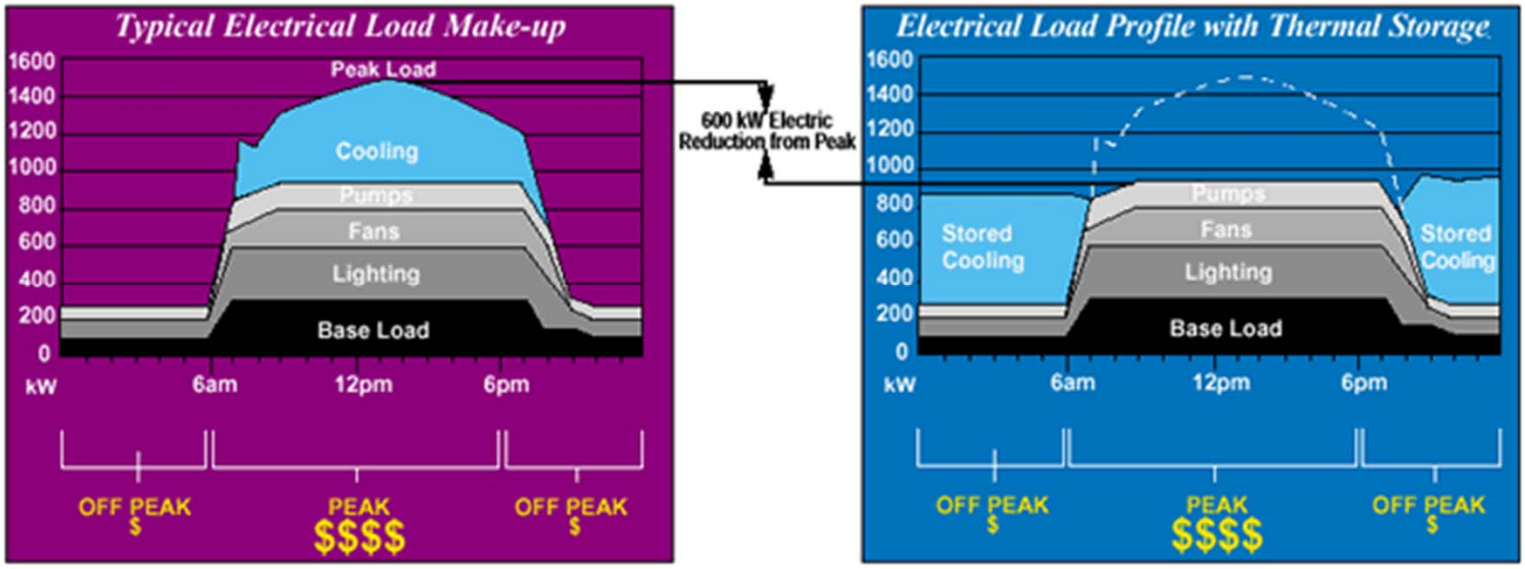




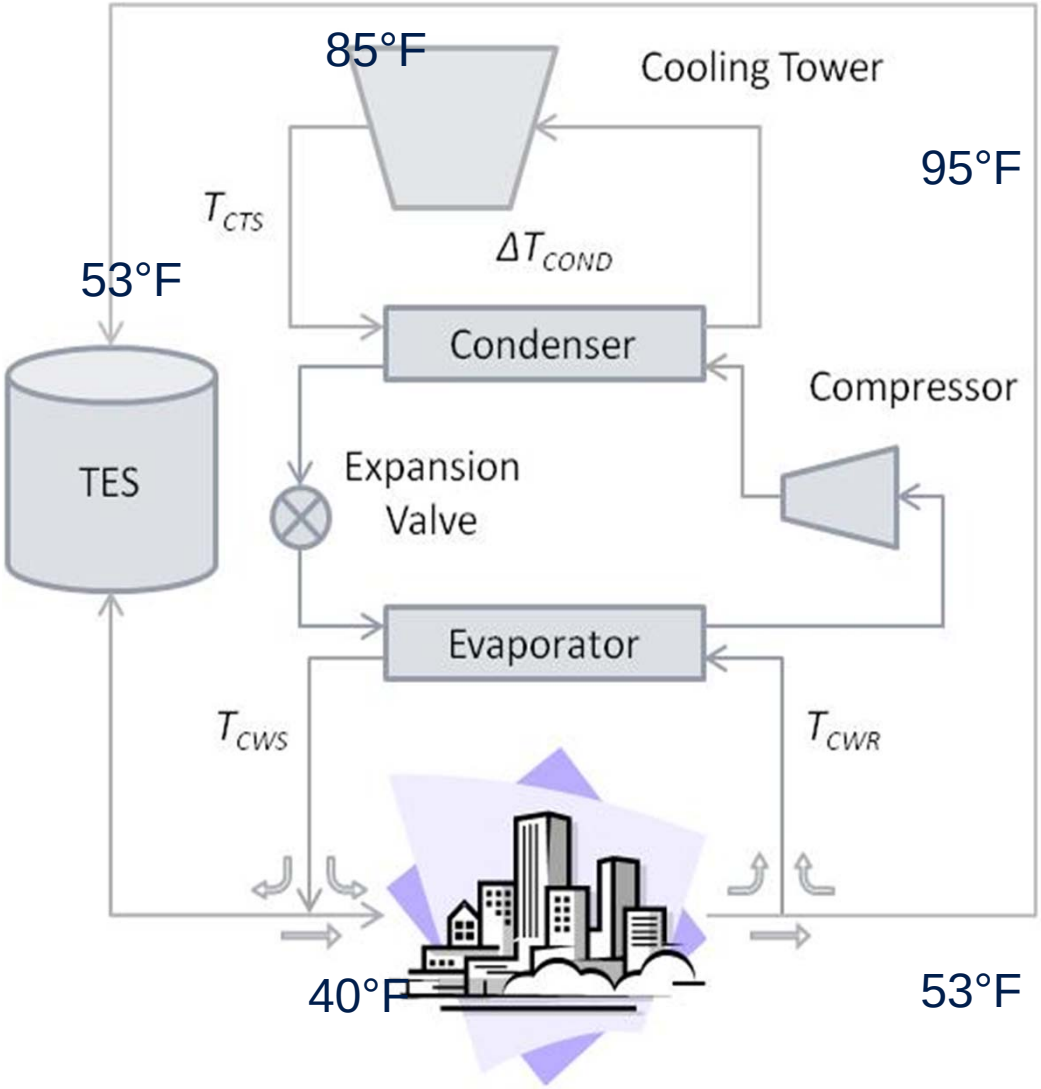


Thermal Energy Storage (TES)





Chiller-TES System



MINLP System
Variables: 672
Integers: 24
Equations: 576

Features
Cold Start Solution

Discrete (24) and Continuous (24) Decisions

Problem Formulation (MINLP)

$$J = \int_0^{t_f} c_{elec}(t) \sum_i P_{chiller,i}(t) dt$$

Subject to:

$$\sum_i y_i L_{chiller,i} = L_{building} - TES$$

$$P_{chiller,i} = y_i f\left(L_{chiller,i}, WBT\right) \qquad f \text{ is nonlinear}$$

$$\frac{dE_{TES}}{dt} = -TES$$

$$0 \le E_{TES} \le 8000$$

$$-2000 \le TES \le 2000$$

$$175 \le L_{chiller,i} \le 1312$$

$$y_i \in 0,1$$

Problem Formulation (Relaxed)

$$J = \min \sum_{i=1}^{24} \left[c_{elec,i} \left(P_{chiller1,i} + P_{chiller2,i} \right) \right]$$

Subject to:

$$L_{chiller1,i} + L_{chiller2,i} = L_{building,i} - TES_i$$

$$P_{chiller1,i} = f\left(L_{chiller1,i}, WBT_i\right) \qquad f \text{ is nonlinear}$$

$$P_{chiller2,i} = f\left(L_{chiller2,i}, WBT_i\right)$$

$$E_{TES,i} = E_{TES,i-1} - TES_i$$

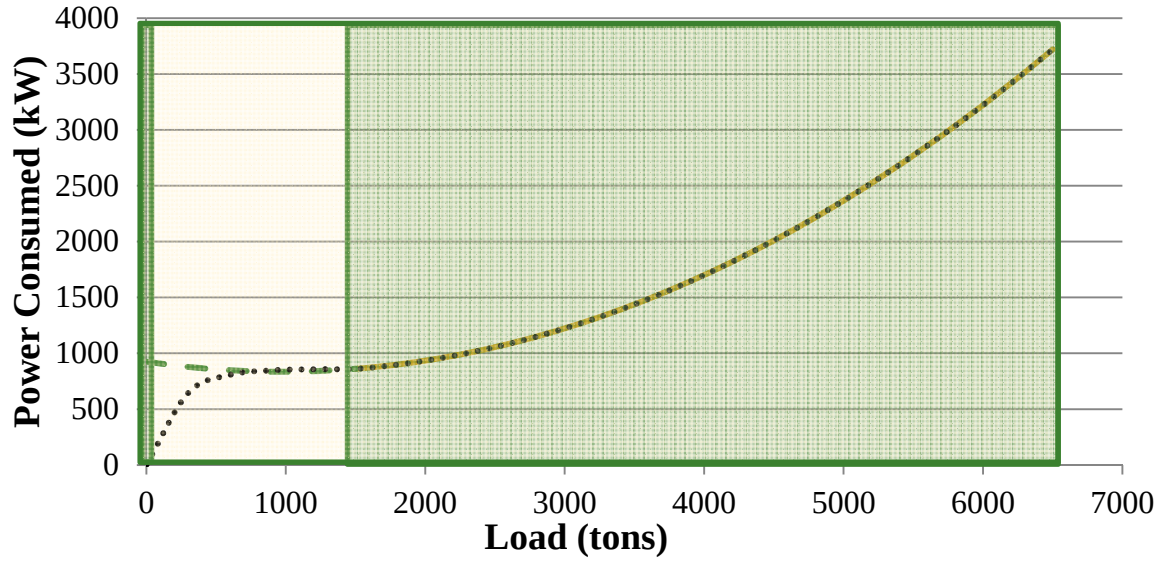
$$0 \le E_{TES,i} \le 8000$$

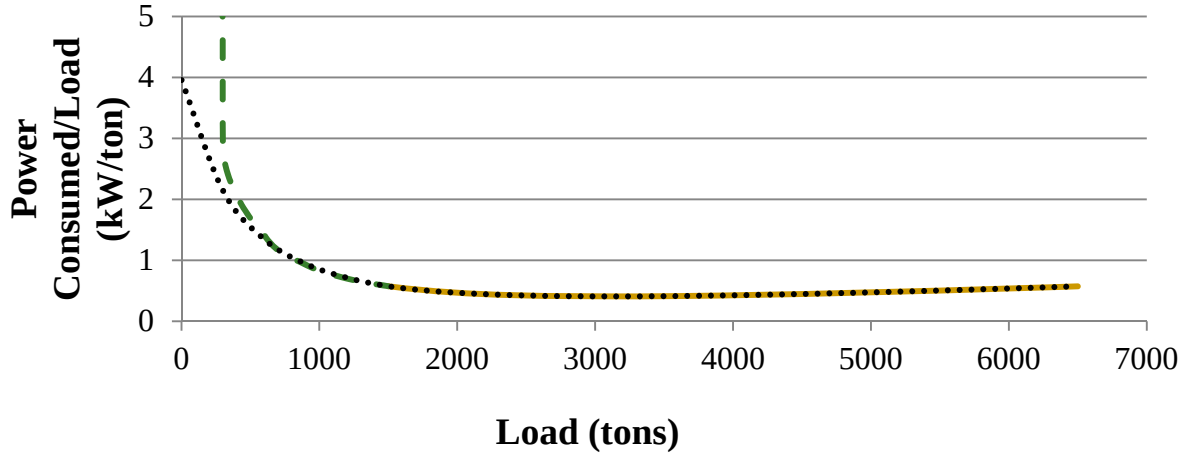
$$-2000 \le TES_i \le 2000$$

Solved using SQP algorithm

Relaxing Binary Constraints

- Mixed integer problem doubles # variables
- Branch and bound technique significantly increases computation time
- Continuous formulation?

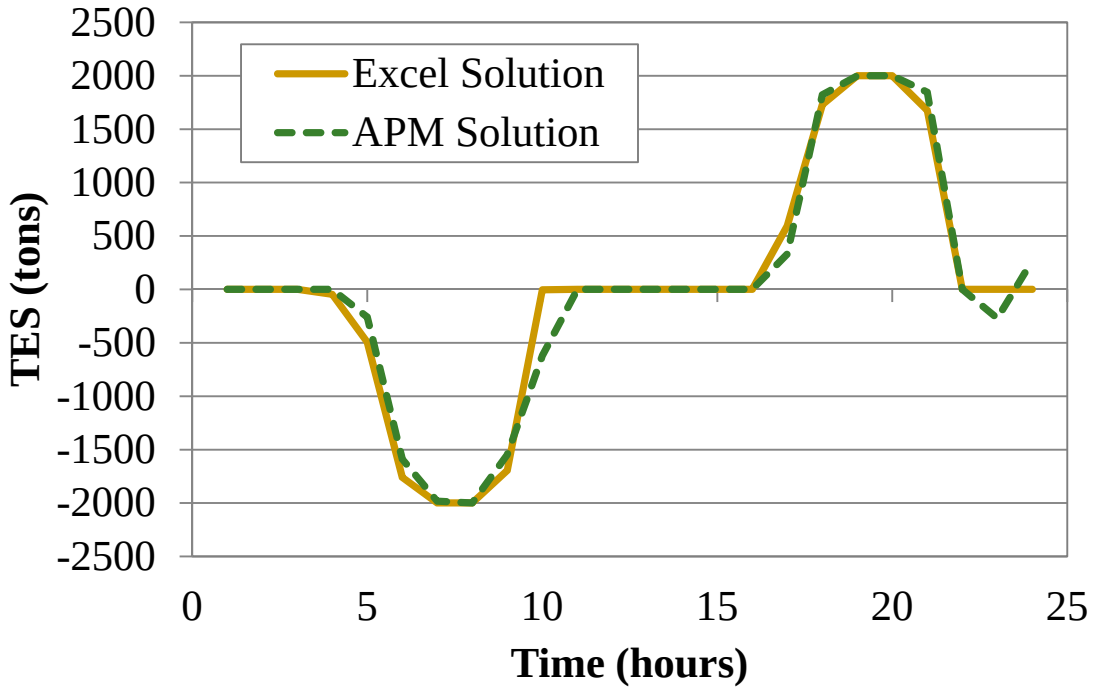




Results

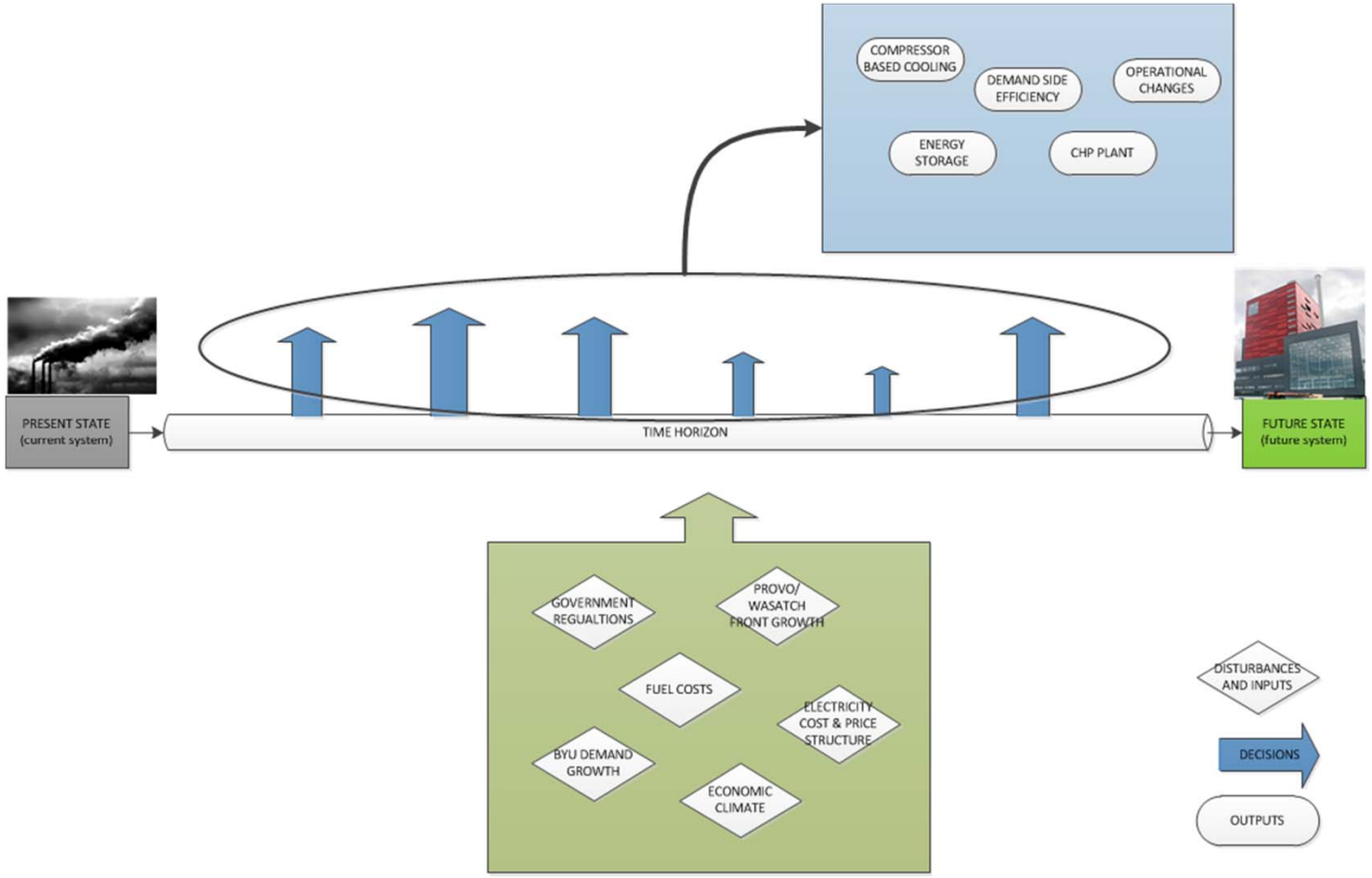
	BONMIN	APOPT	Excel	MATLAB
Cost ($/day)	$ 807.53	$ 804.65	$ 801.93*	$ 802.13*
CPU Time (sec)	11.6	45.0	58.4*	0.1*

* = Relaxed Formulation (NLP)



Optimization of investment decision in energy systems

- Can we apply a similar MPC with MINLP approach to optimize investment decisions for next generation energy systems?



Future Development

- Most flexible and powerful platform for DAEs
  - Need collaborators to create a new interfaces.
- Development influenced by multiple domains:
  - Computational Biology
  - Aerospace Engineering (UAVs)
  - Petrochemical Industry
  - Smart Grid Modeling and Optimization
- Solver Development
  - Mixed Integer Nonlinear Programming for DAEs (MIDAEs)
  - Combine strengths of Active Set (APOPT) and Interior Point (BPOPT) methods