DOE/OE Transmission Reliability Program

Models and Strategies for Optimal Demand Side Management in the Chemical Industries

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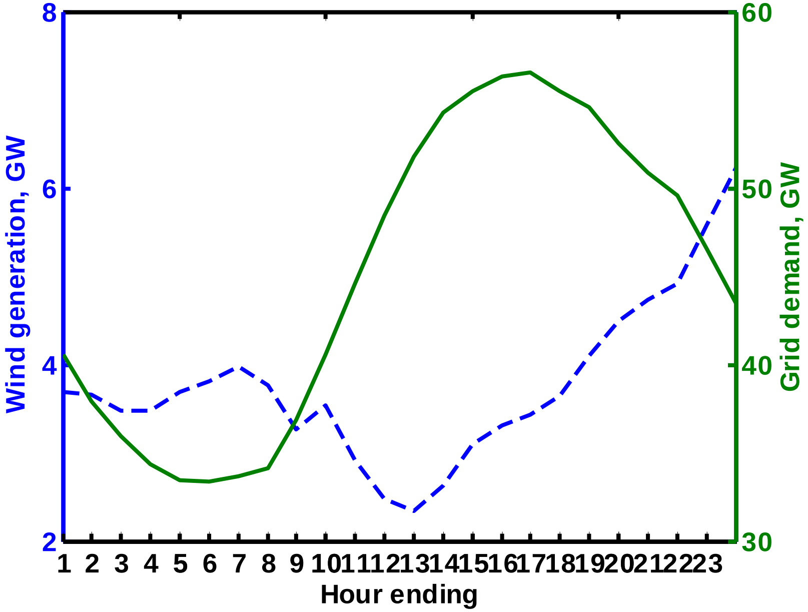
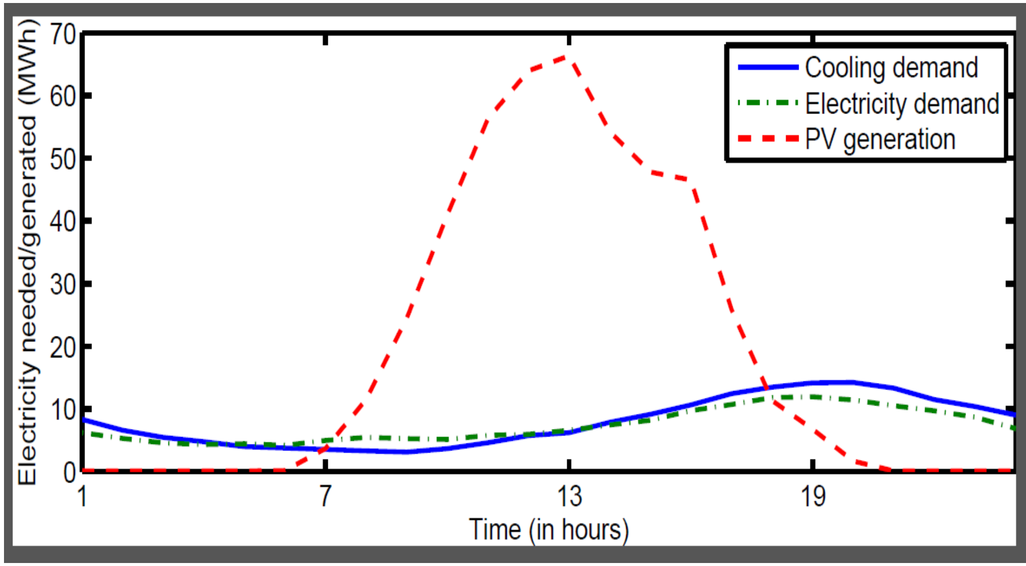
Background and Motivation: Power Grid



Data: www.ercot.com



Ondeck, Edgar, Baldea, Applied Energy, 593-606, 2015

- Significant expansion of renewable generation
  - GW-scale wind generation (~8,200MW in 2016) www.awea.org
  - >1GW of PV solar installed in 2014 www.seia.org
- Increased capacity exacerbates variability issues

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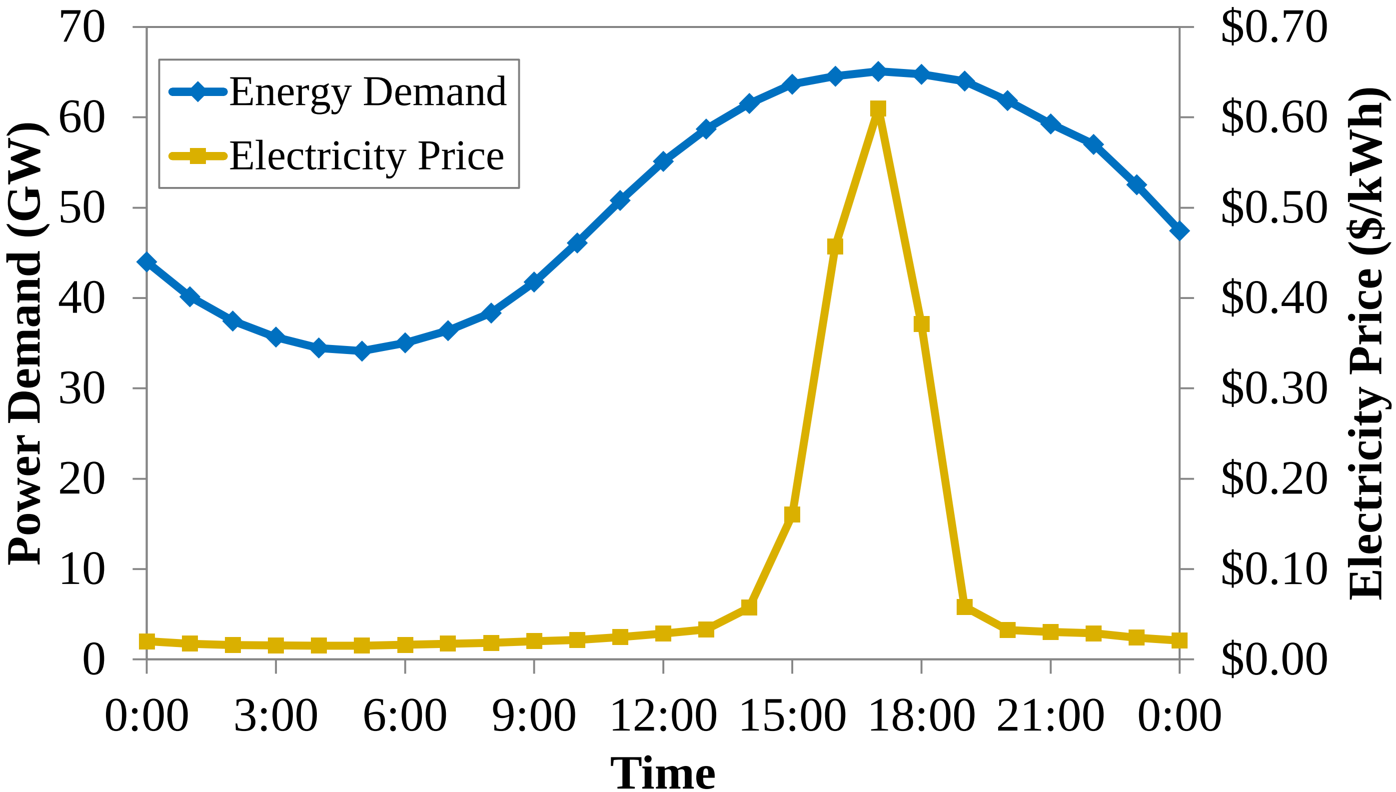
Demand Variability

- Grid demand not synchronized with renewable production
- Peak demand → fast changing and high prices



ERCOT demand and day ahead settlement point prices for June 25, 2012 from www.ercot.com

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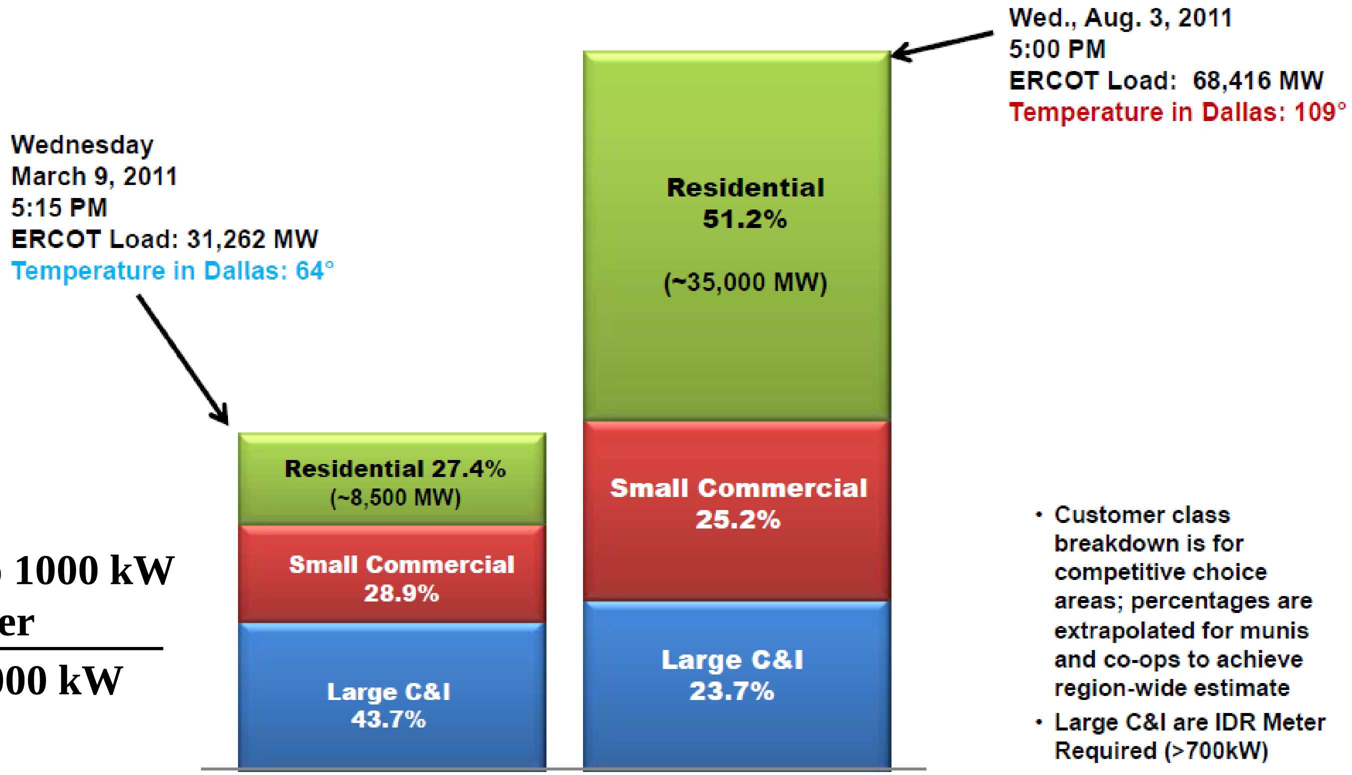
The Peak Demand Problem

- Residential buildings are the primary cause
- Industry could help - how?



$$\frac{\text{Demand up to 1000 kW per user}}{\text{Demand > 1000 kW}}$$

Source: Paul Wattles, ERCOT Overview, Smart Energy Summit, 2012

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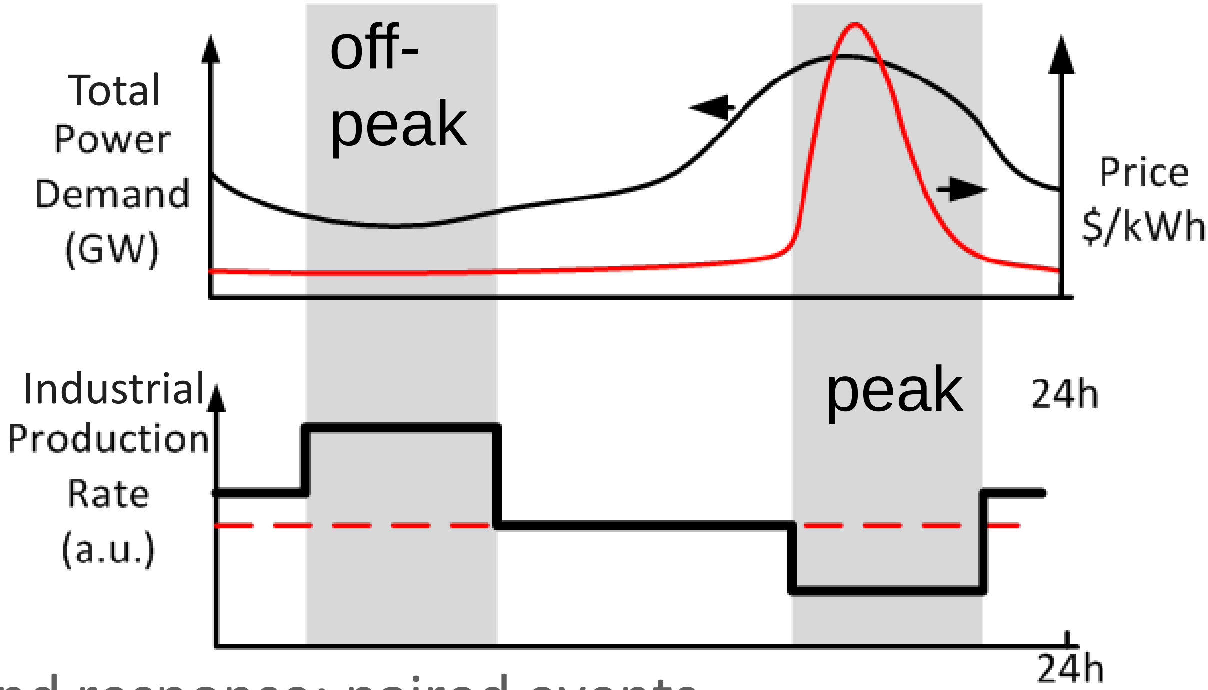
Industrial Demand Response



- Demand response: paired events
  - lower production at peak time, compensate off-peak
  - assumptions: excess capacity available, product storage feasible, transitions are feasible

Soroush and Chmielewski, Comput. Chem. Eng., 51, 86-95, 2013; Paulus and Borggrefe, Applied Energy, 88, 432-441, 2011

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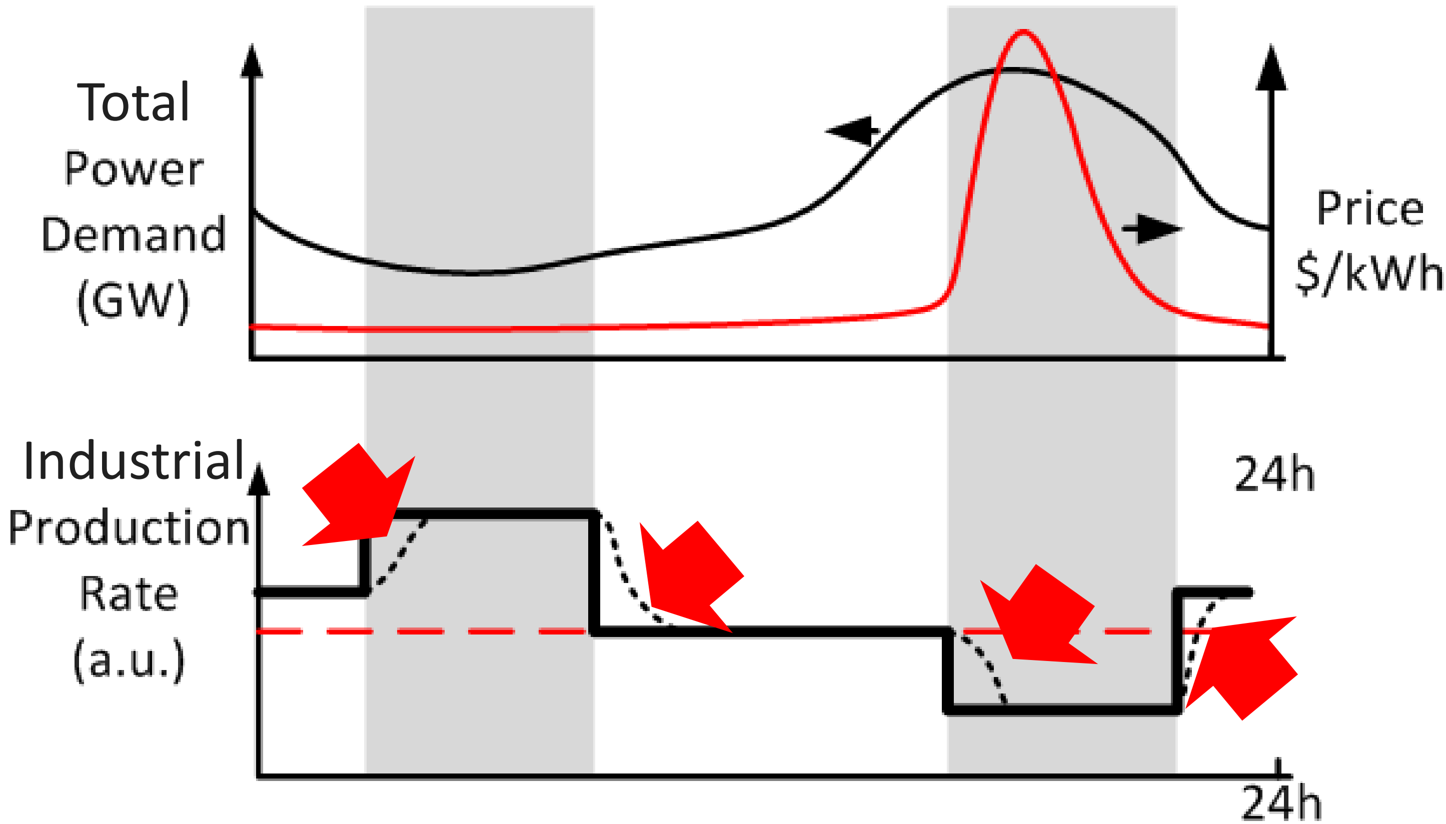
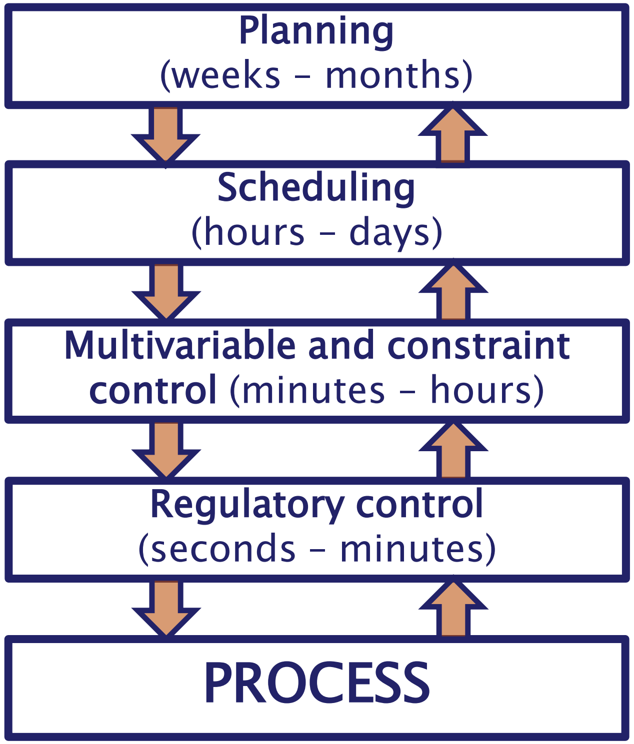
Industrial Demand Response



- Frequent production rate (schedule) changes: process dynamics must be accounted for in production scheduling

Hierarchy of Process Operation Decisions



Production management

- Assume steady-state operation
- Typically carried out off-line

Control

- Account for dynamics
- Online, in real-time

Different time horizons, objectives, personnel: production management and control carried out independently

Seborg et al., Wiley, 2010, Baldea and Harjunkoski, Comput. Chem. Eng., 71, 377-390, 2014, Shobrys and White, Comput. Chem. Eng, 26, 149—160, 2002

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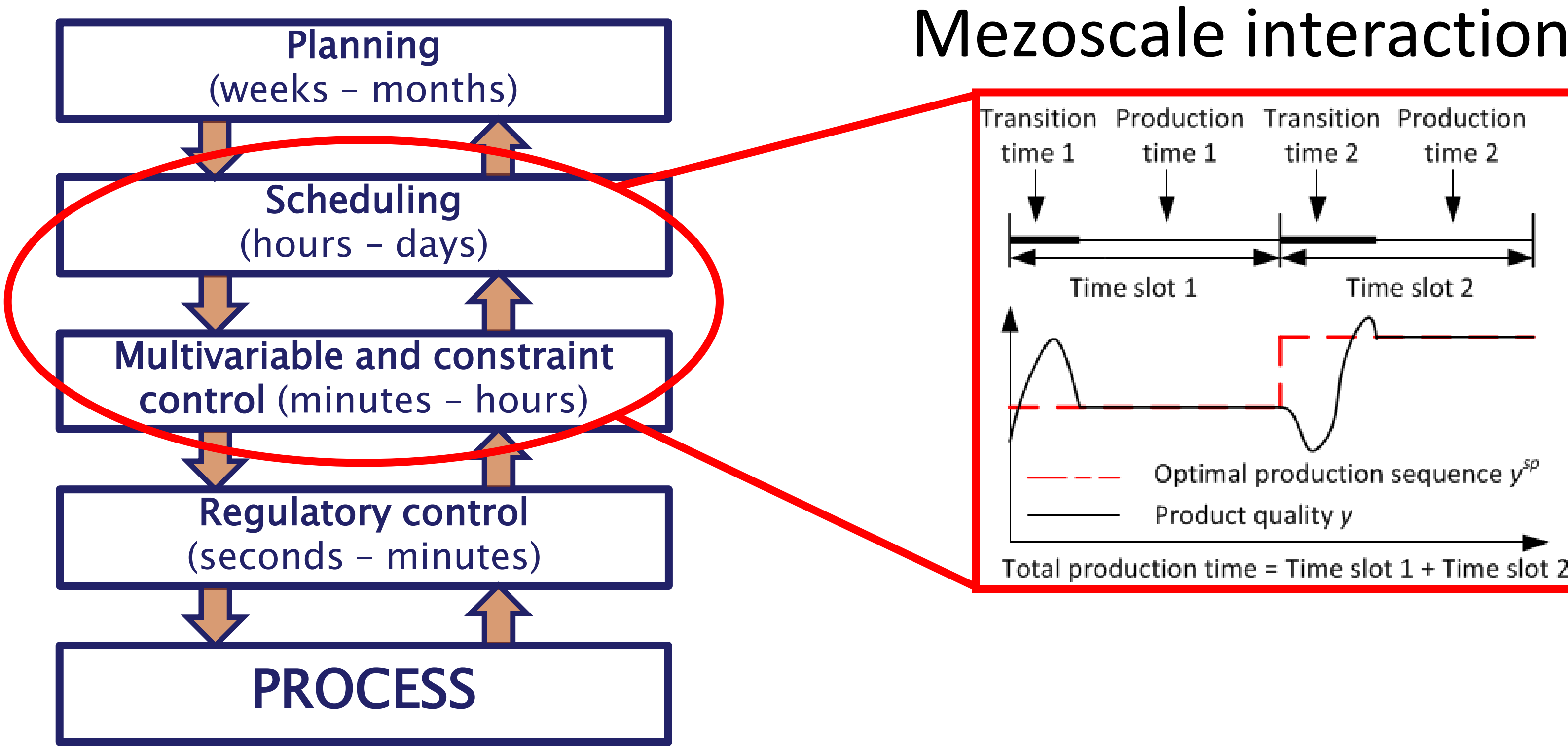
Hierarchy of Process Operation Decisions



Overlap in the time scales of production management and process control motivates considering the integrated problem

Seborg et al., Wiley, 2010, Baldea and Harjunkoski, Comput. Chem. Eng., 71, 377-390, 2014, Shobrys and White, Comput. Chem. Eng, 26, 149—160, 2002

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Overall Project Objective

- Create framework that will enable the safe and extensive utilization of the DR potential of chemical and petrochemical process.
  - Synchronize production scheduling with the control system
  - Account for the dynamic nature of transitions
  - Solvable in real time (deal with model size)
- Case study: air separation unit (ASU)

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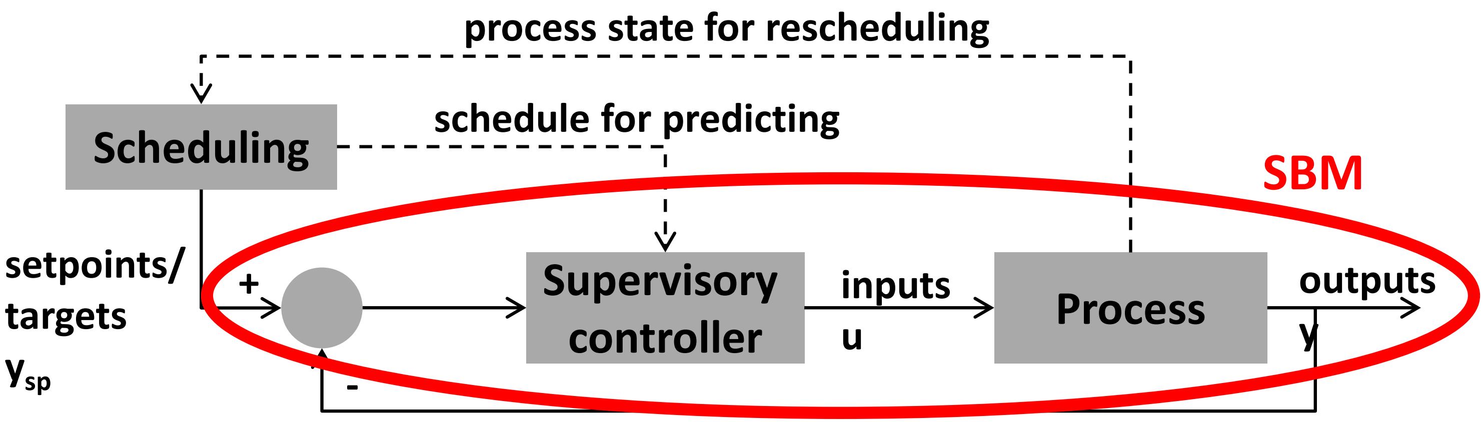
Approach: Scale-Bridging Model



Baldea and Harjunkoski, Comput. Chem. Eng., 71, 377-390, 2014

- Low dimensional
  - Dynamics at scheduling-relevant time scales
- Capture closed-loop input-output dynamics
  - Stability guaranteed
  - Robustness to modeling error
- Data-driven

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Accomplishments during past year

- Theory:
  - development of LINEAR forms for scale-bridging models (based on Hammerstein Wiener models)
  - Initial MILP production scheduling formulation
- Air separation case study:
  - Transition data for range of production rates were generated from a detailed model
  - Continuous HW models identified for scheduling-relevant variables
  - Discretized and linearized continuous HW models
  - 0.01-0.24% error

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Scale-Bridging Model Development

1. Acquire relevant data
   - Simulate detailed model and control system, or use operating data from the plant model
   - Cover full range of set-point changes
2. Identify nonlinear SBMs
   - Hammerstein-Wiener (HW) models

$$h = H(u)$$ Input nonlinearity

$$\frac{d\vec{x}}{dt} = A\vec{x} + Bh$$ State space model

$$y = C\vec{x}$$ Output nonlinearity

$$w = W(y)$$

3. **Develop linearization strategies**
   - Can be exact in specific cases (e.g., piecewise linear)

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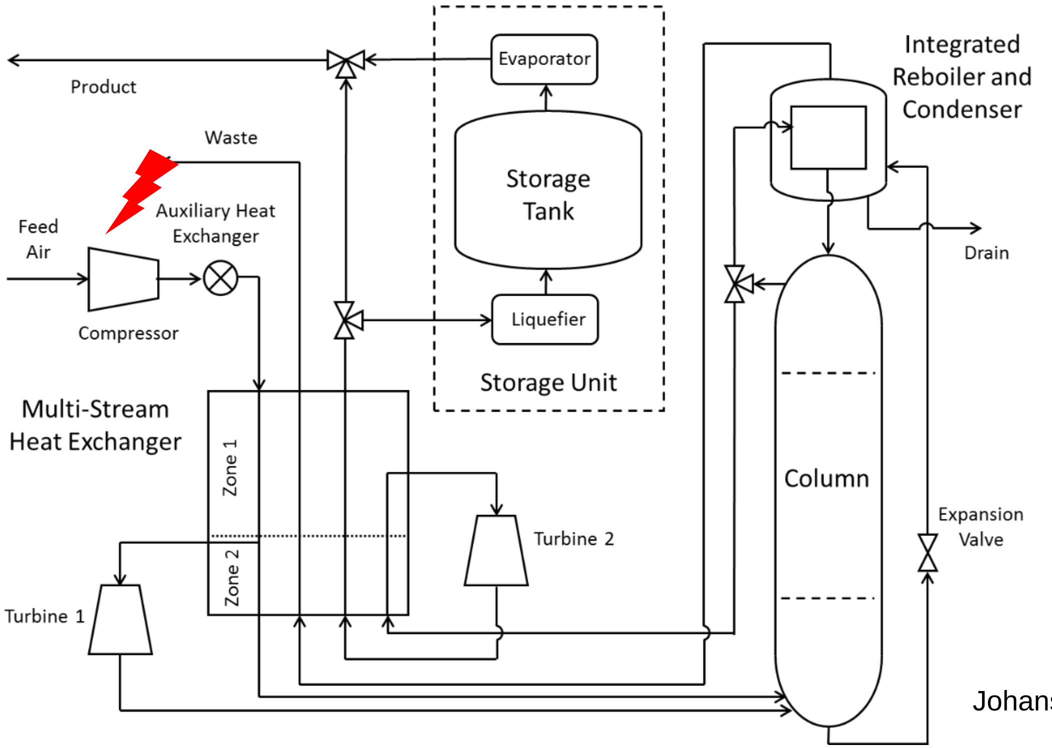
Linearization Strategies

1. Binary variables + Big-M
   - Binary variable generated for each breakpoint—Substantial increase in problem size
2. Special Ordered Sets of type 2 (SOS2)
   - Utilizes linear interpolation and assigned weights (SOS2 variables) for active segment
3. Ongoing: reduced SOS2 using upper/lower bounds for variables not in objective function
   - Only requires 2 breakpoints (endpoints)

Case Study: DR of Air Separation Unit



Johansson, MSc thesis, KTH/UT Austin, 2015

- Separate components of air via cryogenic distillation: high purity (>99%)
- Refrigeration via thermal expansion and energy recovery
- Large energy consumers: 19.4 TWh in US in 2010
- Store energy as liquefied molecules: potential to shift grid load

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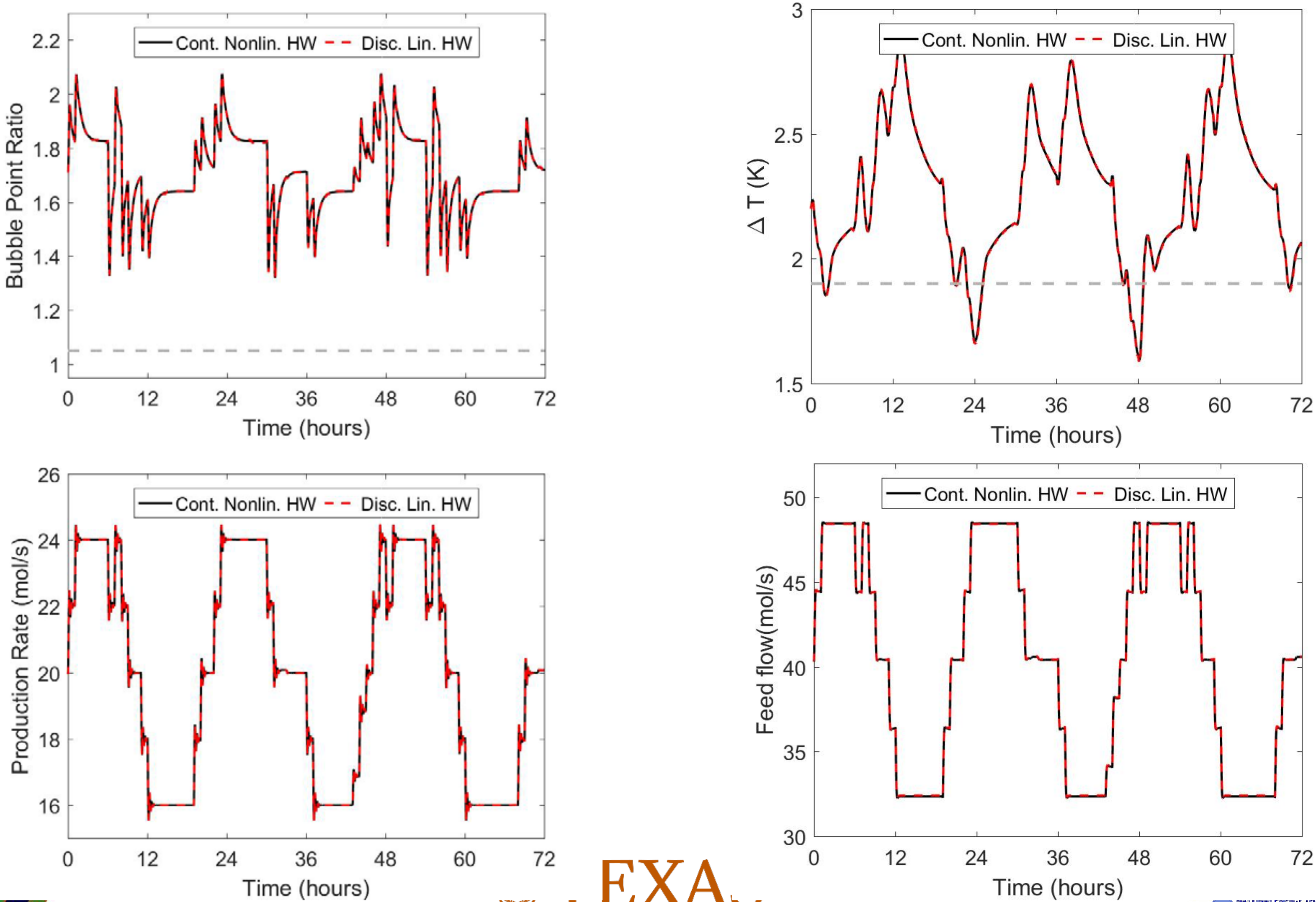
Performance of Linear Reformulation



Preliminary Results: ASU Scheduling

- Goal: Modulate production rate to track real-time electricity pricing

$$\min_{u_i} J = \sum_i \sum_j \phi(p_{ij}, w_{ij}^{Fp}, w_{ij}^{Ff}, w_{inv})$$

s.t.

HW models

Inventory model

Initial Conditions

Process Constraints

Quality Constraints

Symbol	Definition
i	Scheduling time step
j	Dynamics time step
J	Operating Cost
p_{ij}	Electricity prices
w_{ij}	HW output
w_{inv}	Inventory output
u_i	System inputs (set-points)
F_p	Production rate
F_f	Feed flowrate

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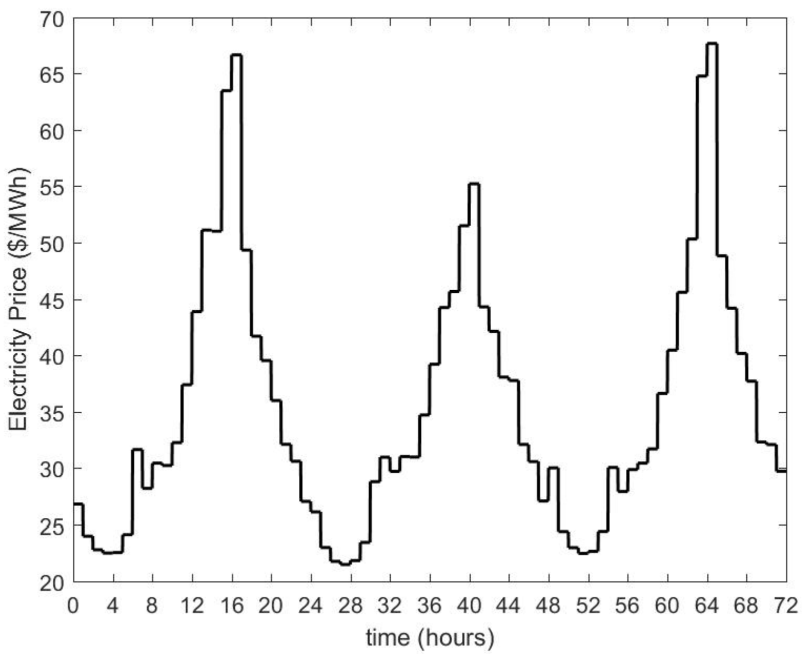
Preliminary Results: ASU Scheduling

- Goal: Modulate production rate to track real-time electricity pricing
- Target solution time:
  - Less than 1 hour for 72 h horizon
- Problem size (after pre-solve):
  - 82,201 continuous variables
  - 10,658 SOS variables
- **Expected benefits:**
  - **20% reduction in peak demand**
  - **3% reduction in operating cost (considerable for ASU)**



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Remaining Deliverables: FY16

- Improve scheduling formulation
  - Lagrangian relaxation/decomposition, reduce solution time to less than 1 hour
- Simulate schedule on detailed model
  - Assess constraint violations, refine HW models if needed or modify (back-off) constraints
- Peer reviewed publication:
  - Linear surrogate dynamical models for embedding process dynamics in optimal production scheduling calculations, Comput. Chem. Eng., in prep.

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Accepted publications/presentations

- Accepted peer reviewed presentations:
  - Linear Surrogate Dynamical Models for Embedding Process Dynamics in Optimal Production Scheduling Calculations: AIChE Annual Meeting, Minneapolis, MN, November 2017
  - Demand response operation of air separation units utilizing an efficient MILP modeling framework: AIChE Annual Meeting, Minneapolis, MN, November 2017

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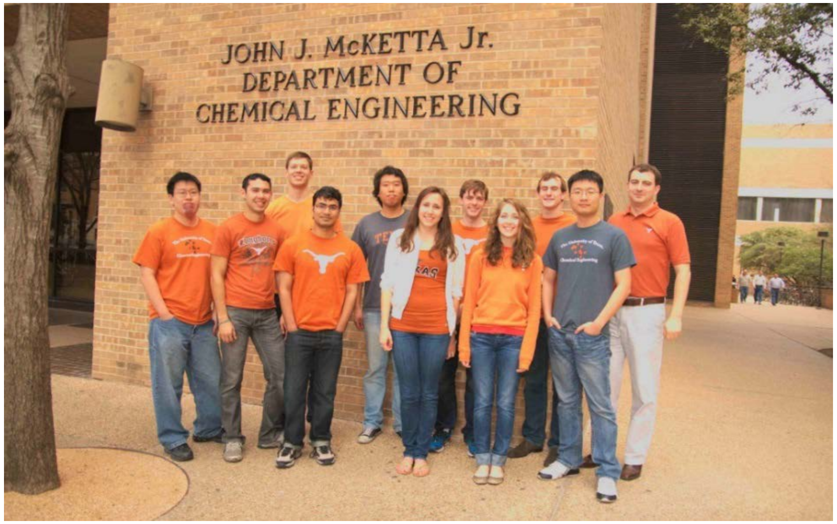
Planned Activities and Schedule

Year 2:

1. Algorithms for linearizing low-order data-driven models of DR scheduling-relevant dynamics
   1. Peer reviewed publication #1
2. General scheduling model for DR operations of chemical processes with dynamic constraints
   1. Peer reviewed publication #2
   2. Peer reviewed presentation

Acknowledgements



- DOE: DE-OE0000841

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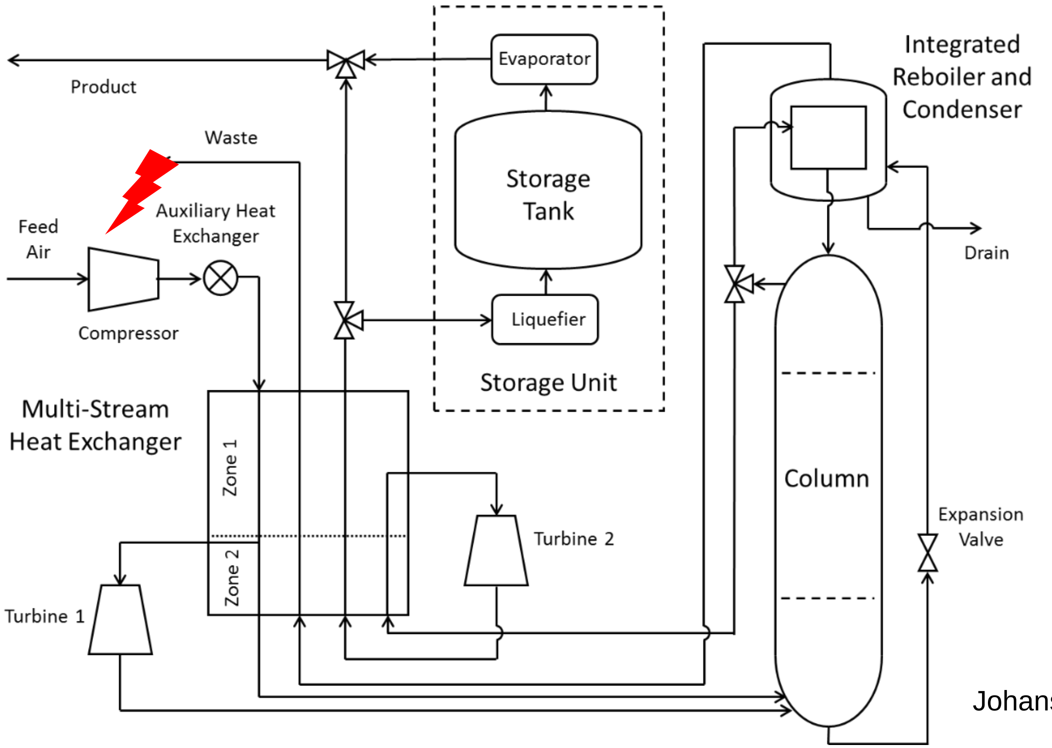
Case Study: DR of Air Separation Unit



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- Refrigeration via thermal expansion and energy recovery
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Big-M Linearization

$$PW_{i,k}^{H} = \frac{pw_{k+1}^{H} - pw_{k}^{H}}{bp_{k+1}^{H} - bp_{k}^{H}}(u_i - bp_k^H) + pw_k^H$$

$$bp_k^H < u_i \leq bp_{k+1}^H$$

$$h_i = PW_{i,k=0}^{H} + \sum_k [(PW_{i,k}^{H} - PW_{i,k-1}^{H}) z_{i,k}^{H}] = PW_{i,k=0}^{H} + \sum_k A_{i,k}^{H} z_{i,k}^{H} = PW_{i,k=0}^{H} + \sum_k B_{i,k}^{H}$$

Symbol	Definition
H	Hammerstein designation
k	Breakpoint index
i	Scheduling time step (index)
pw	Value of function at breakpoint
bp	breakpoint
u	inputs (set-points)
h	Hammerstein output
z	Binary variable

$$B_{i,k}^{H} \geq A_{i,k}^{H} - M(1 - z_{i,k}^{H})$$

$$B_{i,k}^{H} \leq A_{i,k}^{H} + M(1 - z_{i,k}^{H})$$

$$B_{i,k}^{H} \geq -M z_{i,k}^{H}$$

$$B_{i,k}^{H} \leq M z_{i,k}^{H}$$

Bilinear term takes value of $A_{i,k}$ when $z_{i,k}$=1 and zero when $z_{i,k}$=0

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Linearization Example (using Big-M)

$$h_i = PW^H_{i,0} + (PW^H_{i,1} - PW^H_{i,0})(z^H_{i,1}) + (PW^H_{i,2} - PW^H_{i,1})(z^H_{i,2}) + (PW^H_{i,3} - PW^H_{i,2})(z^H_{i,3}) + \cdots$$

1 1 0

$$PW^H_{i,k} = \frac{pw^H_{k+1} - pw^H_k}{bp^H_{k+1} - bp^H_k}(u_i - bp^H_k) + pw^H_k$$

$$bp^H_k < u_i \leq bp^H_{k+1}$$

Symbol	Definition
k	Breakpoint index
i	Scheduling time step
pw	Value of function at breakpoint
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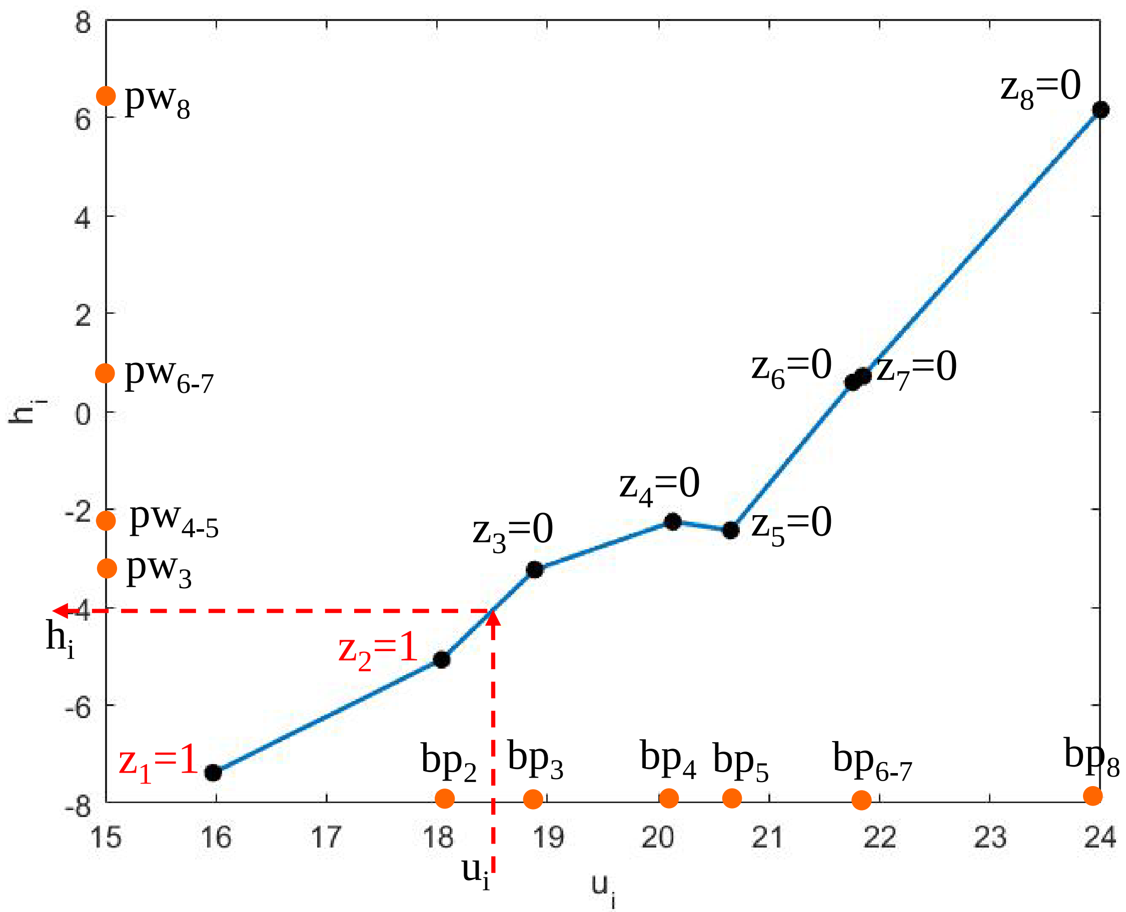
u	inputs (set-points)
h	Hammerstein output
z	Binary variable



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SOS2 Linearization

Symbol	Definition
H	Hammerstein designation
k	Breakpoint index
i	Scheduling time step (index)
pw	Value of function at breakpoint
bp	breakpoint
u	inputs (set-points)
h	Hammerstein output
b	Binary variable
λ	SOS2 variable

Enforced by Cplex

$$\lambda_{i,k}^H \leq b_{i,k}^H$$

$$\sum_k b_{i,k}^H = 2$$

$$b_{i,k}^H + b_{i,k'}^H \leq 1 \ \forall k' > k + 1$$

$$\sum_k \lambda_{i,k}^H = 1$$

$$u_i = \sum_k [\lambda_{i,k}^H bp_{i,k}^H]$$

$$h_i = \sum_k [\lambda_{i,k}^H pw_{i,k}^H]$$

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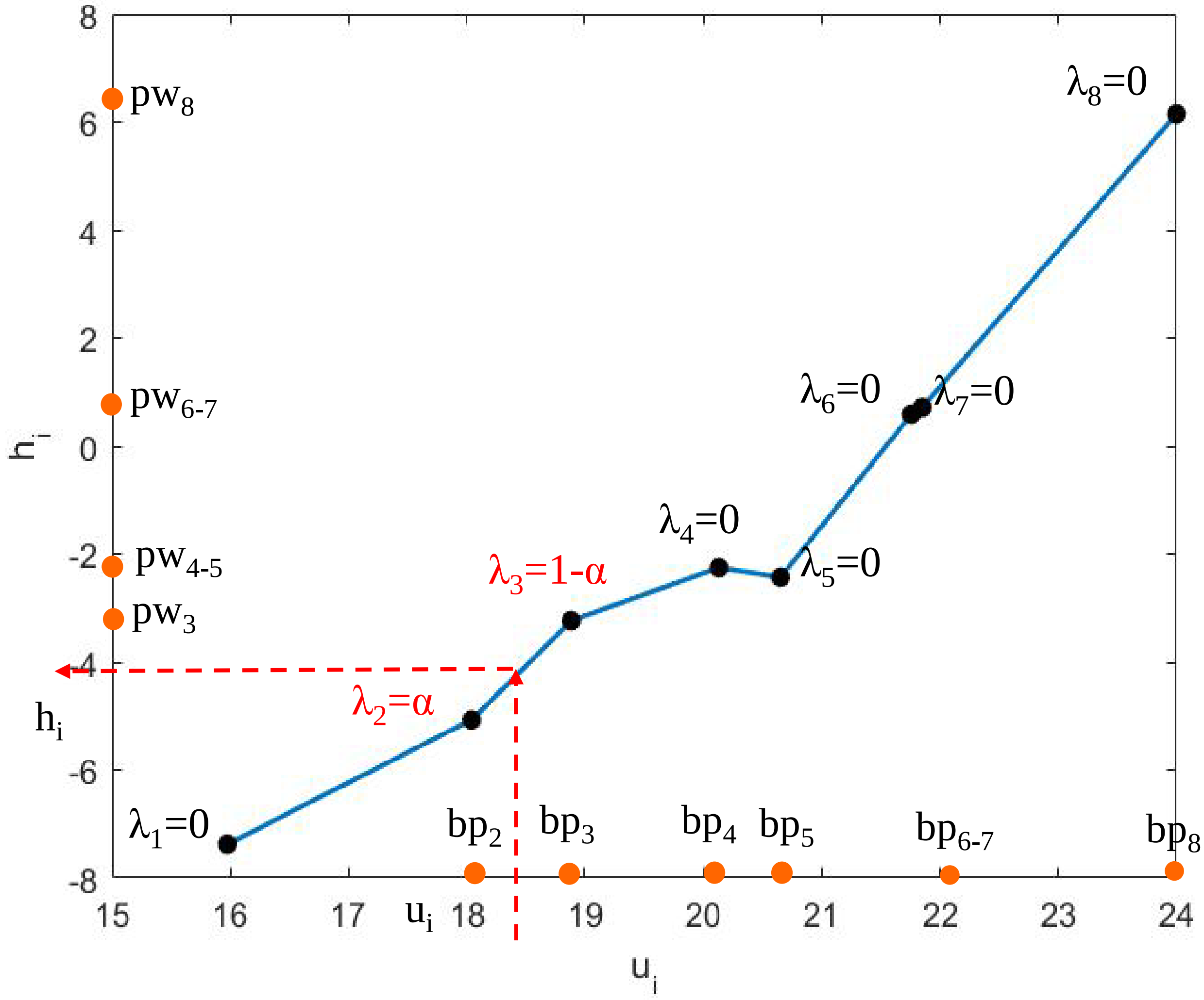
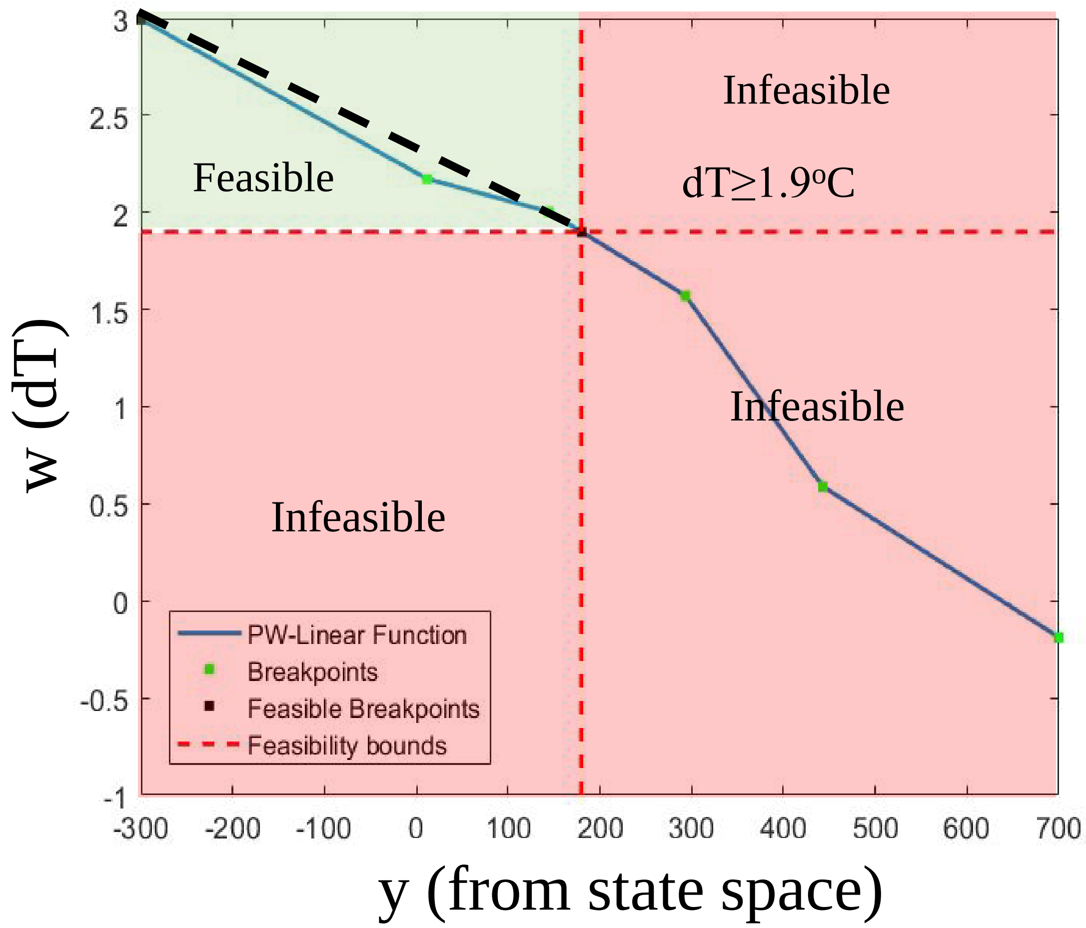
SOS2 Linearization Example



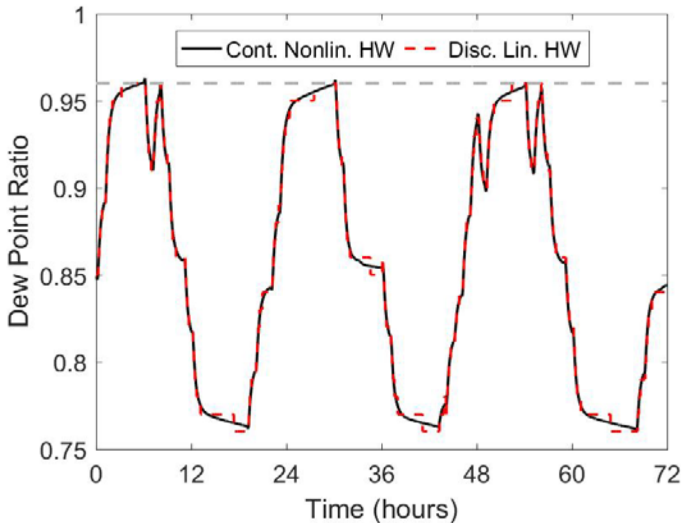
SOS2 Reduction (Wiener Block)

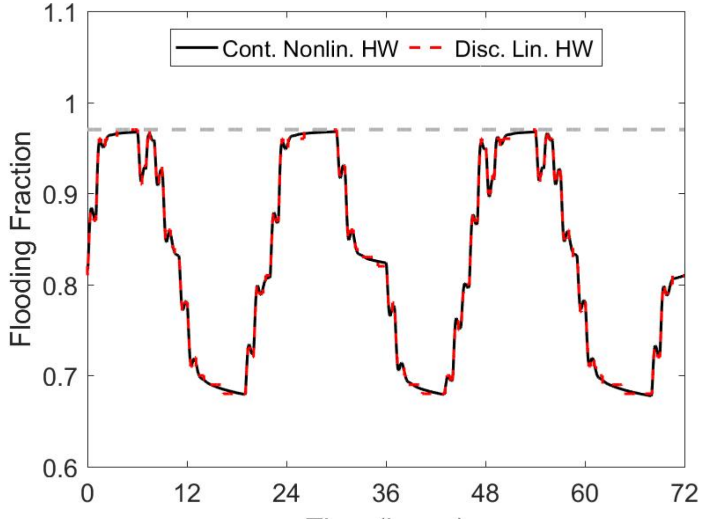


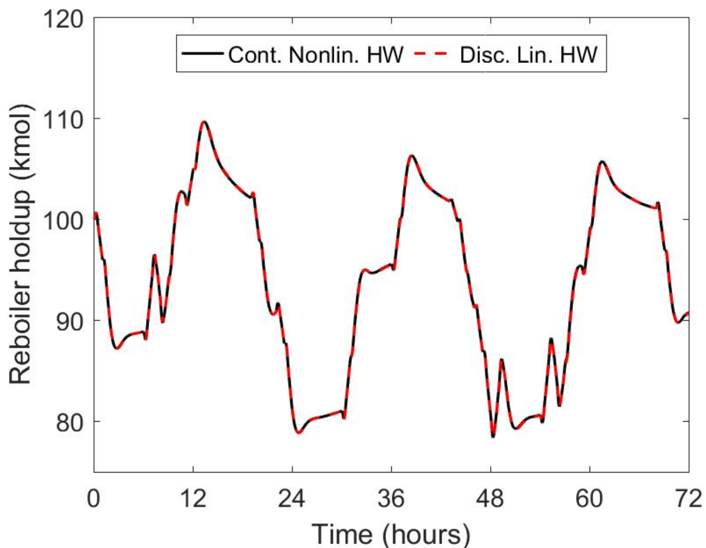
For variables not in the objective function:

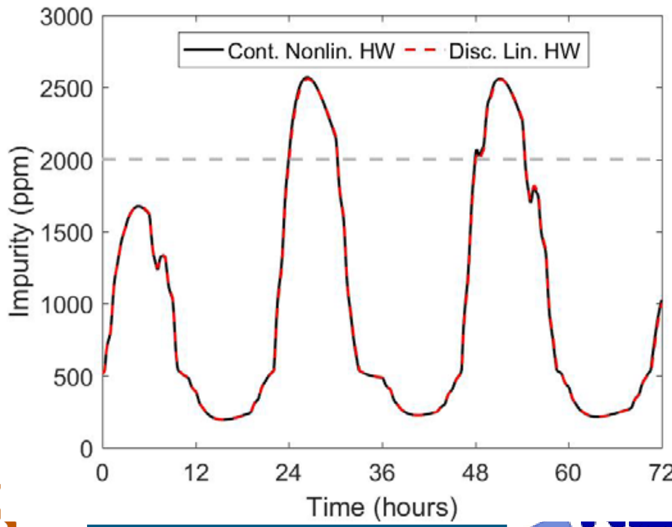
- *Output* nonlinearity can be estimated by endpoints at the upper and lower bounds
  - Variable stays between bounds
  - Eliminates many breakpoints

Discrete vs. Continuous HW Models









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Planned Activities and Deliverables

Year 3:

1. Representation of DR in Power Systems Models
   – Mathematical modelling
   – Electricity pricing algorithms
   – Peer reviewed publication #1
2. Electricity pricing algorithm and validation on ERCOT model
   – Peer reviewed publication #2
3. Peer reviewed presentation

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