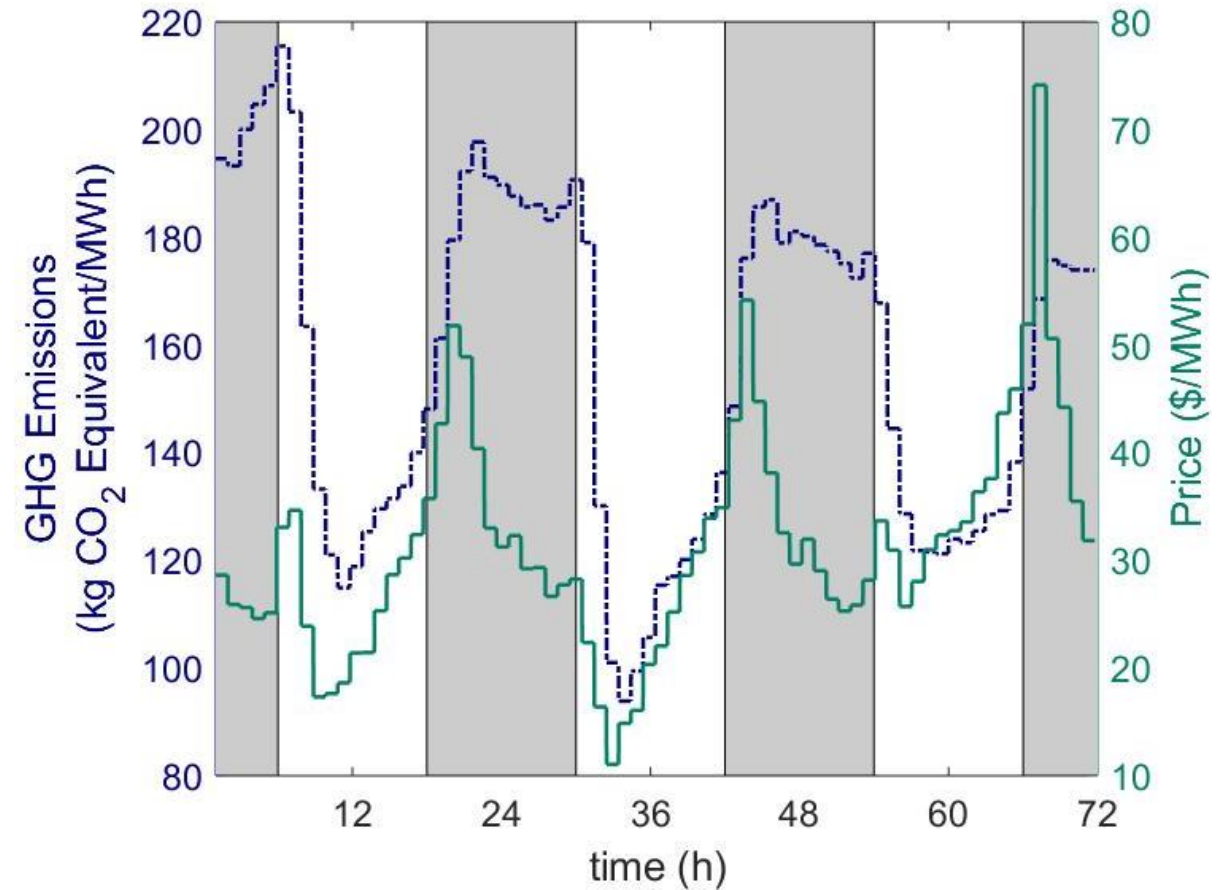
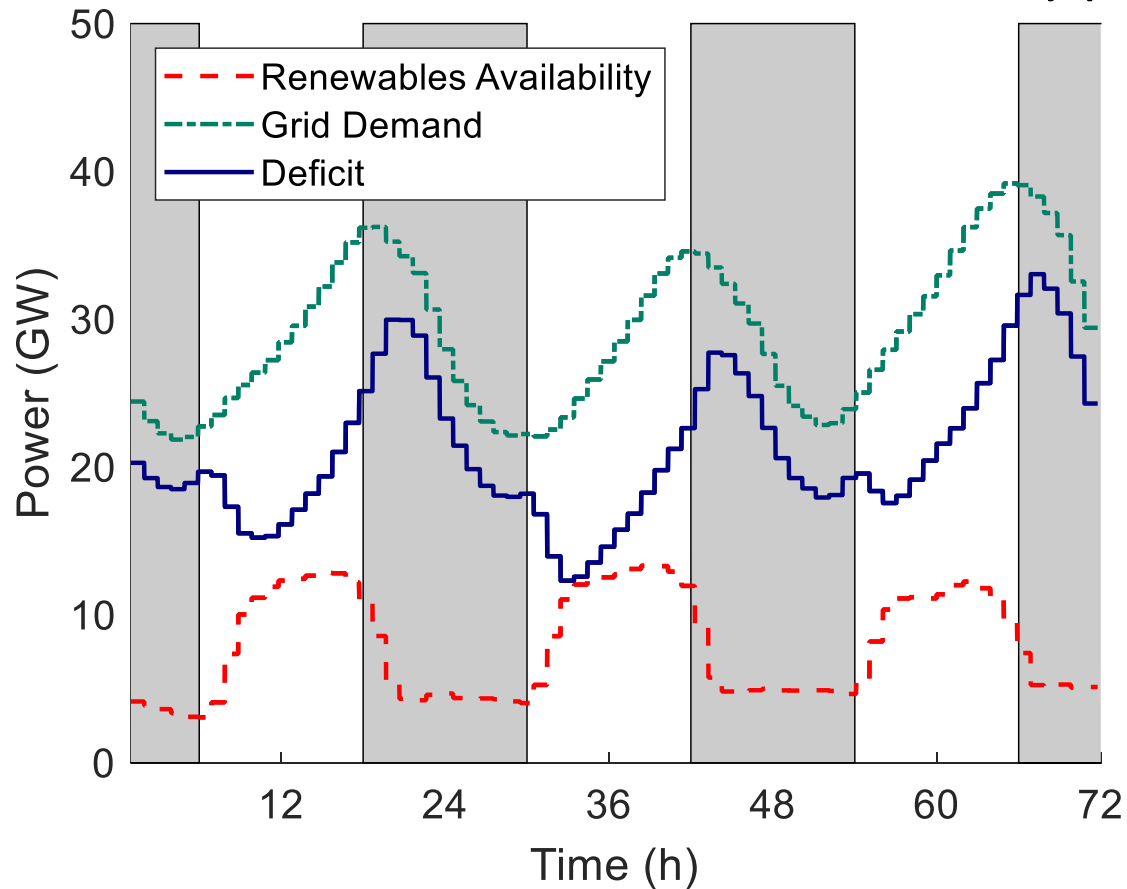


# **Modeling and optimization of complex industrial systems for application to demand response**

**Morgan Kelley, Dr. Ross Baldick, Dr. Michael Baldea**  
DOE CSGF Program Review  
Summer 2021

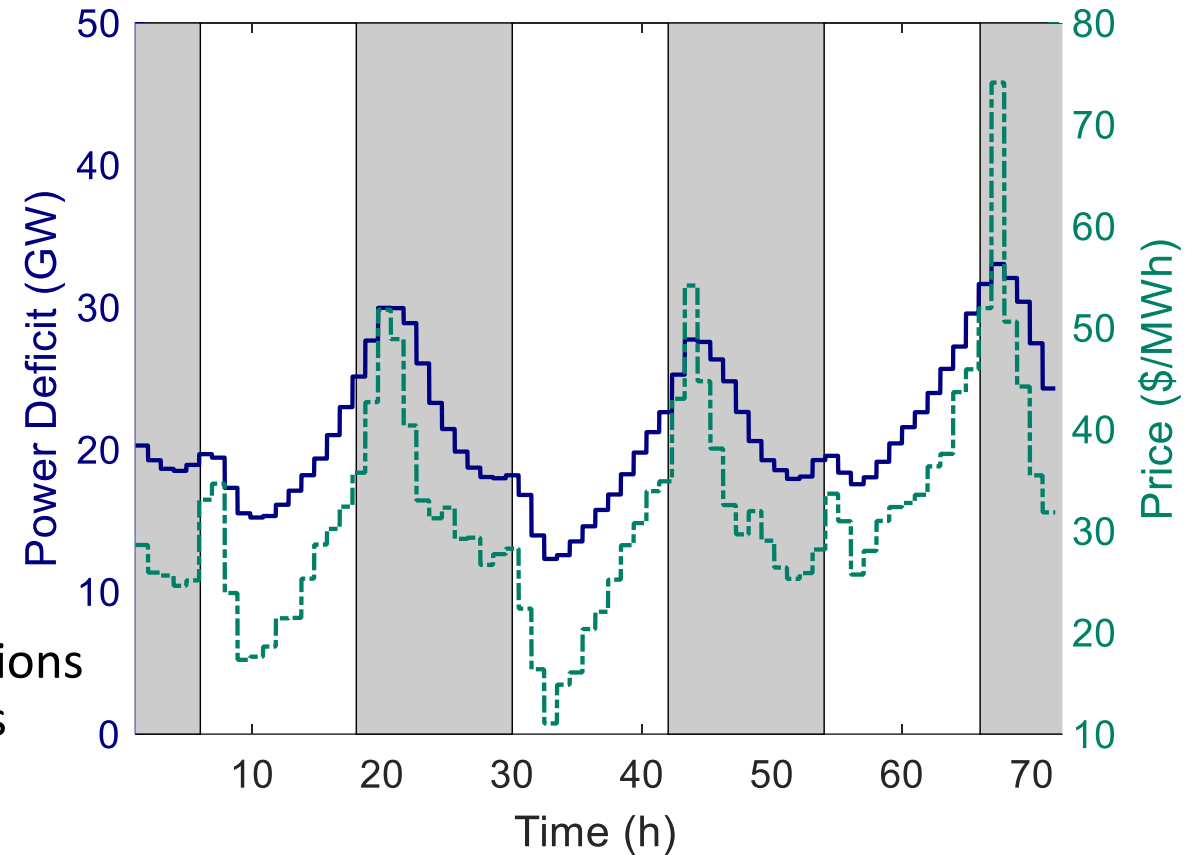
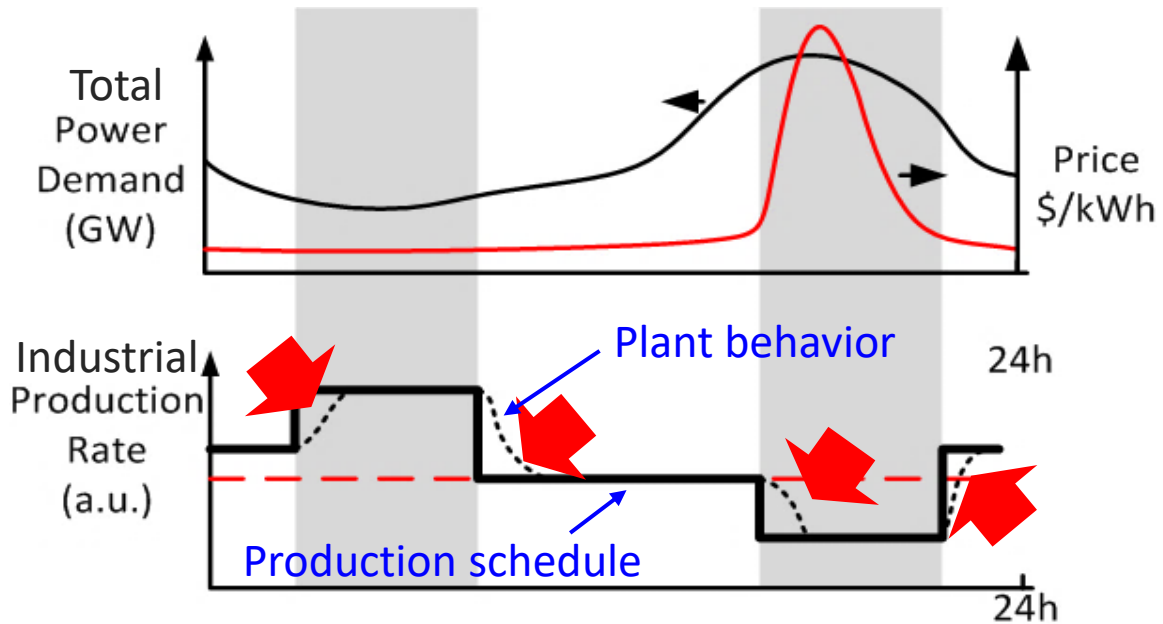
# Demand, Availability, and Price

- Increased capacity from renewables exacerbates variability issues
- This deficit is reflected in the electricity prices



Renewables contribution, grid demand, and prices for July 3-5 2017 from data supplied by CAISO

# Load Shifting: Industrial Participation

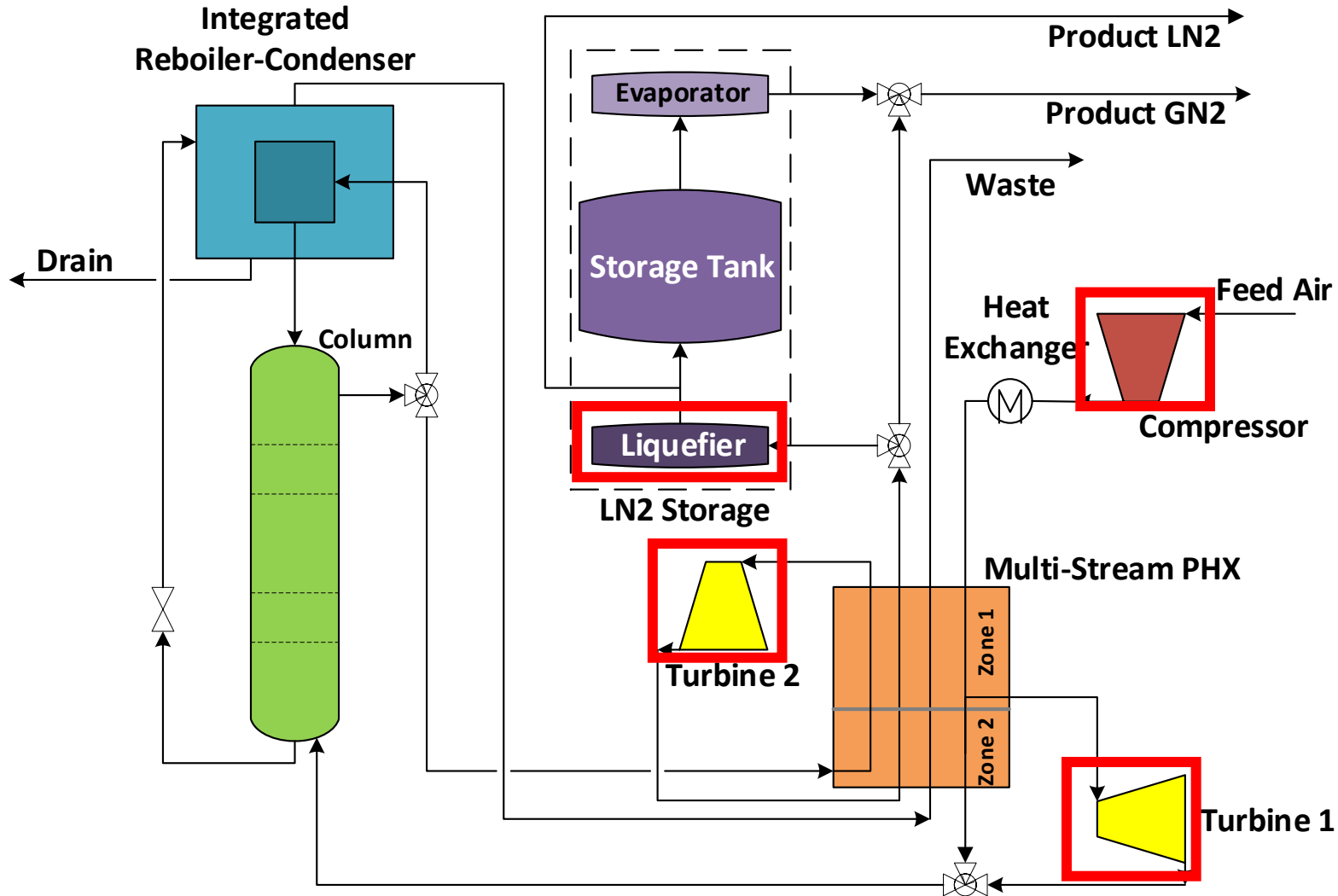


Renewables contribution, grid demand, and prices for July 3-5 2017 from data supplied by CAISO

- **Paired events:** overproduce during low demand/emissions times and store extra product to use during peak hours when production is lower
  - Frequent schedule changes, account for process dynamics (same time scale as scheduling decisions)
  - Assumptions: excess capacity, product storage, fast transitions are possible

CAISO. (2017). California Independent System Operator. Retrieved from <http://www.caiso.com/Pages/default.aspx>

# Case study: Cryogenic Air Separation



Industrial gas sector accounted for 2.62% of industrial electricity consumption in 2014[5]

Products: LN<sub>2</sub>, GN<sub>2</sub>

Vary the inlet feed flowrate to modulate production levels

Longer time horizon=more savings

[5] US EIA. (2017). *Manufacturing Energy Consumption Survey 2014*. Washington, D.C.

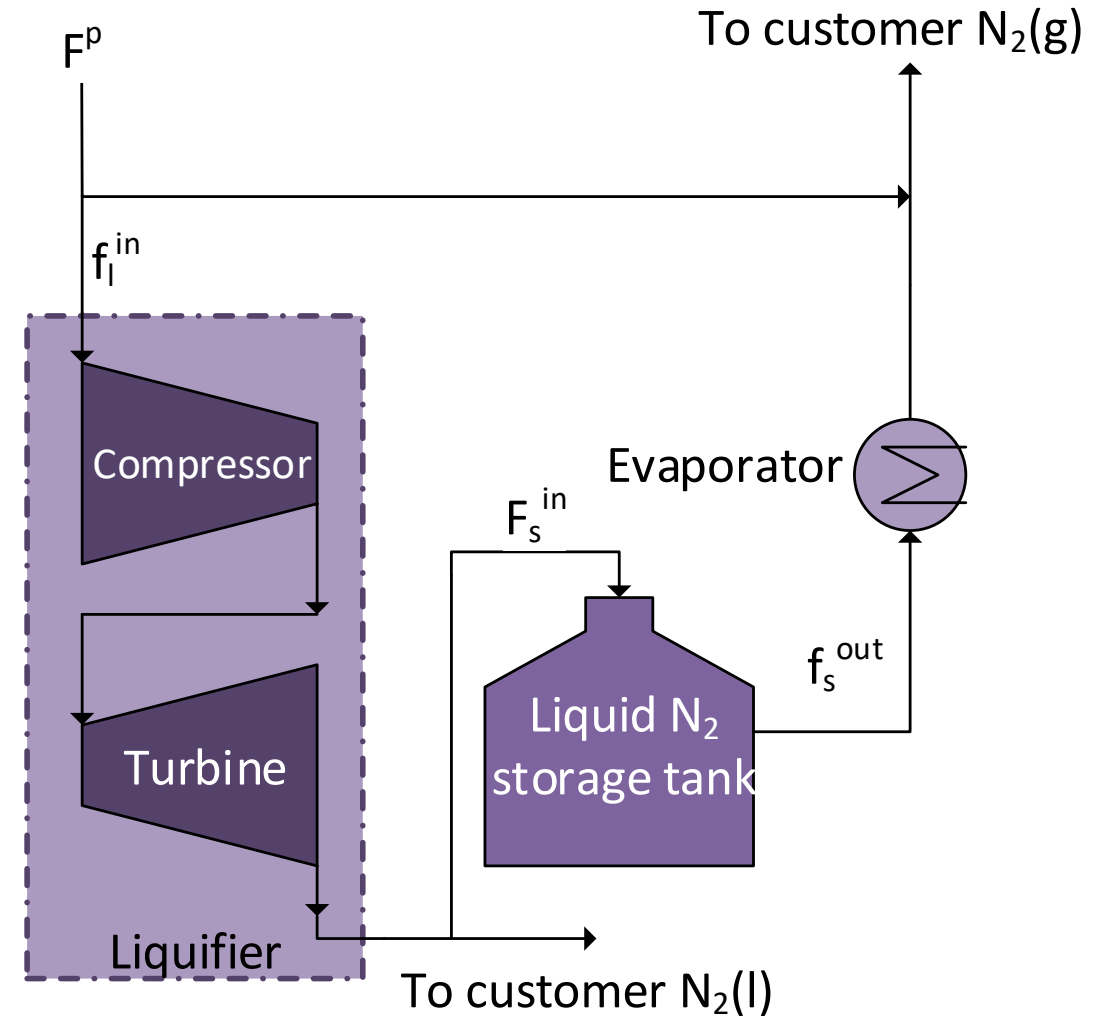
# Storage System and Power Consumption

## Storage system:

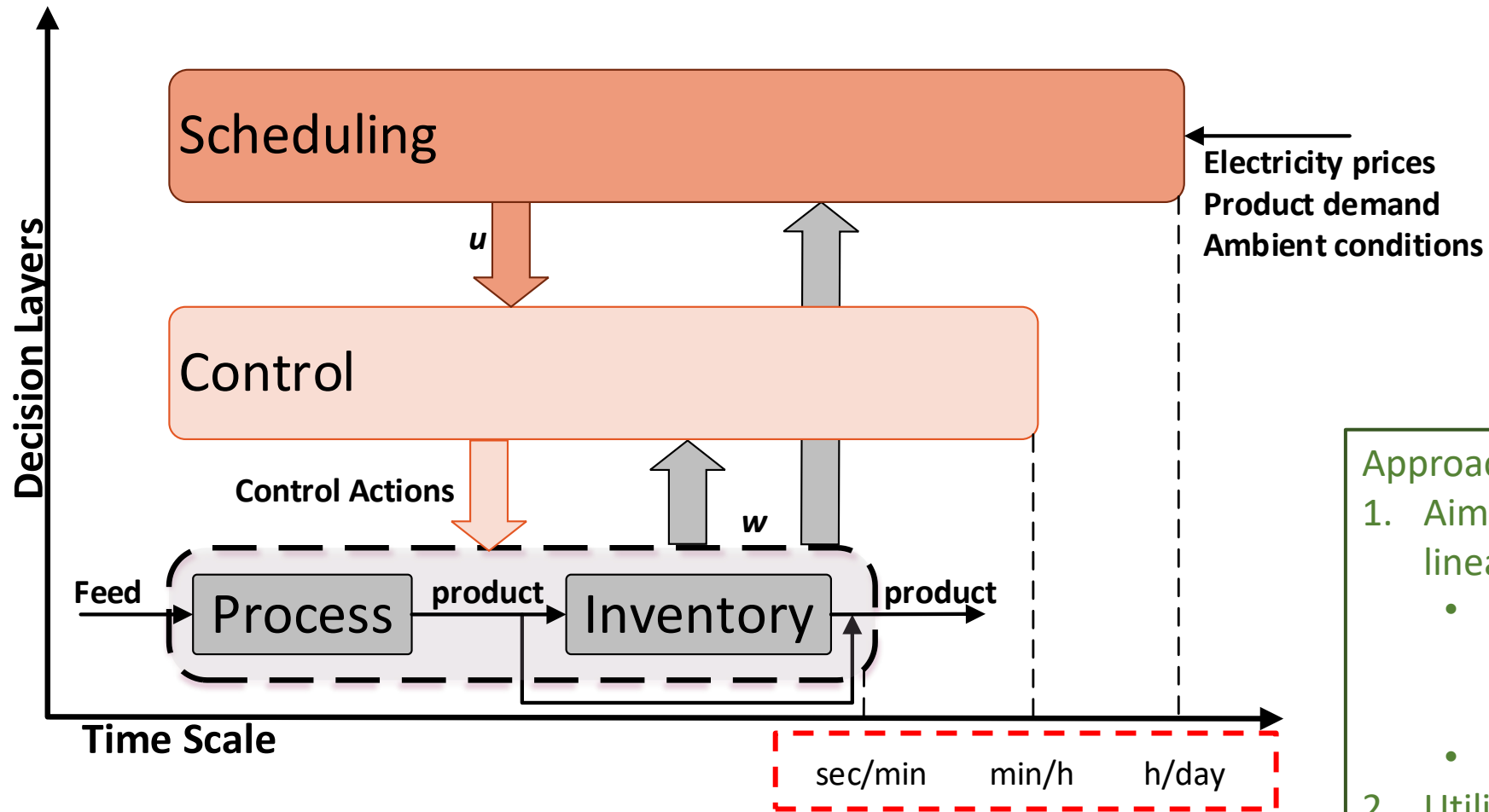
- Product in excess of gas demand is liquefied
  - Product is removed from liquefier and sent to meet liquid demand
  - Excess is sent to storage (as liquid)

## Power consumption:

- Linear relationship between net work and flow through unit



# Hierarchy of Process Decisions



Key goal:  
Solve the optimal  
scheduling problem in  
less than an hour on a  
standard computer

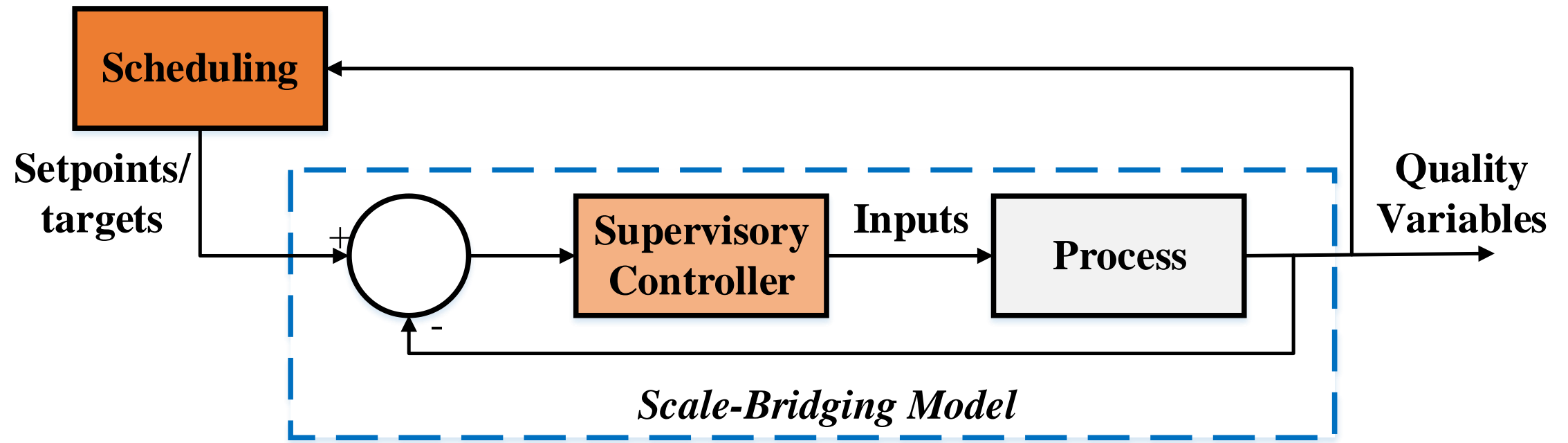
## Approach:

1. Aim for a linear (or mixed-integer linear) program
  - Linear programs have guaranteed optimality and fast solution times
  - Grid models are MILPs
2. Utilize problem structure that enables parallel computing

# Reduced-order modeling

Bridge disparate time scales between scheduling and process dynamics/control

- Low-order
- Utilize input/output (closed-loop) operating data
- Only capture scheduling-relevant variables



[7] J. Du, J. Park, I. Harjunkoski, and M. Baldea, "A time scale-bridging approach for integrating production scheduling and process control," *Comput. Chem. Eng.*, vol. 79, pp. 59–69, Aug. 2015.

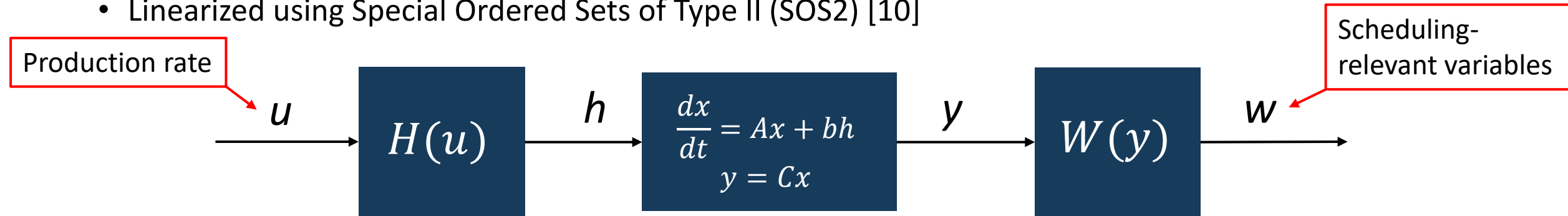
# Scale Bridging Models

## Finite Step Response (FSR) Models (Linear)

- Data-driven non-parametric models used for unknown model order and time delay

## Hammerstein-Wiener (HW) Models (Nonlinear)

- Linear State-space block
- Static input/output nonlinearities: piece-wise linear (PWL)
  - Linearized using Special Ordered Sets of Type II (SOS2) [10]



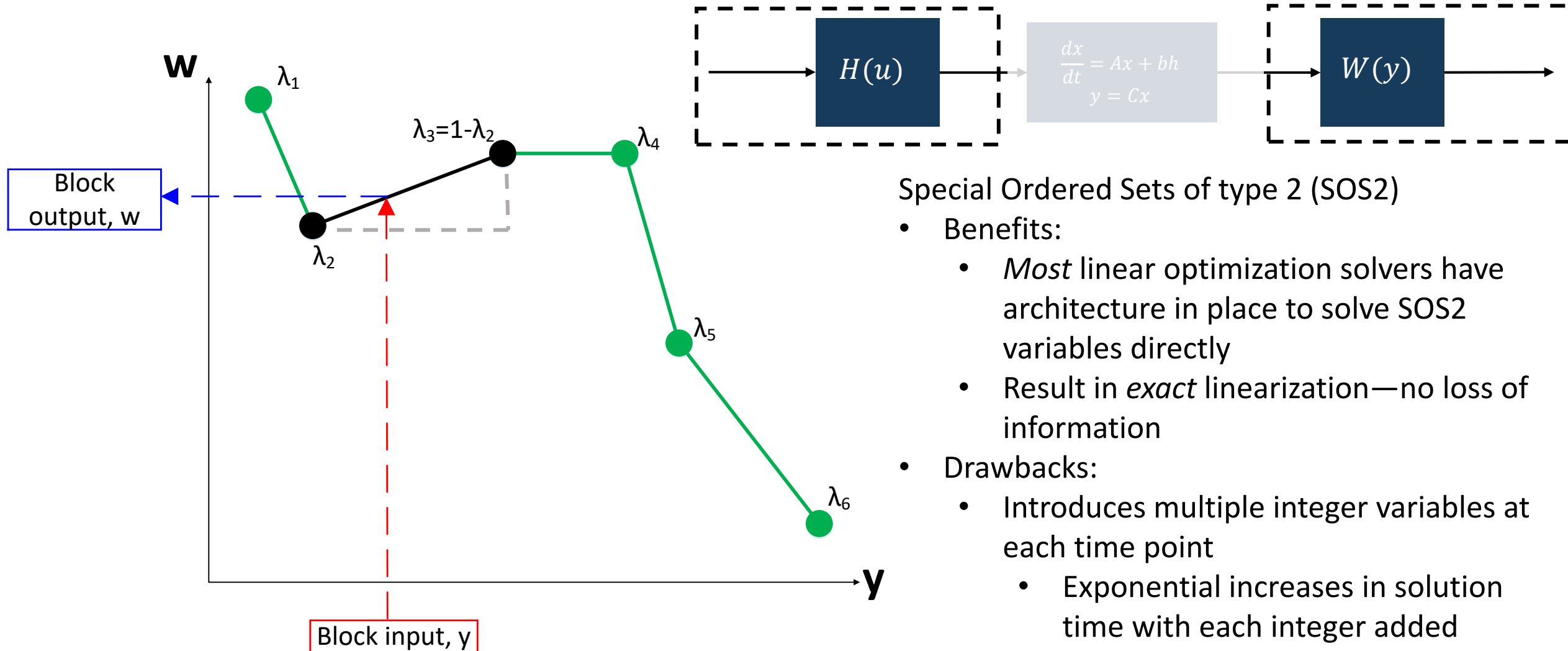
Billings, S. A. (2013). *Nonlinear system identification : NARMAX methods in the time, frequency, and spatio-temporal domains*. Chichester, West Sussex: John Wiley & Sons.

MATLAB. (2016). MATLAB 2016a. Natick, MA, USA: The Mathworks, Inc.

M. T. Kelley, R. C. Pattison, R. Baldick, and M. Baldea, "An MILP framework for optimizing demand response operation of air separation units," *Appl. Energy*, vol. 222, pp. 951–966, Jul. 2018.



# Static blocks: Linearize nonlinearities



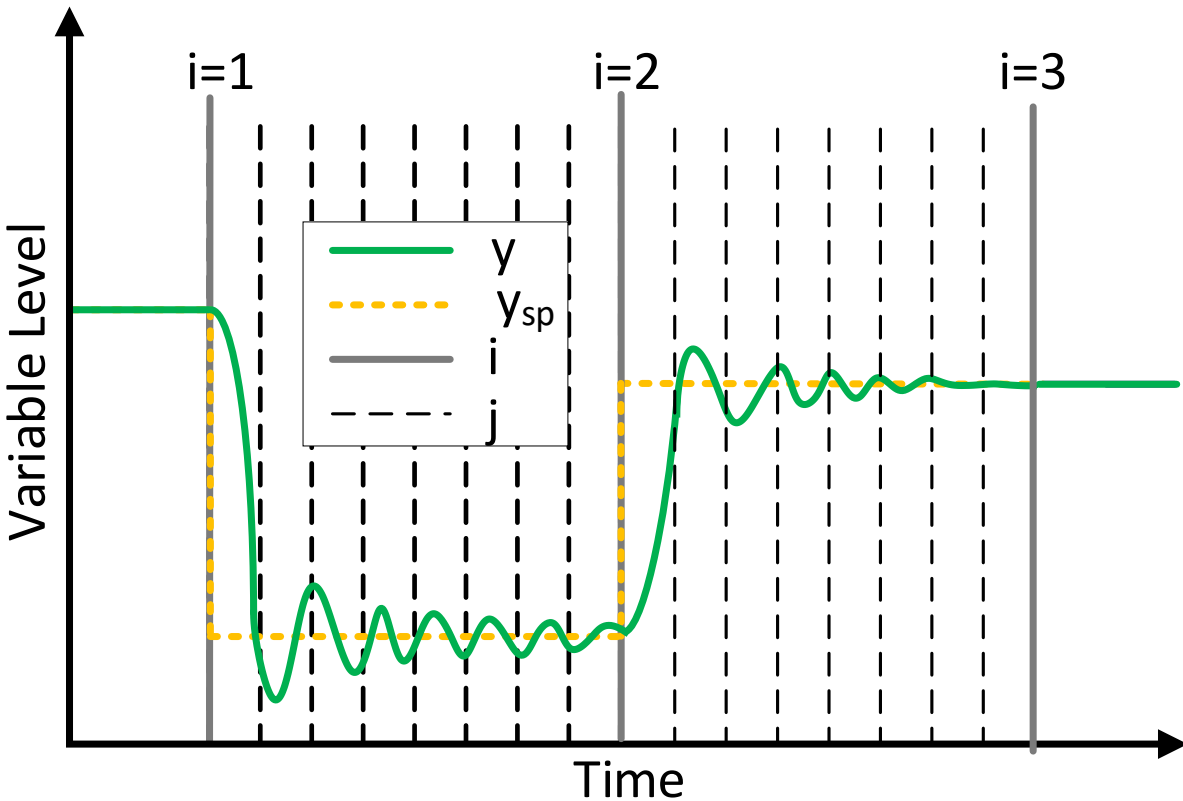
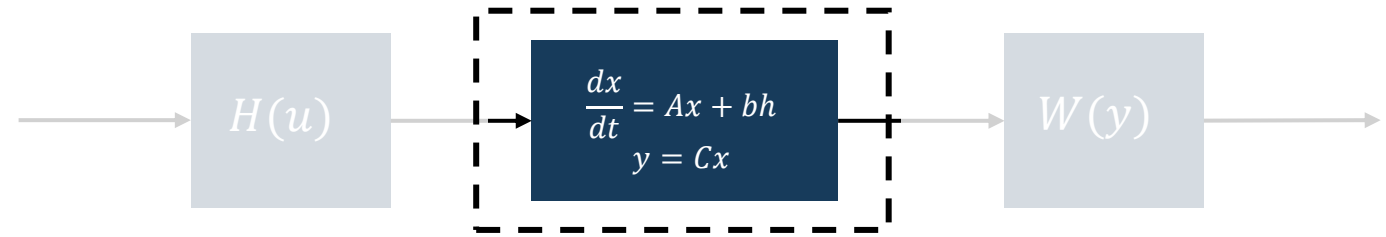
## Special Ordered Sets of type 2 (SOS2)

- Benefits:
  - *Most* linear optimization solvers have architecture in place to solve SOS2 variables directly
  - Result in *exact* linearization—no loss of information
- Drawbacks:
  - Introduces multiple integer variables at each time point
    - Exponential increases in solution time with each integer added

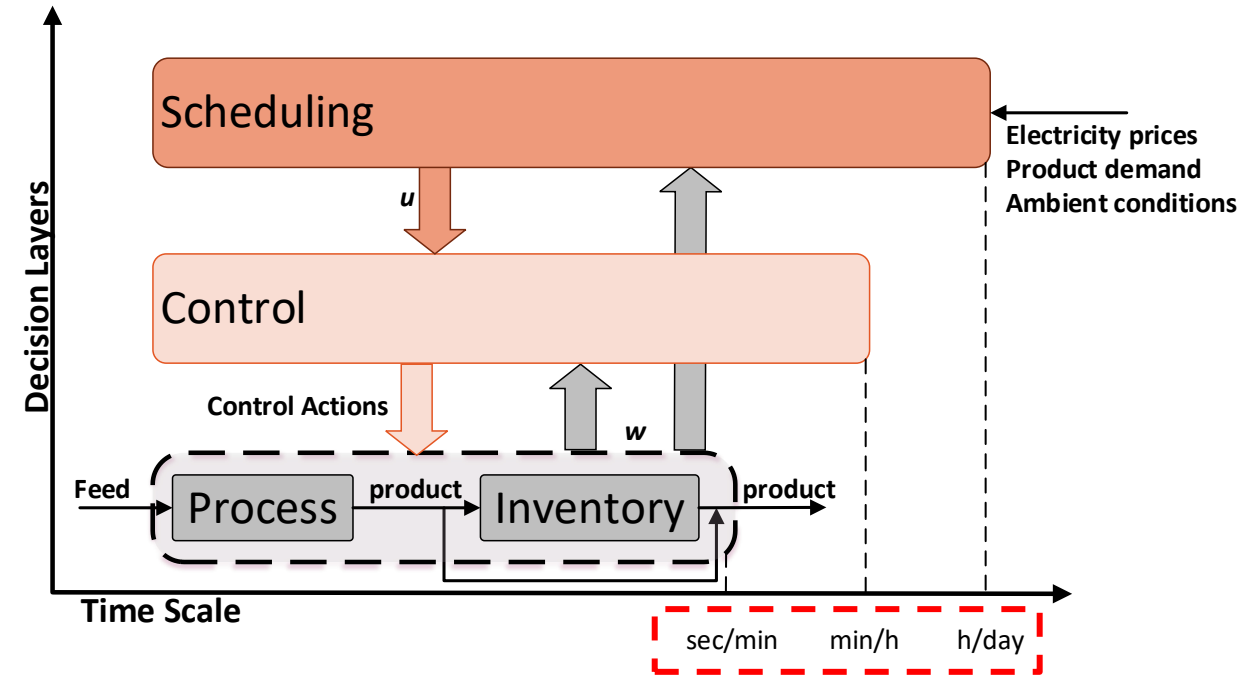
# Dynamic block: Define discrete time grids

i: Scheduling time slots

j: time points for discretized dynamics



$y_{sp}$  is supplied by the scheduling layer, and  $y$  is how the process reacts to  $y_{sp}$



# MILP Reformulation: Discretization

- Discretization:

$$h_i = H(u_i)$$

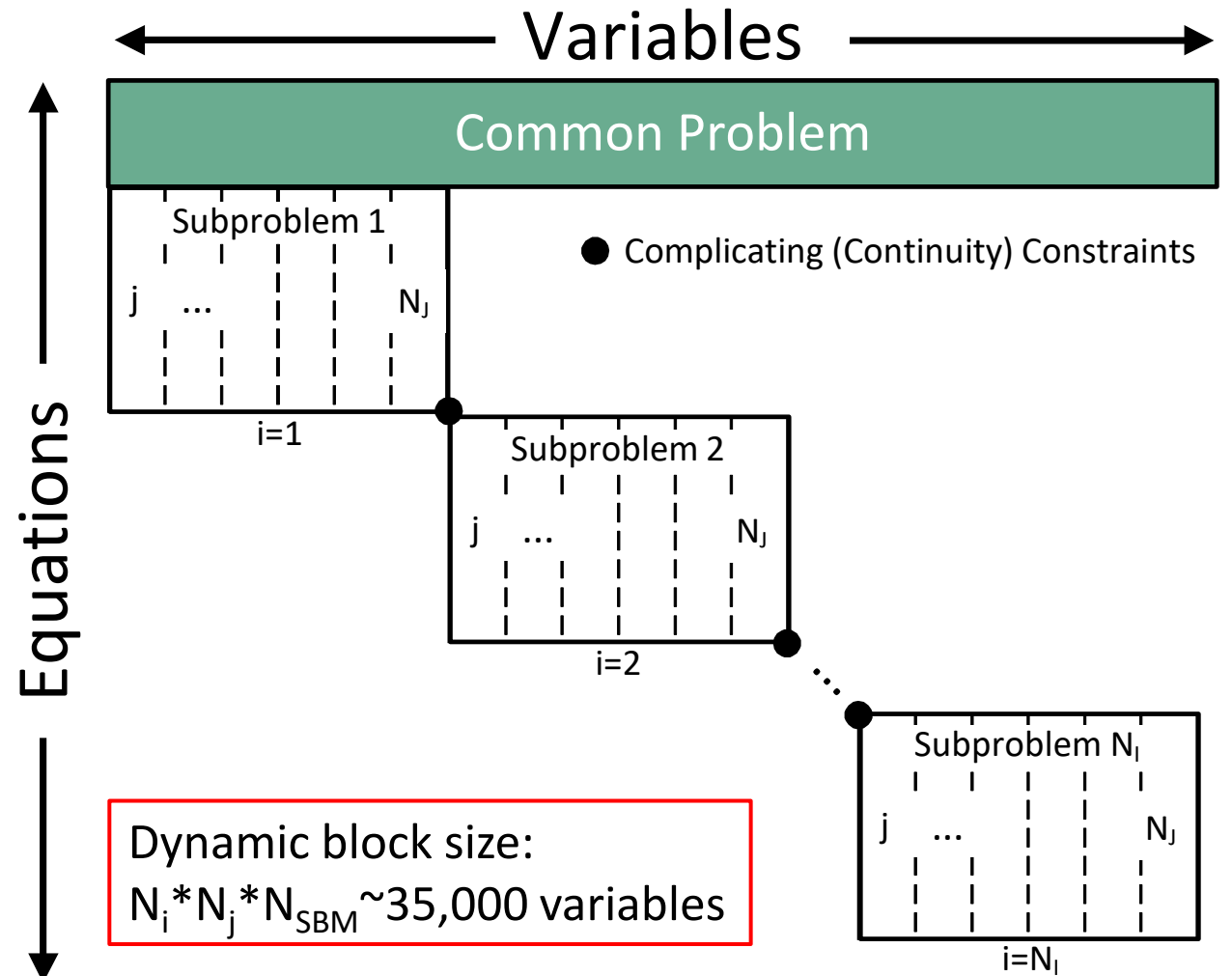
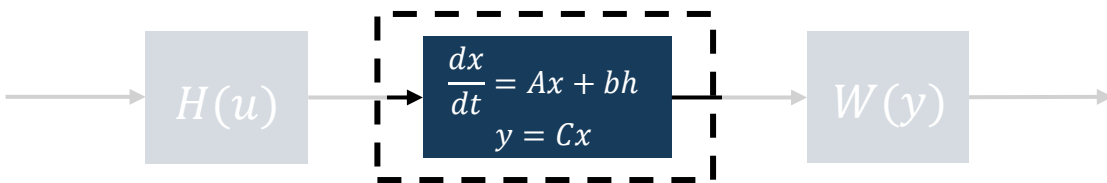
$$\vec{x}_{i,j+1} = A\vec{x}_{ij} + Bh_i$$

$$y_{ij} = C\vec{x}_{ij}$$

$$w_{ij} = W(y_{ij})$$

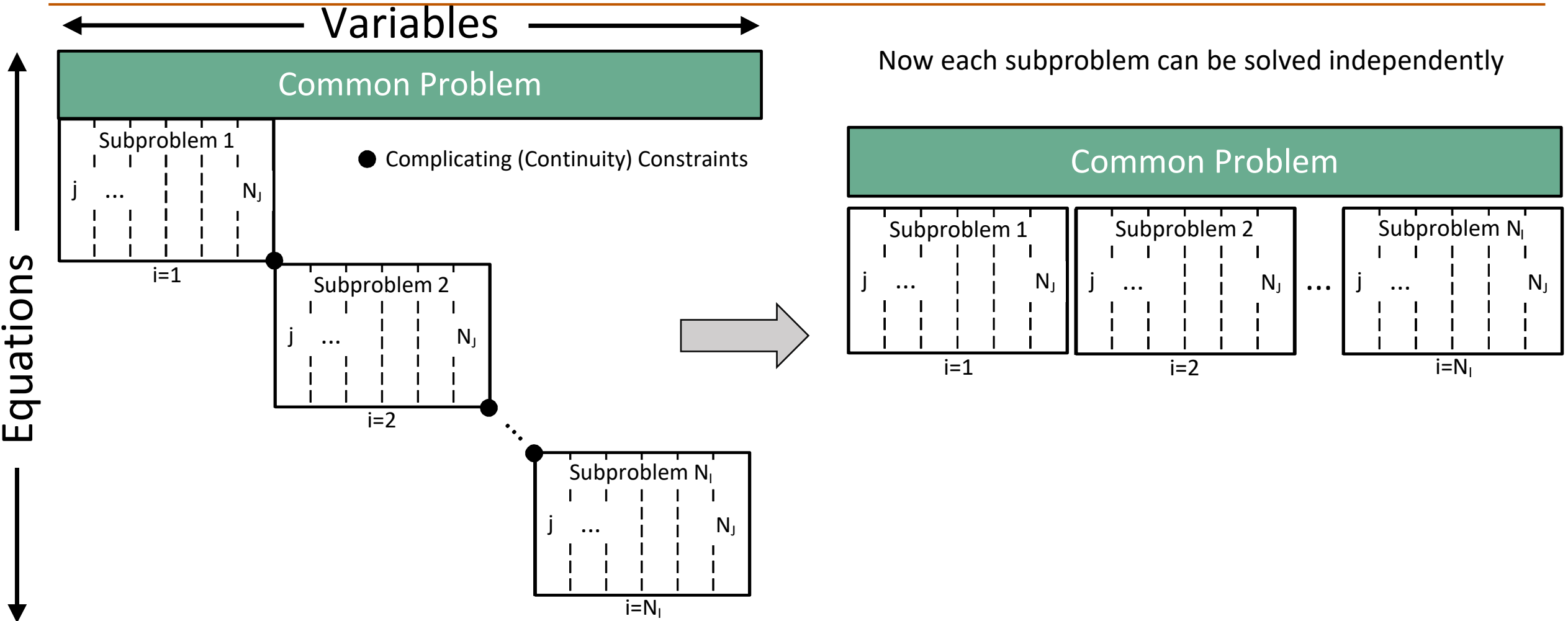
- Requires state continuity constraint between scheduling time slots:

$$x_{i,j+1} = x_{i-1,j=N_j}$$



Kelley, M. T., Pattison, R. C., Baldick, R., & Baldea, M. (2018). An MILP framework for optimizing demand response operation of air separation units. *Applied Energy*, 222, 951–966. <https://doi.org/10.1016/j.apenergy.2017.12.127>

# Parallelization



Kelley, M. T., Pattison, R. C., Baldick, R., & Baldea, M. (2018). An MILP framework for optimizing demand response operation of air separation units. *Applied Energy*, 222, 951–966. <https://doi.org/10.1016/j.apenergy.2017.12.127>

# Lagrangian Relaxation

Re-write complicating constraints (continuity conditions):

$$x_{i,j+1} = x_{i-1,j=N_j} \quad \rightarrow \quad |x_{i,j+1} - x_{i-1,j=N_j}| = \lambda_{i,m}$$

Designate a Lagrangian multiplier:  $\gamma_{i,m} = f(\gamma_{i,m-1})$

Optimization problem (m is iteration number):

$$\min_{u_i} J_m = \sum_i \sum_j Price_i P_{ijm} + \gamma_{im} \gamma_{im}$$

s.t.

Timing constraints

Process model (HW/FSR)

Inventory model

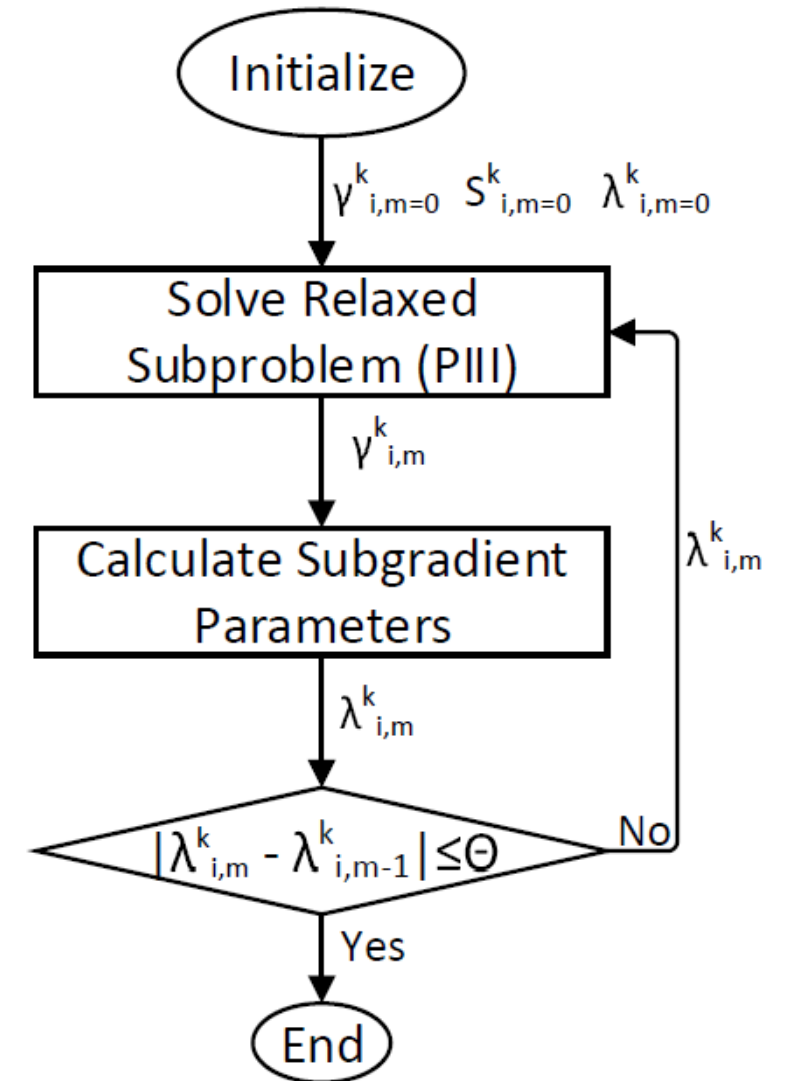
Initial Conditions

Process and Quality Constraints

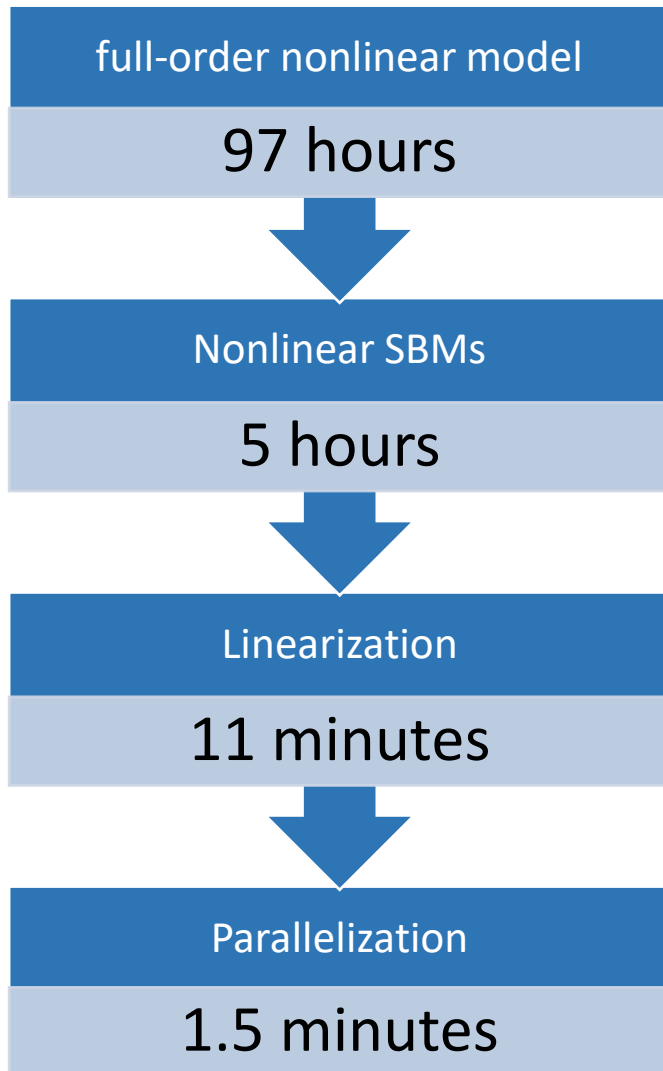
Kelley, M. T., Pattison, R. C., Baldick, R., & Baldea, M. (2018). An MILP framework for optimizing demand response operation of air separation units. *Applied Energy*, 222, 951–966. <https://doi.org/10.1016/j.apenergy.2017.12.127>

**Solution time:** 1.5 mins  
**Optimal operating cost:** \$1,014  
**Cost savings:** 1.12%  
**Optimality gap:** 0.09%

**Continuous Variables:** 90,325  
**SOS2 Variables:** 1,512



# Evolution of the solution time



## 1. Demand response scheduling

Kelley, M. T., Pattison, R. C., Baldick, R. & Baldea, M. An MILP framework for optimizing demand response operation of air separation units. *Appl. Energy* 222, 951-966 (2018).

## 2. Grid-side emissions minimization

Kelley, M. T., Baldick, R. & Baldea, M. Demand Response Operation of Electricity-Intensive Chemical Processes for Reduced Greenhouse Gas Emissions: Application to an Air Separation Unit. *ACS Sustain. Chem. Eng.* 7, 1909-1922 (2019).

## 3. Consideration of electricity price and product demand uncertainty

Kelley, M. T., Baldick, R. & Baldea, M. Demand response scheduling under uncertainty: Chance-constrained framework and application to an air separation unit. *AIChE J.* 66, (2020).

Kelley, M. T., Baldick, R. & Baldea, M. An empirical study of moving horizon closed-loop demand response scheduling. *J. Process Control* 92, 137-148 (2020).

## 4. Additional case studies: Ammonia production, batch reactors

Kelley, M. T., Pattison, R. C., Baldick, R. & Baldea, M. An efficient MILP framework for integrating nonlinear process dynamics and control in optimal production scheduling calculations. *Comput. Chem. Eng.* 110, 35-52 (2018).

Evaluating the Demand Response Potential of Ammonia Plants, submitted

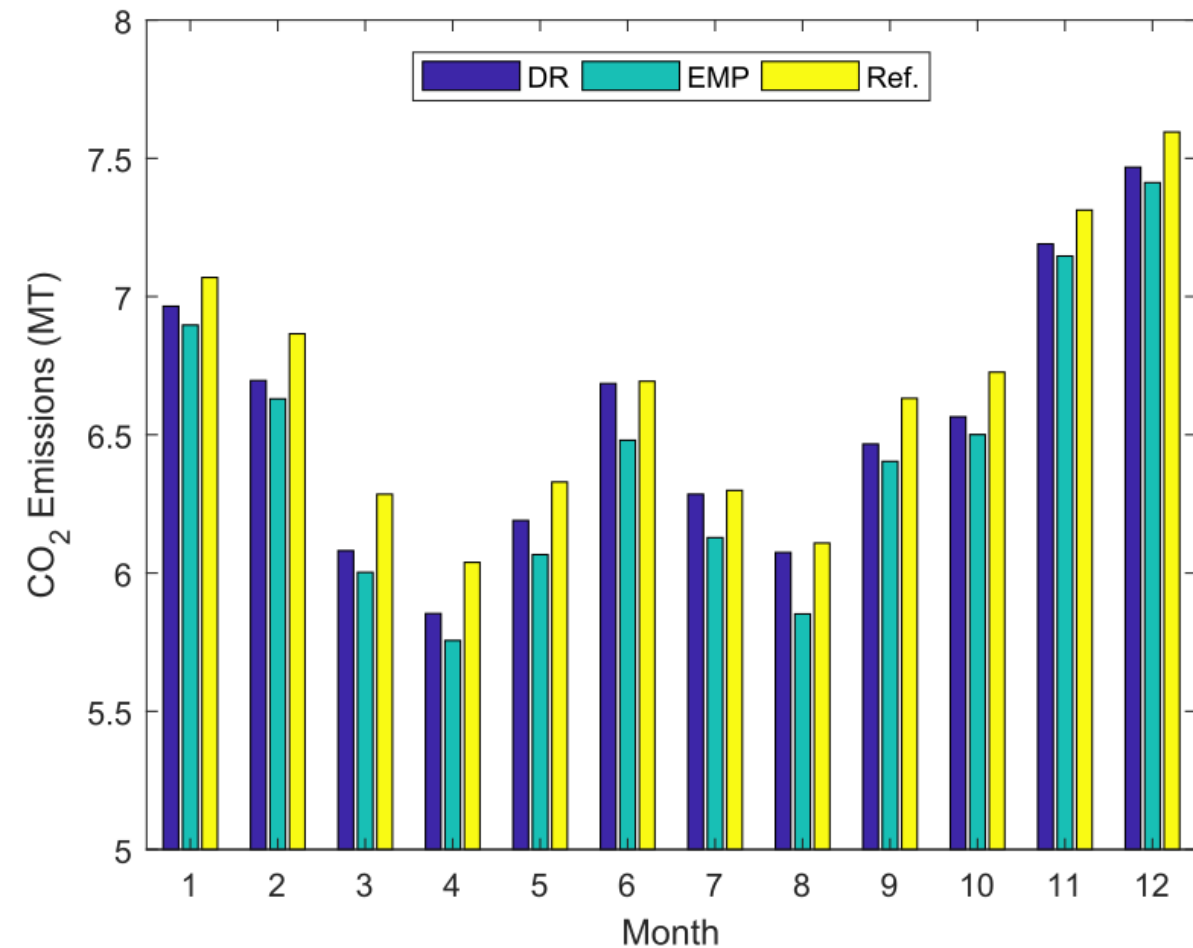
## 5. Identified SBMs for a year's worth of historical plant data from an industry partner for industrial DR scheduling

A linear programming formulation for demand response scheduling problem for an industrial air separation unit, in preparation

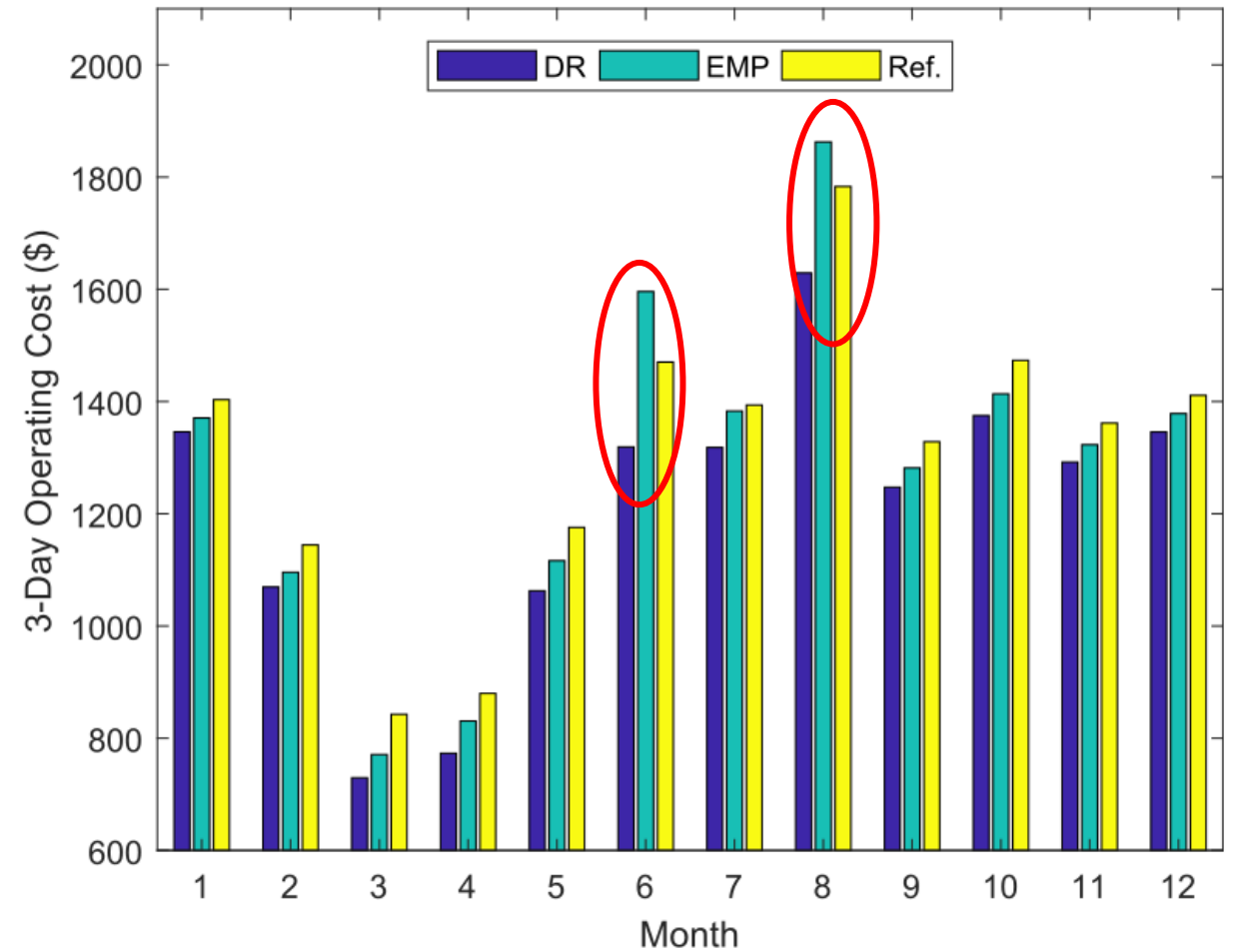
## 6. Extension to nonlinear problems

Kelley, M. T., Baldick, R. & Baldea, M. A direct transcription-based multiple shooting formulation for dynamic optimization. *Comput. Chem. Eng.* 140, 106846 (2020).

# Grid-side emissions reduction

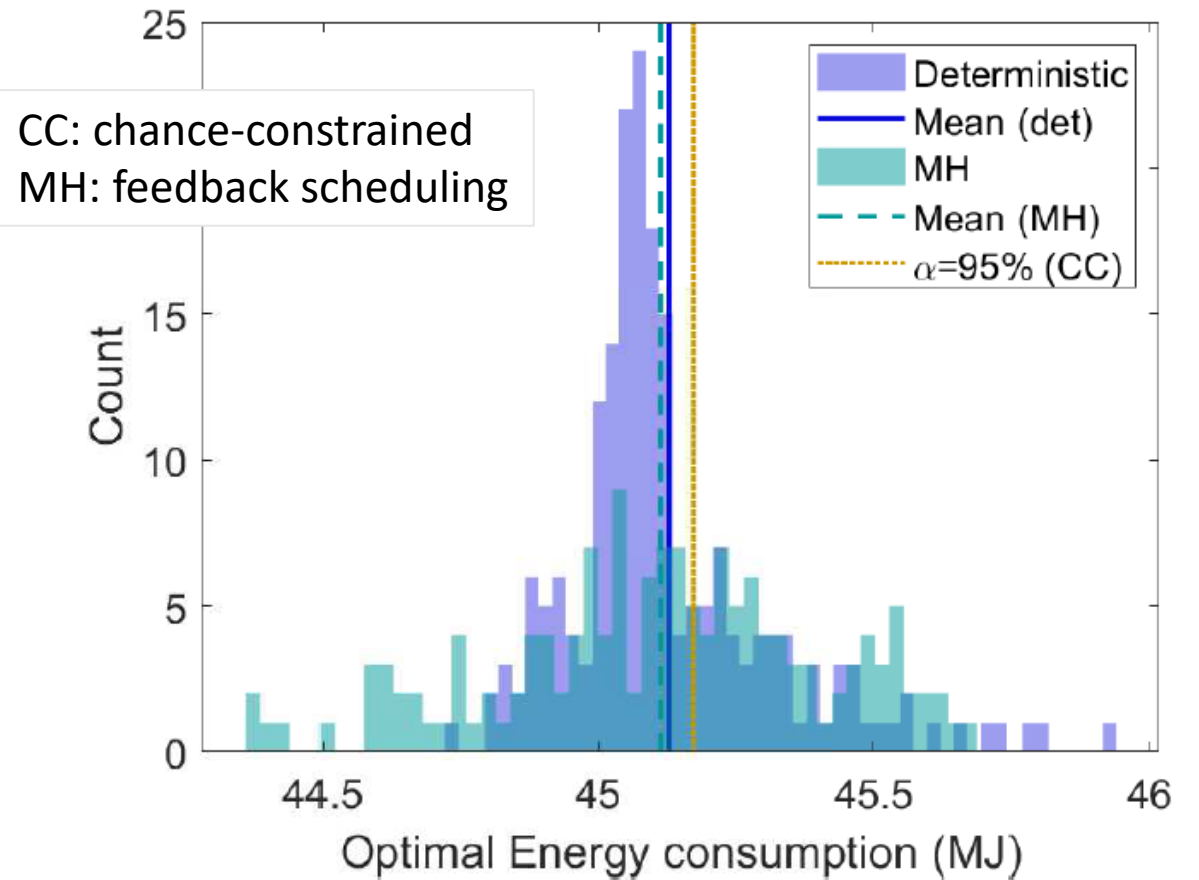
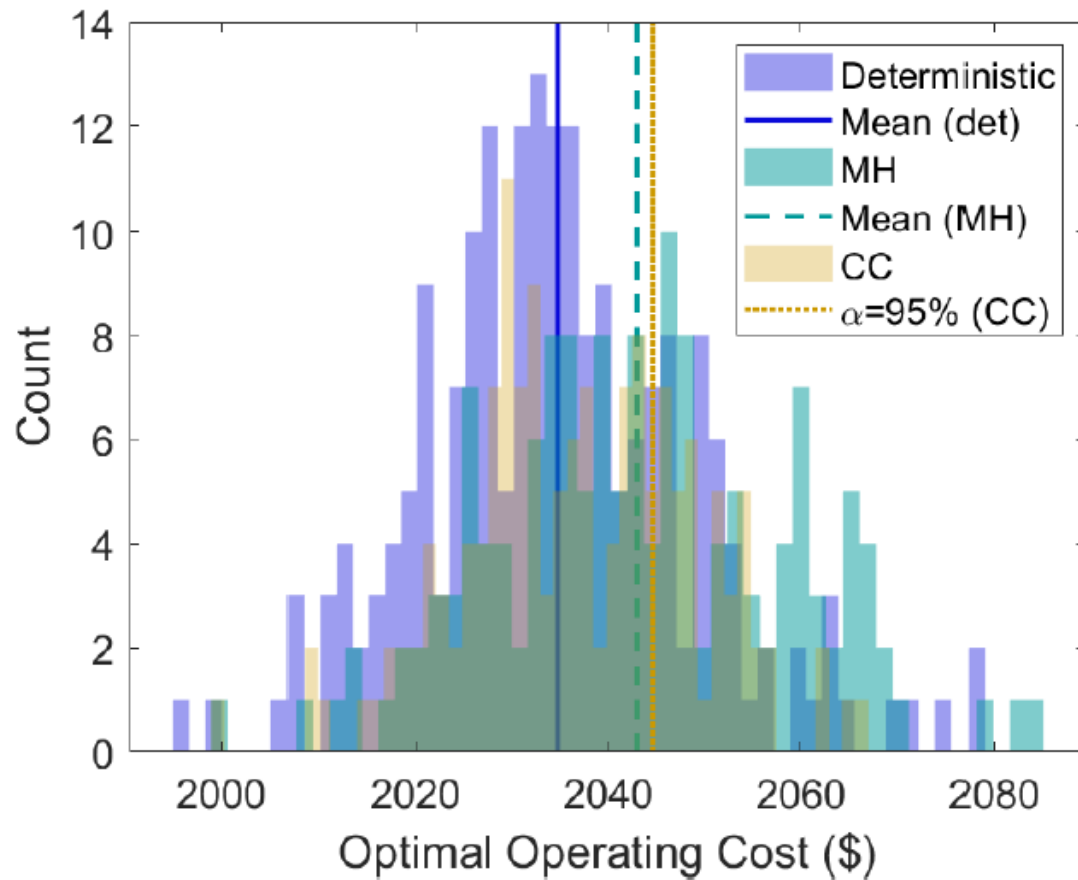


**DR consistently lowers emissions even though its aim is to minimize operating cost**



**Minimizing emissions can increase operating cost during summer months**

# Consideration of uncertainty



MH and CC methods are comparable, with the MH method allowing more room for correction at rescheduling points

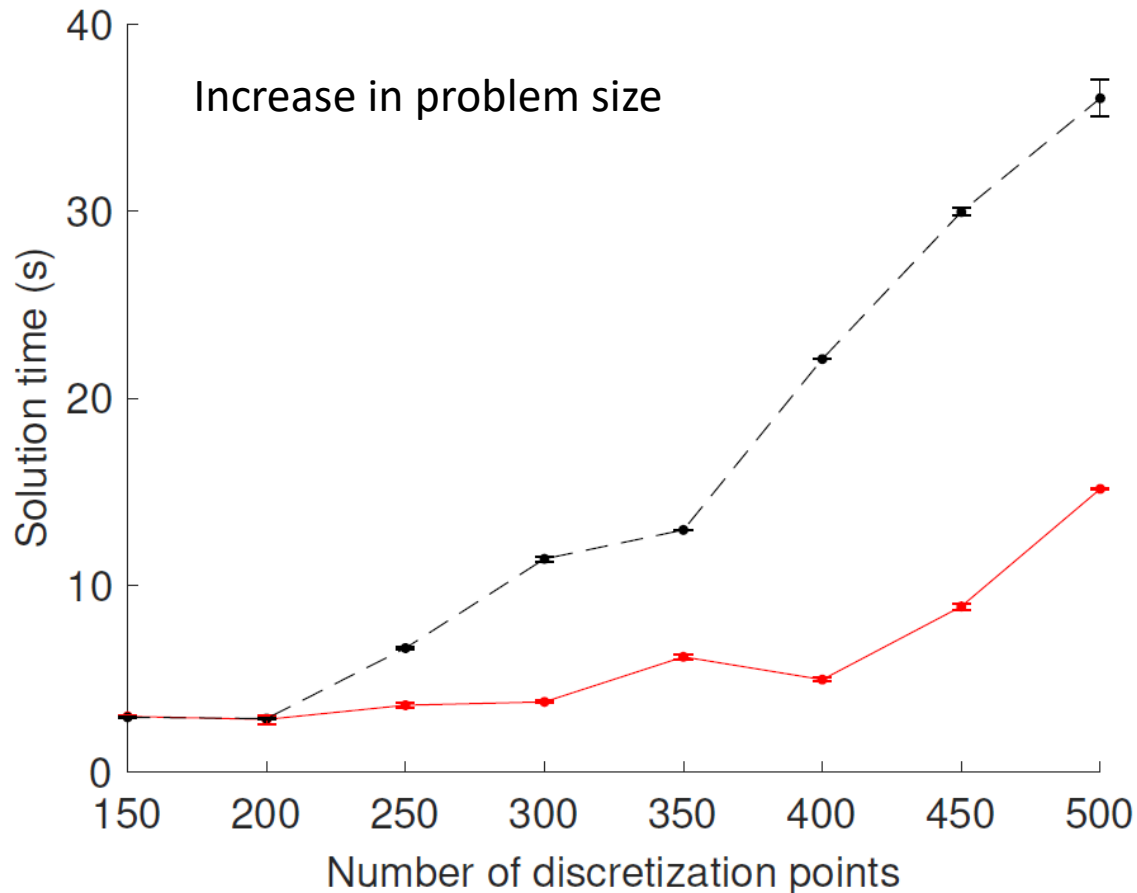


# Extension of parallel framework to nonlinear problems

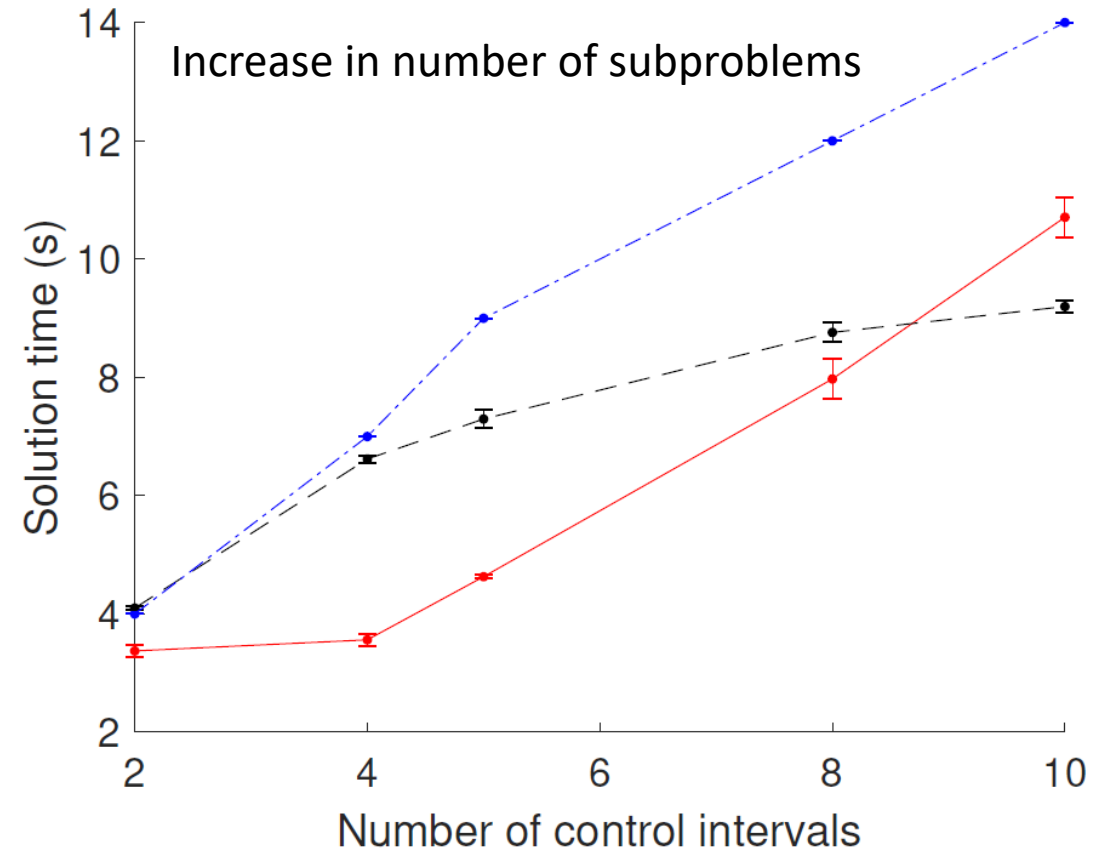
Continuous Sequential: **Blue** dash-dot

Discrete sequential: **Black** dash

Parallel solution: **Red** solid



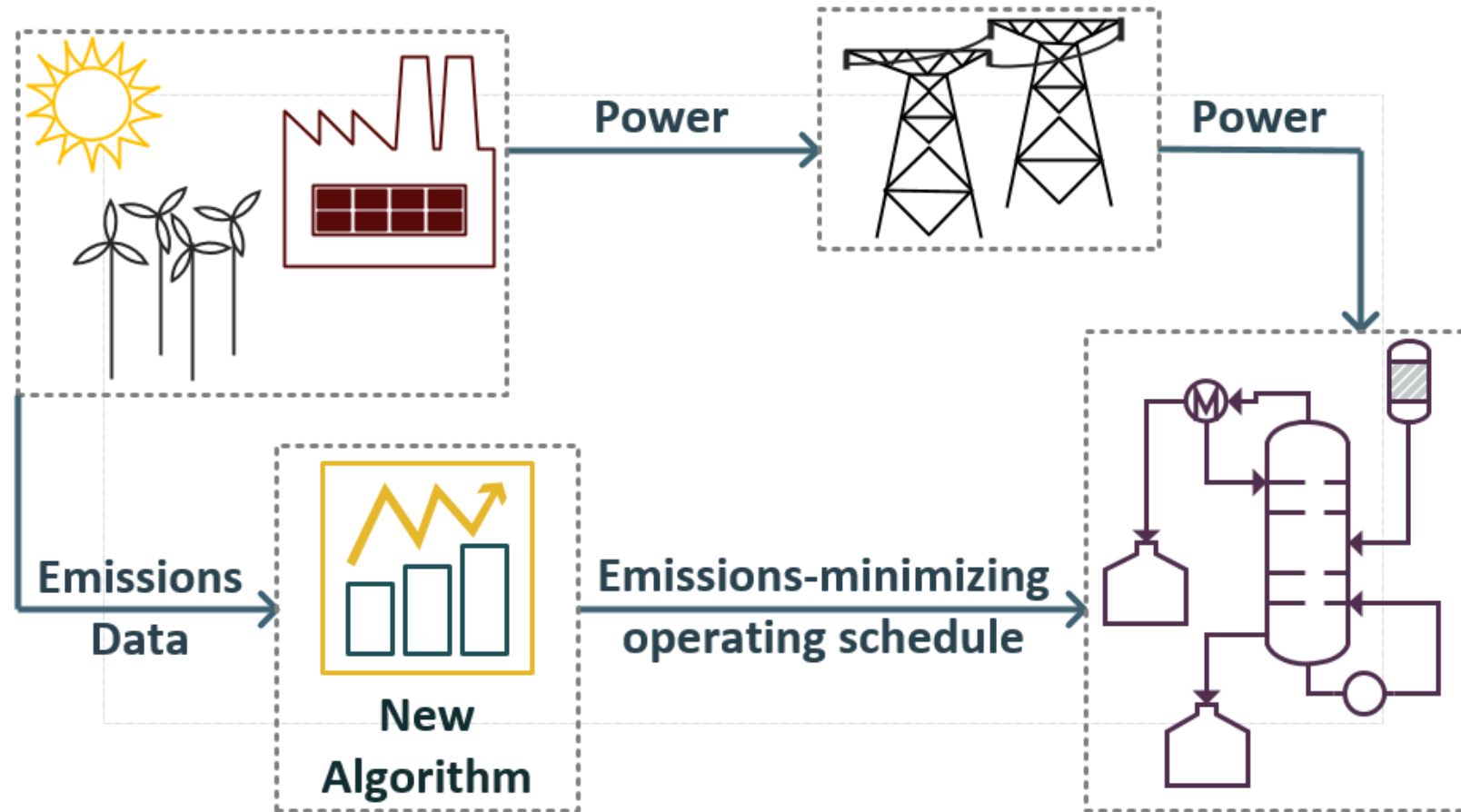
Parallel solution can handle increase in problem size much better than the sequential problem



Parallel solution is beneficial up until a point, where the overhead at generating each independent subproblem is too much

# Conclusions

- Developed framework to do optimal scheduling of large chemical entities for participation in load shifting
- Parallelization made a significant difference in terms of solution time and problem flexibility
- The fast solution time enabled many different directions of research



# Acknowledgements

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- Baldea and Edgar research groups
- Funding support from:
  - Department of Energy Computational Science Graduate Research Fellowship (DOE CSGF) award DE-FG02-97ER25308

