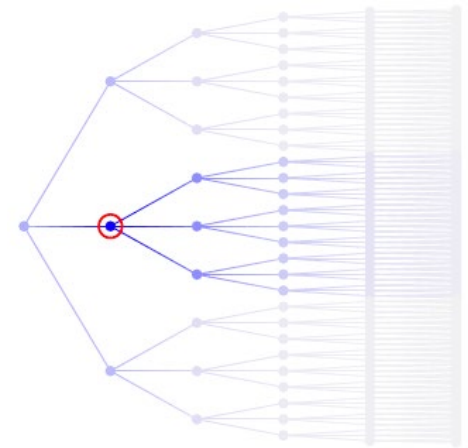


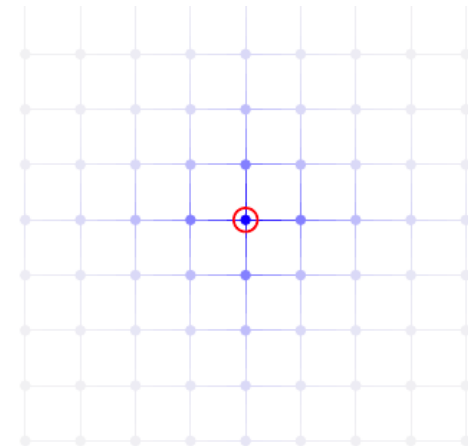
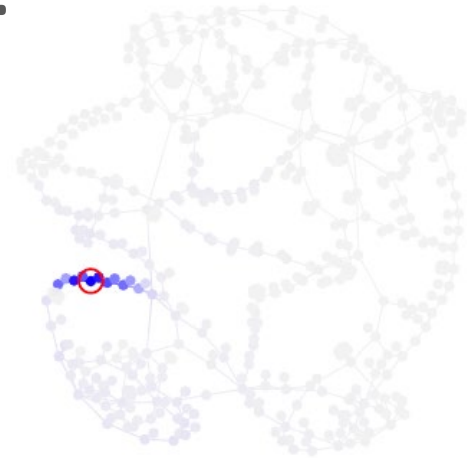


A Graph-Theoretic Perspective on Optimization: Theory, Modeling, Algorithms, and Applications

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University of Wisconsin-Madison

Mathematics and Computer Science Division
Argonne National Laboratory



Work with: Sungho Shin, Mihai Anitescu, Jordan Jalving, David Cole

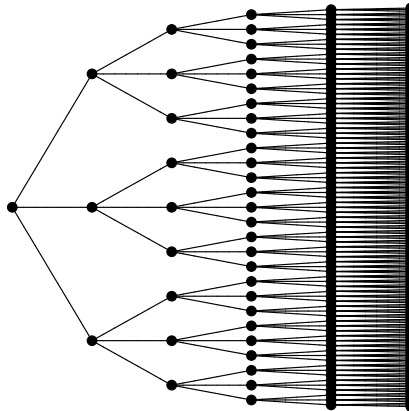
Motivation

What is a General Math Abstraction of these Problem Classes?

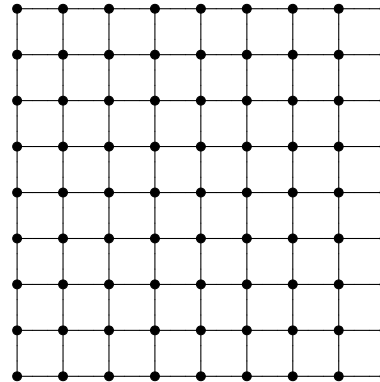
Dynamic Optimization



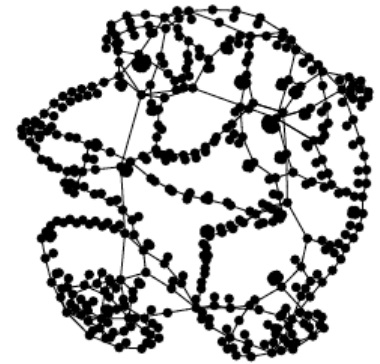
Stochastic Optimization



PDE Optimization

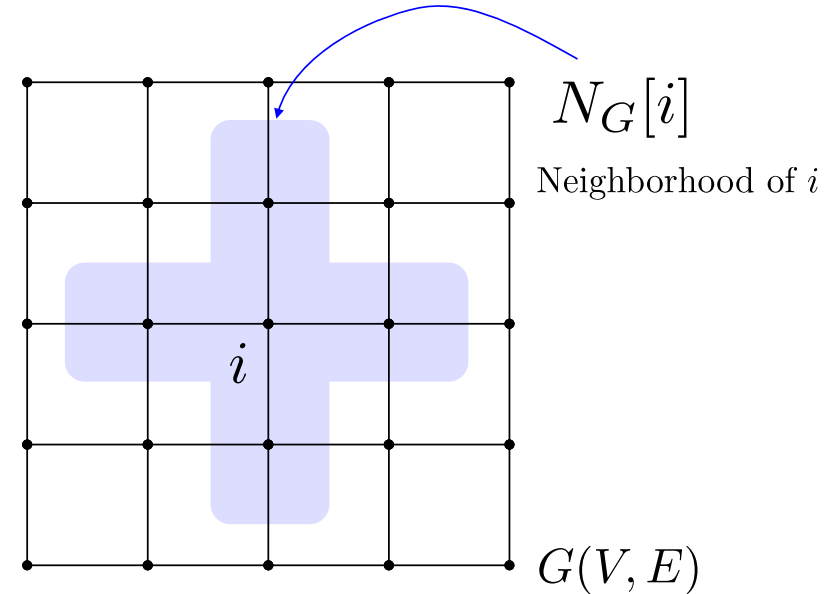


Network Optimization



Graph-Structured Nonlinear Programs (gsNLP)

$$\begin{aligned} \min_{\{z_i\}_{i \in V}} \quad & \sum_{i \in V} f_i(\{z_j\}_{j \in N_G[i]}, p_i) \\ \text{s.t.} \quad & g_i(\{z_j\}_{j \in N_G[i]}, p_i) \geq 0, \quad i \in V \end{aligned}$$

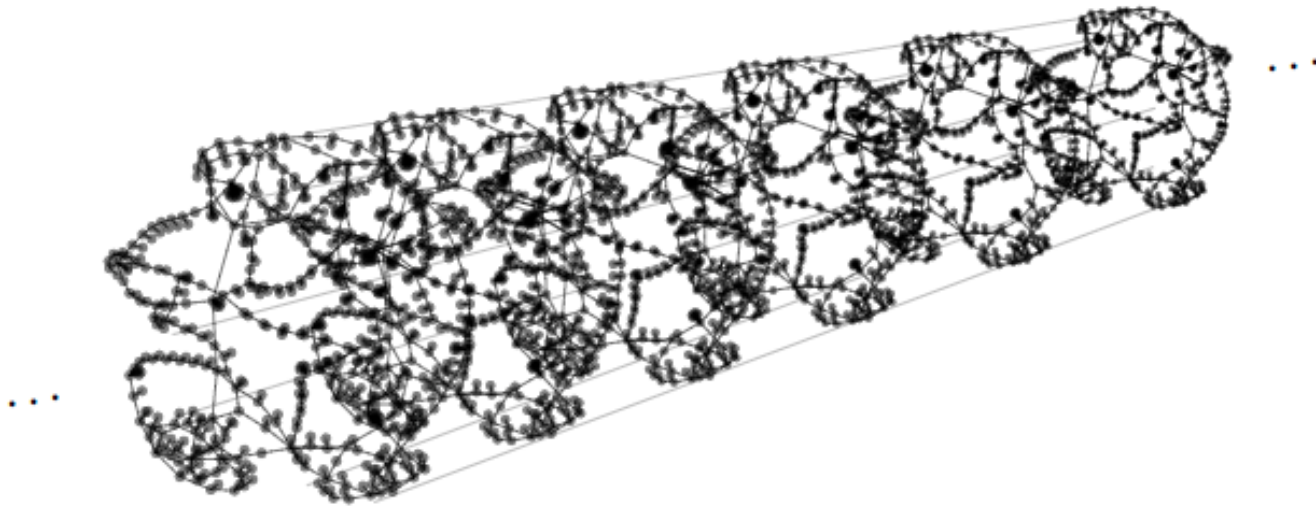


- Problem domain given by graph $G(V, E)$.
- Each node $i \in V$ has local objective, constraints, and **data**.
- Each node $i \in V$ has local variables (e.g., states and controls).
- Node $i \in V$ is coupled to its neighbors $N_G[i] \subseteq V$



Dynamic Network Optimization

(e.g., natural gas, power, water, transportation networks)



Exponential Decay of Sensitivity (EDS)

Sensitivity of NLPs (Classical)

How does solution z^* change when data p changes?

$$p, p' \Rightarrow \begin{array}{l} \min_z f(z, p) \\ \text{s.t. } g(z, p) \geq 0 \end{array} \Rightarrow z^*(p), z^*(p')$$

Assumptions:

- Consider base data p and perturbation p' .
- Assume base solution $z^*(p)$ satisfies SSOC and LICQ (regularity conditions).

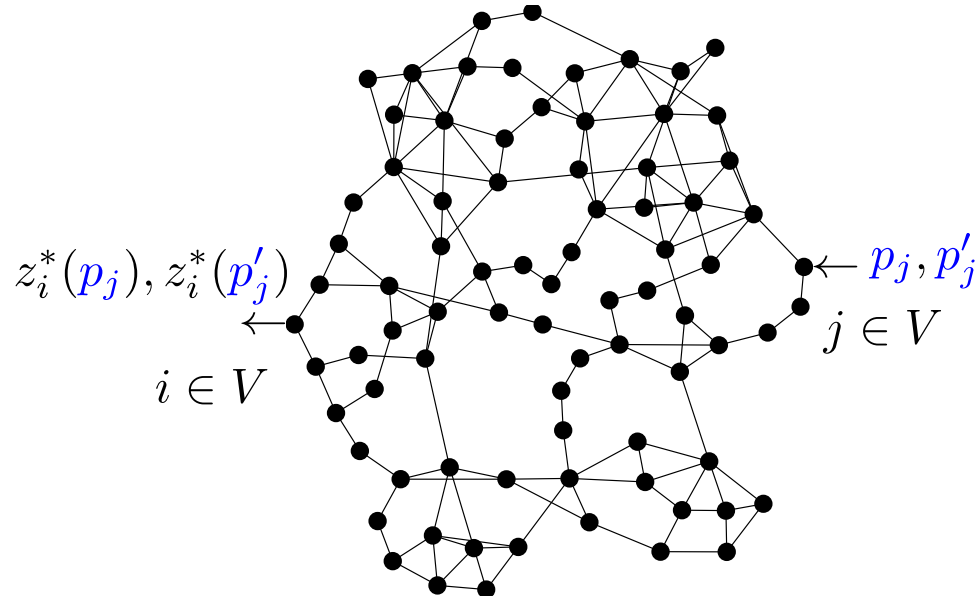
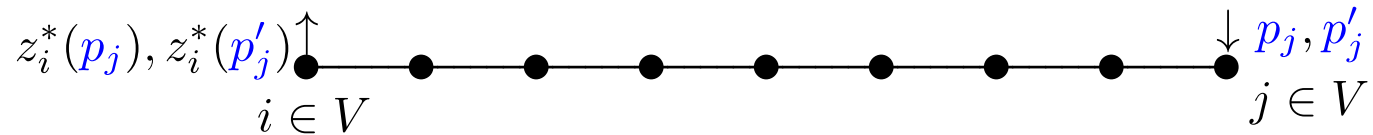
Theorem: There exists a continuous solution mapping $z^*(\cdot)$ and:

$$\|z^*(p) - z^*(p')\| \leq C\|p - p'\|$$

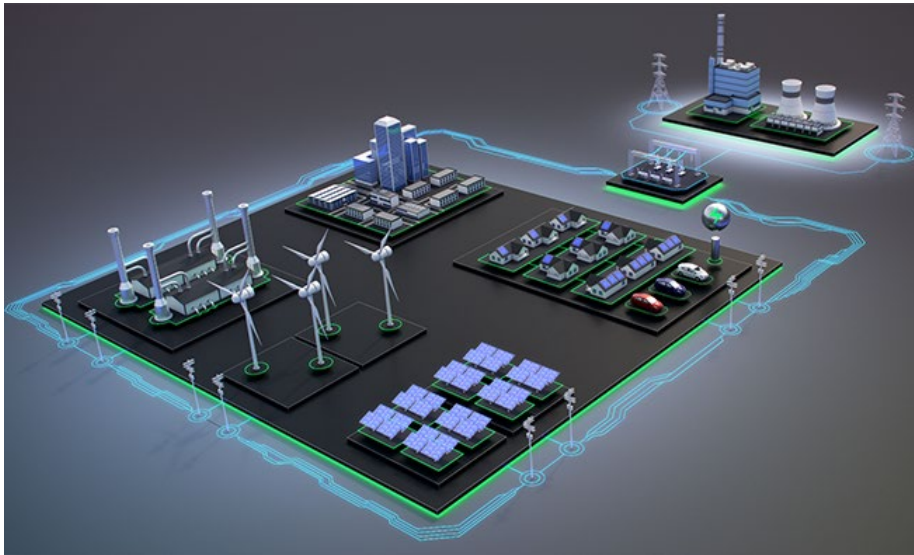
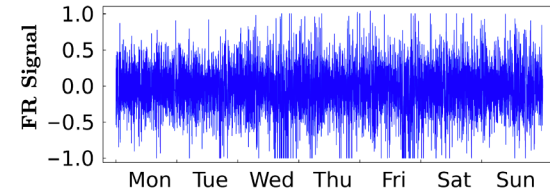
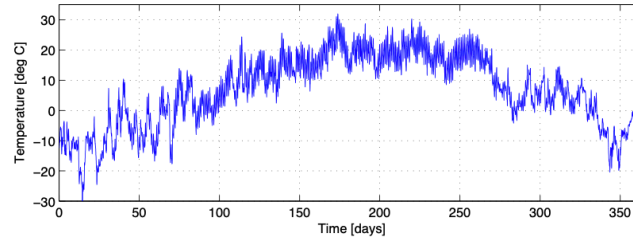
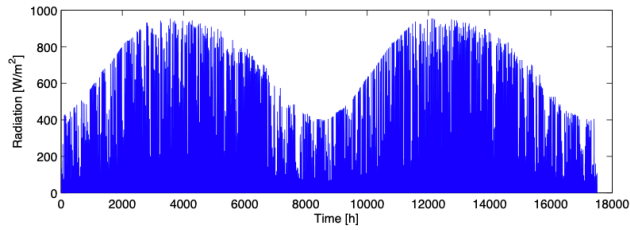
with Lipschitz Constant C .

Sensitivity of gsNLPs

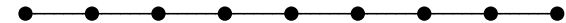
How does solution z_i^* (at node $i \in V$) change when data p_j (at node $j \in V$) changes?



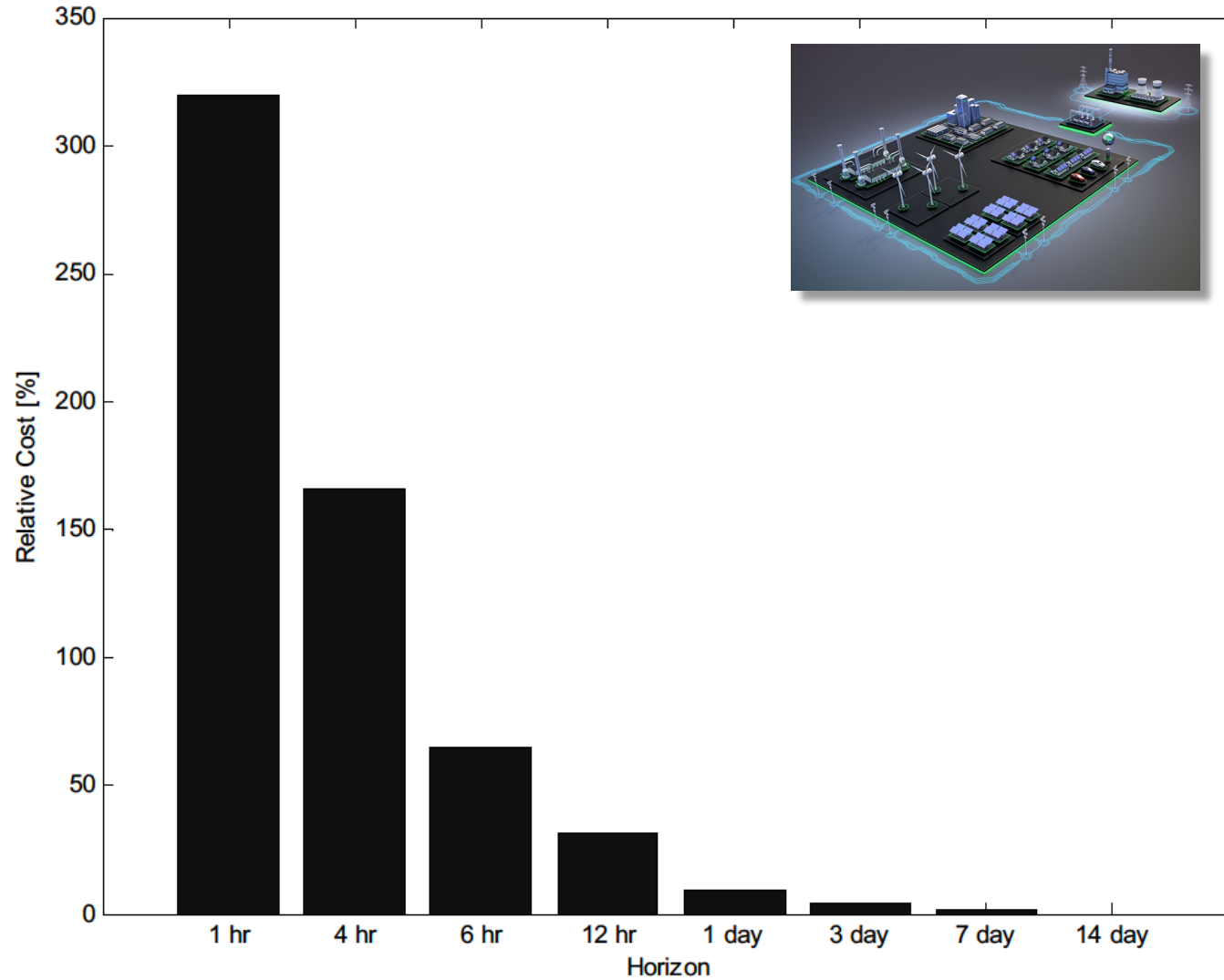
Exponential Decay of Sensitivity (EDS): Temporal



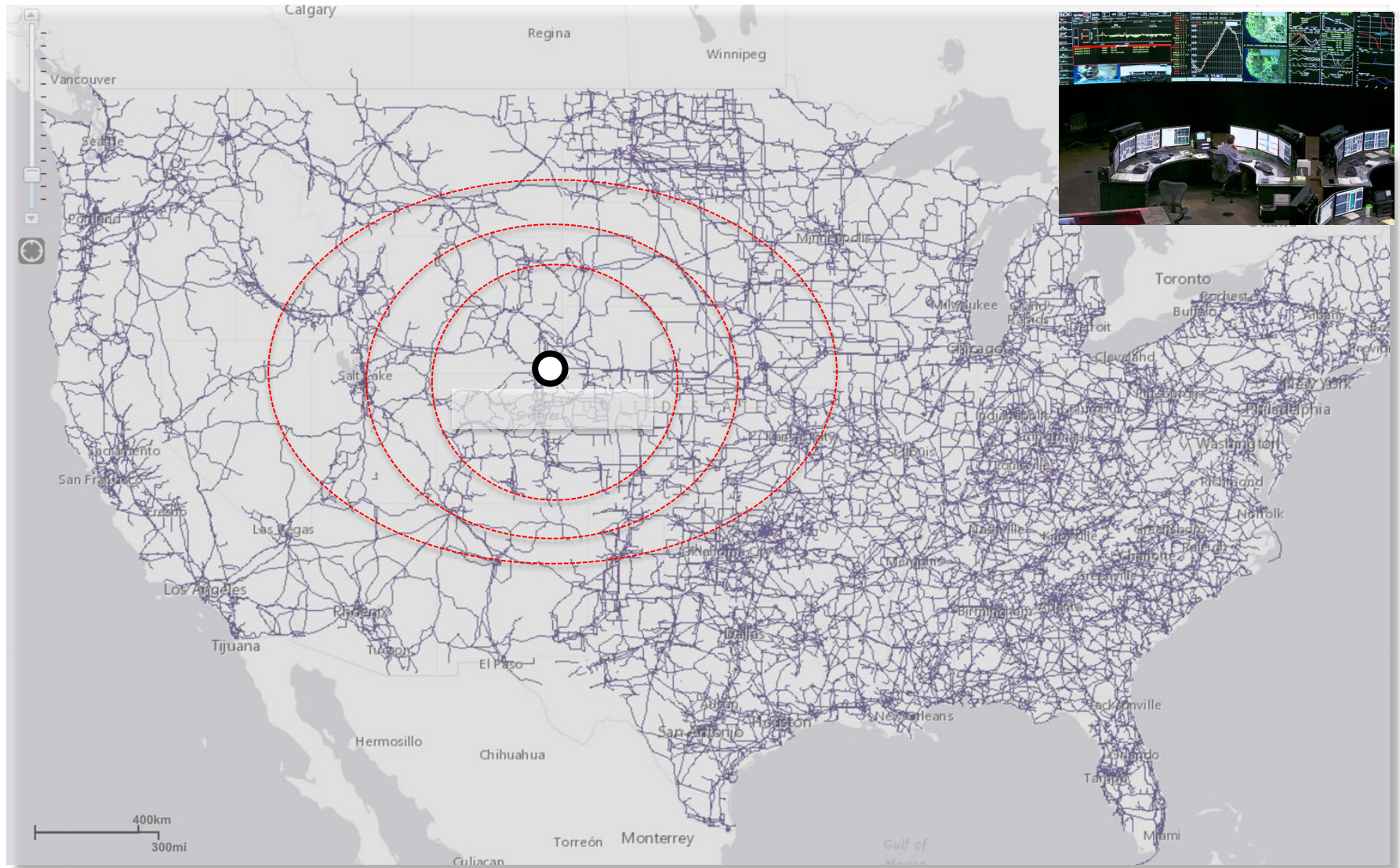
$$\begin{aligned} \min_{u(\cdot)} \quad & \int_0^T \varphi(z(\tau), u(\tau), p(\tau)) d\tau \\ \text{s.t.} \quad & \dot{z}(\tau) = f(z(\tau), u(\tau), p(\tau)) \end{aligned}$$



Exponential Decay of Sensitivity (EDS): Temporal



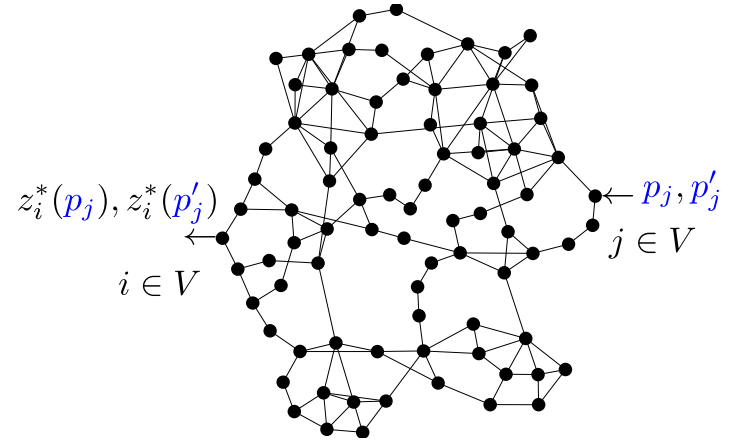
Exponential Decay of Sensitivity (EDS): Spatial



EDS in gsNLPs

How does solution z_i^* (at node $i \in V$) change when data p_j (at node $j \in V$) changes?

$$\begin{aligned} \min_{\{z_i\}_{i \in V}} \quad & \sum_{i \in V} f_i(\{z_j\}_{j \in N_G[i]}, p_i) \\ \text{s.t.} \quad & g_i(\{z_j\}_{j \in N_G[i]}, p_i) \geq 0, \quad i \in V \end{aligned}$$



Assumptions:

- Assume base solution $z^*(p)$ satisfies SSOC and LICQ (regularity conditions).

Theorem: The solutions at node $i \in V$ satisfy:

$$\|z_i^*(p_j) - z_i^*(p'_j)\| \leq C \rho^{d(i,j)} \|p_j - p'_j\|$$

with $\rho \in (0, 1)$, C independent of size of G , and $d(i, j)$ is geodesic distance.

Key: - Solution Sensitivity Decays *Exponentially* with Geodesic Distance.

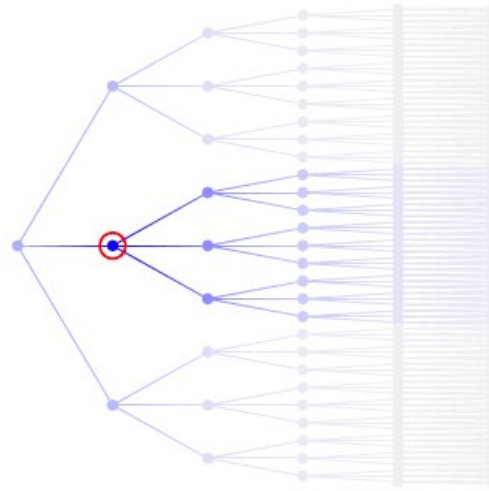
- Result Obtained from Sparsity Analysis of the KKT Matrix Inverse

EDS in gsNLPs

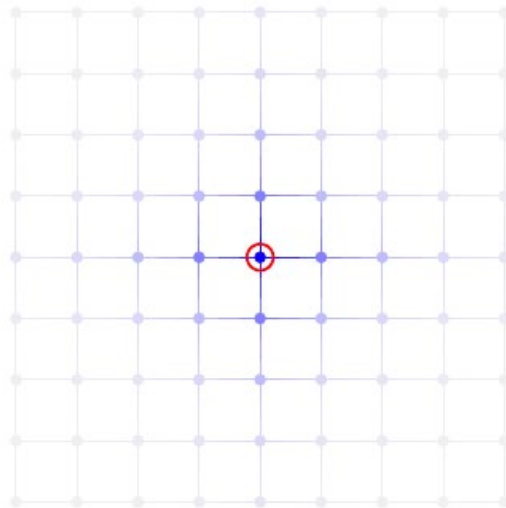
Dynamic Optimization



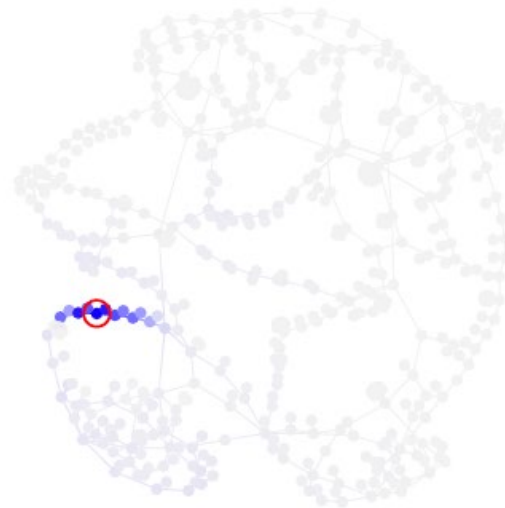
Stochastic Optimization



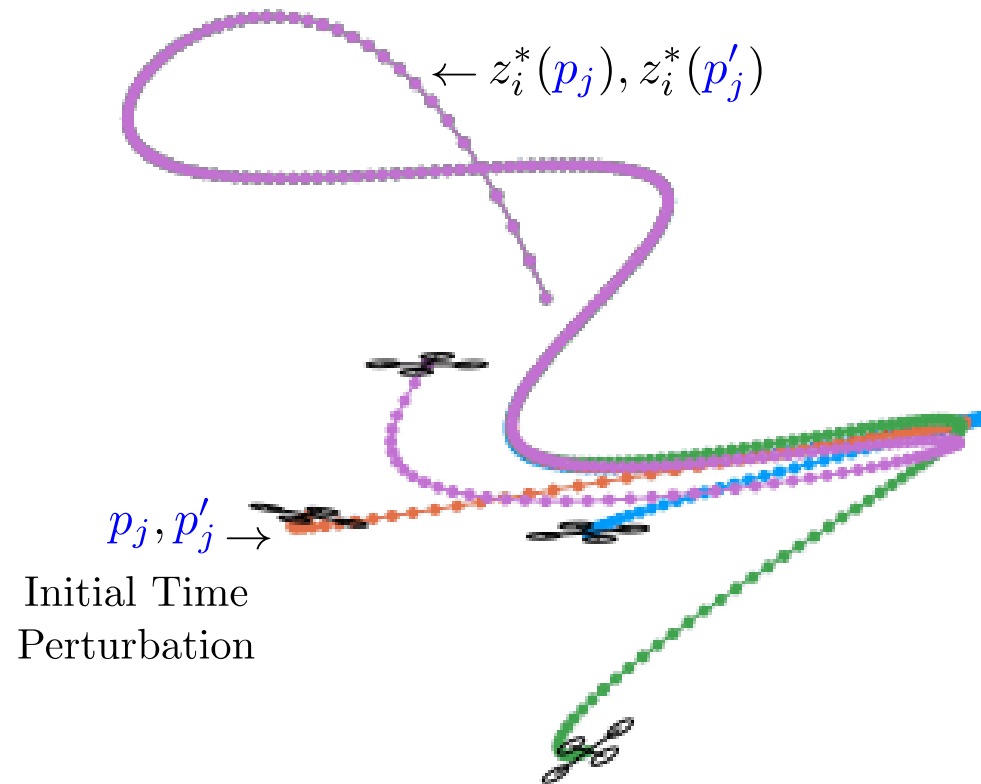
PDE Optimization



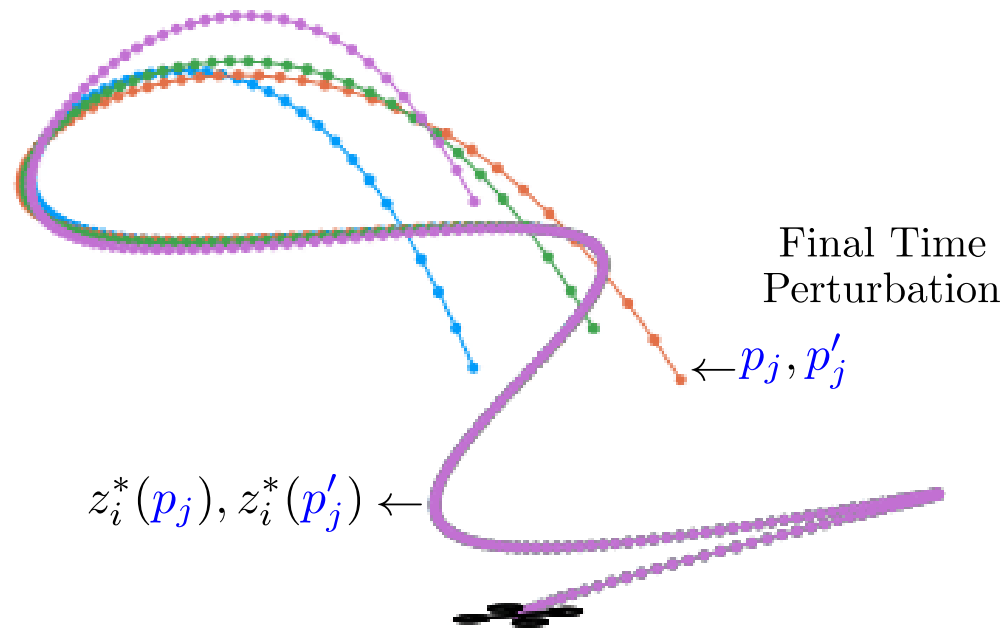
Network Optimization



EDS in gsNLPs



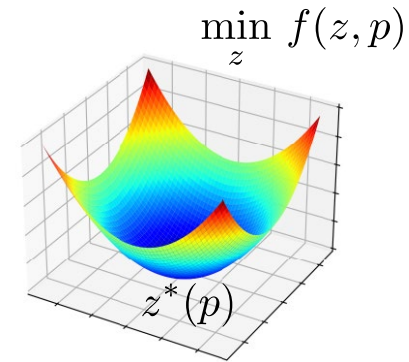
EDS in gsNLPs



EDS in gsNLPs

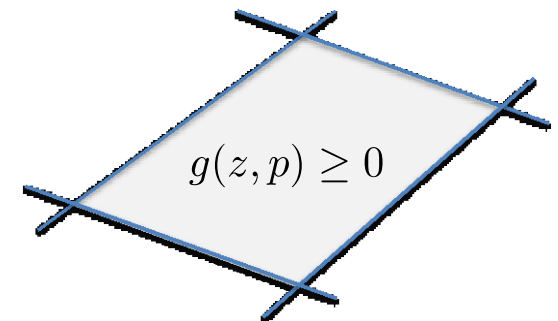
Key: SSOC and LICQ provide Sufficient Conditions for EDS

- Strong Second Order Condition (**SSOC**) Ensures z Impacts Objective
- Smallest Singular Value of Reduced Hessian is a Measure of “Attraction”
- Related to Observability in Optimal Control



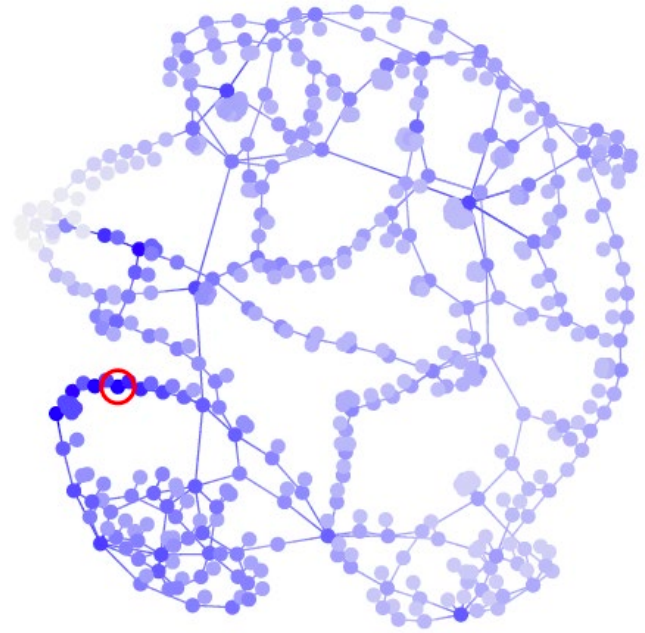
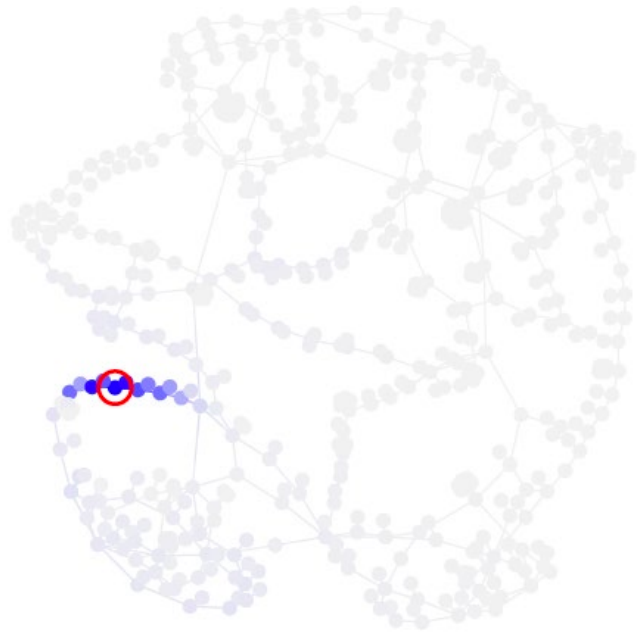
$$\sigma_{\min}(N^T \nabla^2 \mathcal{L}(z^*(p), p) N) > 0 \quad \text{with} \quad \nabla g(z^*(p), p) N = 0$$

- Linear Independence Constraint Qualification (**LICQ**) Ensures z Impacts Constraints
- Smallest Singular Value of Jacobian is a Measure of “Flexibility”
- Related to Controllability in Optimal Control



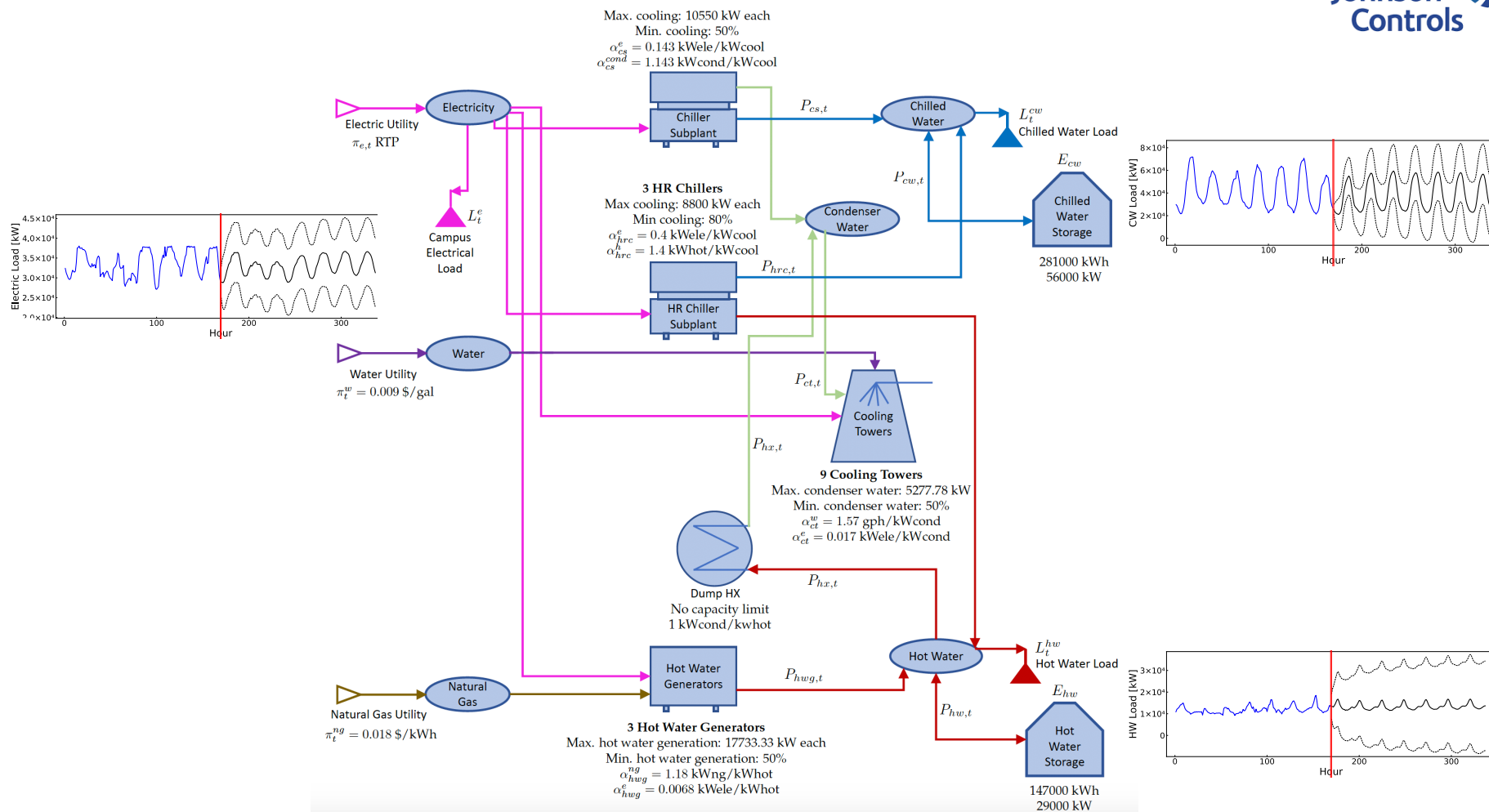
$$\sigma_{\min}(\nabla g(z^*(p), p)) > 0$$

Effect of Regularity



Algorithms

MPC for Utilities Plant



MPC Problem

Objective: Minimize Expected Total Cost and Demand Charge

$$\min \mathbb{E} \left[\sum_{k \in \mathcal{T}} (\pi_k(\xi)^T u_k(\xi) + \mu^T s_k(\xi)) + \frac{\pi^D}{\sigma_t} D(\xi) \right]$$

Load & Energy Balance Constraints:

$$C u_k(\xi) + s_k(\xi) = L_k(\xi)$$

Storage Dynamics:

$$x_{k+1}(\xi) = A x_k(\xi) + B u_k(\xi)$$

$$x_0(\xi) = \hat{x}_t$$

Demand Charges:

$$D(\xi) \geq \beta u_k(\xi)$$

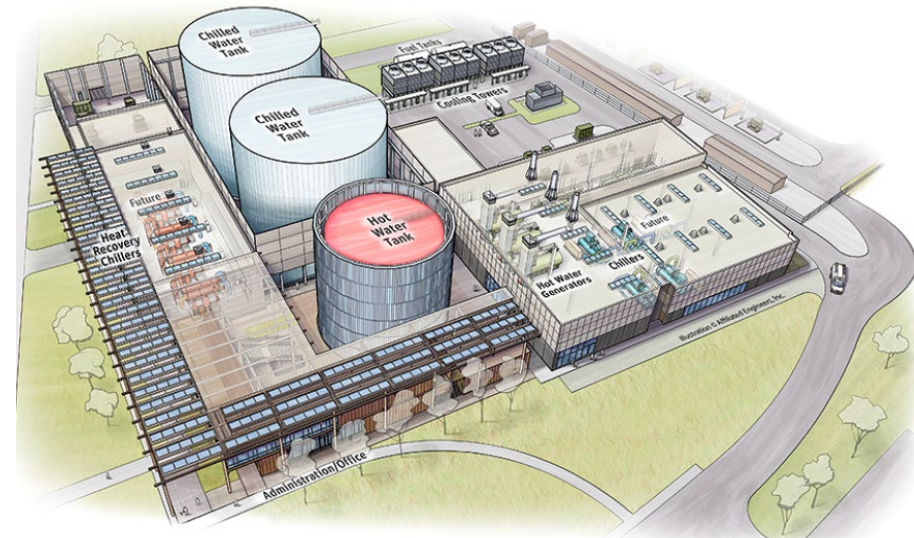
$$D(\xi) \geq \hat{D}_t$$

Bounds:

$$0 \leq x_k(\xi) \leq \bar{x}$$

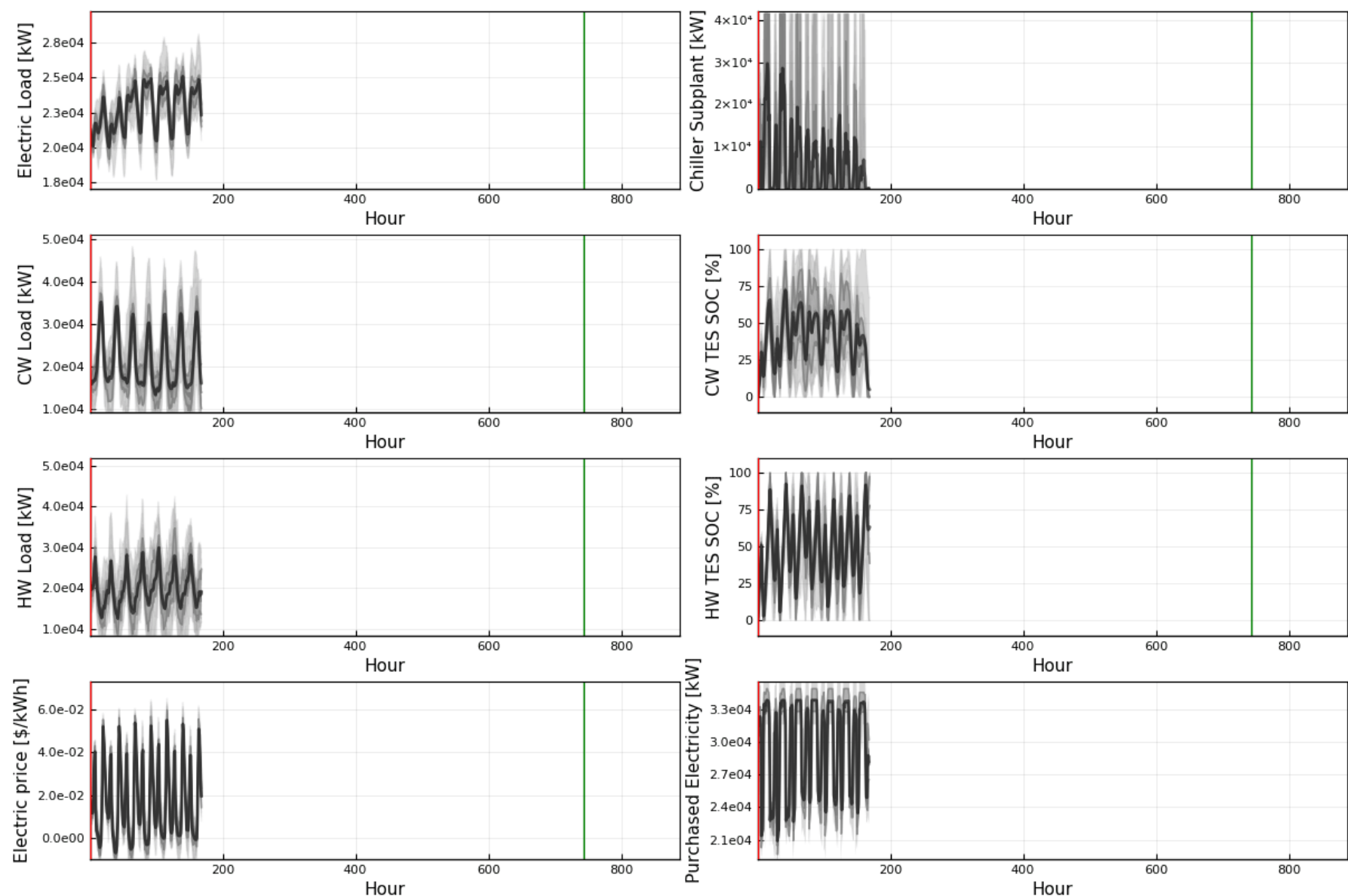
$$\underline{u} \leq u_k(\xi) \leq \bar{u}$$

$$s_k(\xi) \geq 0$$



Closed-Loop System

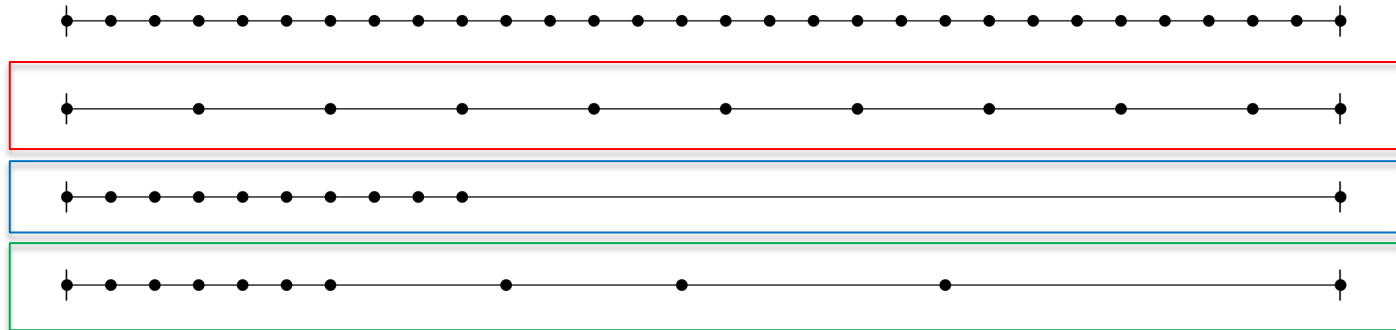
Closed-Loop Simulation (One Year)



Key: A single year-long simulation takes ~ 3 hours.

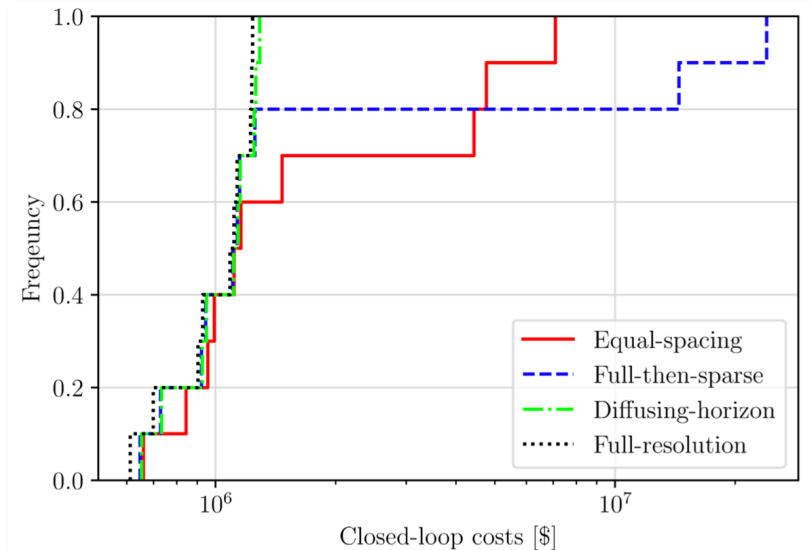
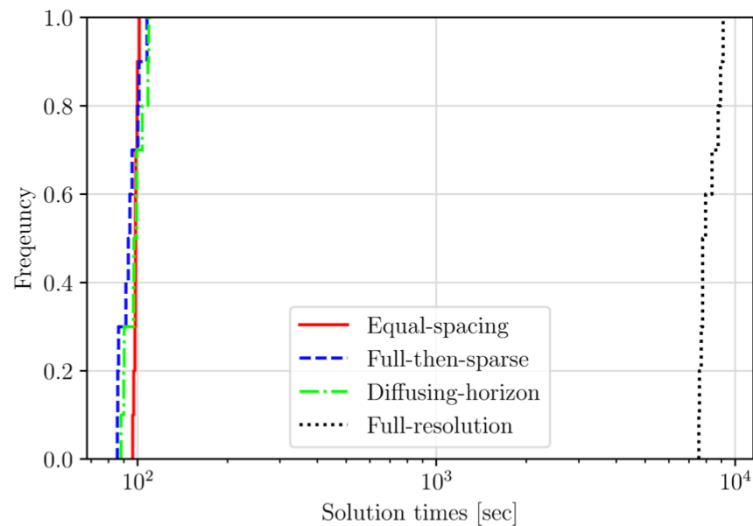
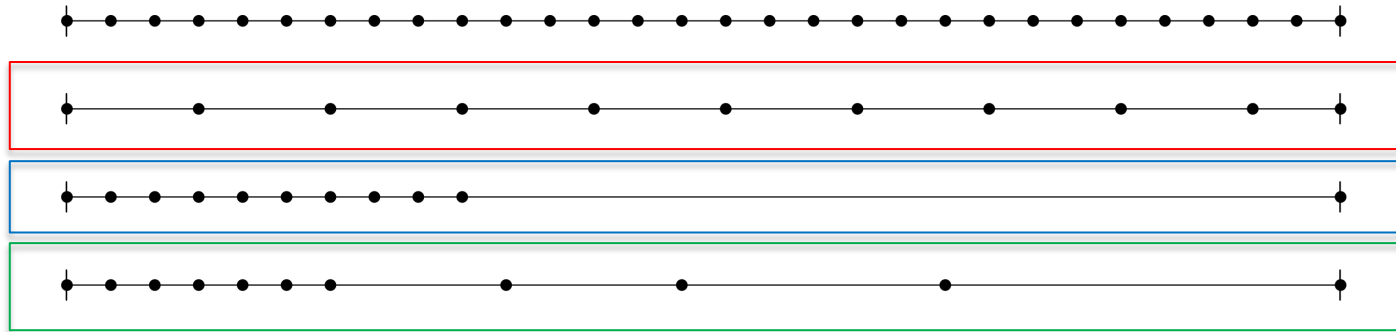
Graph-Based Approximation (Diffusing Horizon MPC)

Horizon Coarsening Strategies



Graph-Based Approximation (Diffusing Horizon MPC)

Horizon Coarsening Strategies



Key: Diffusing-horizon decreases times by 2 orders of magnitude.

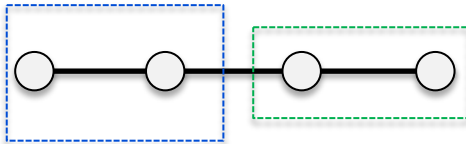
Overlapping Schwarz Decomposition

Full Problem



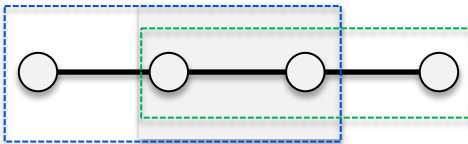
$$\begin{bmatrix} Q_{11} & Q_{12} & & \\ Q_{21} & Q_{22} & Q_{23} & \\ & Q_{32} & Q_{33} & Q_{34} \\ & & Q_{43} & Q_{44} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix}$$

Standard Partitioning



$$\begin{bmatrix} Q_{11} & Q_{12} & & \\ Q_{21} & Q_{22} & Q_{23} & \\ & Q_{32} & Q_{33} & Q_{34} \\ & & Q_{43} & Q_{44} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix}$$

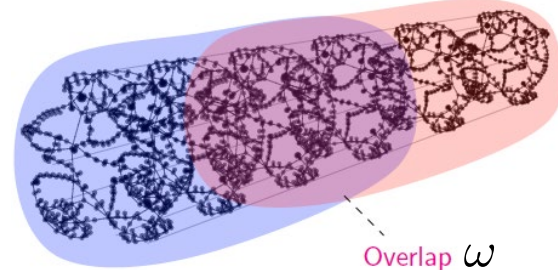
Overlapping Partitioning



$$\begin{bmatrix} Q_{11} & Q_{12} & & \\ Q_{21} & Q_{22} & Q_{23} & \\ & Q_{32} & Q_{33} & Q_{34} \\ & & Q_{43} & Q_{44} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix}$$

Key: Eliminate Redundancy in Overlapping Region via Restriction

Overlapping Schwarz for QP

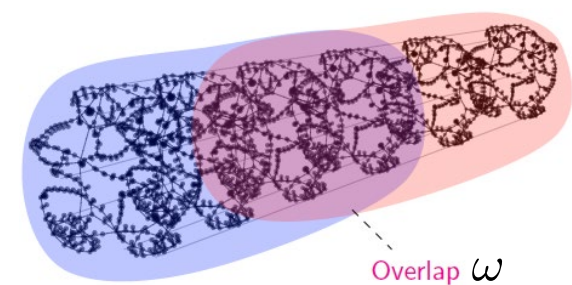


Consider graph-structured problem:

$$\min_z \frac{1}{2} z^T Q z + c^T z$$

$Q \succ 0$ embeds graph structure $G(V, E)$

Overlapping Schwarz for QP



Consider graph-structured problem:

$$\min_z \frac{1}{2} z^T Q z + c^T z$$

$Q \succ 0$ embeds graph structure $G(V, E)$

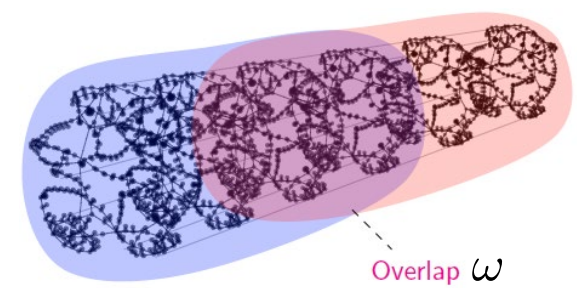
Partition domain V into V_k , $k = 1, \dots, K$ and construct overlapping domains:

$$V_k^\omega := \{v \in V \mid d(v, V_k) \leq \omega\}$$

ω is size of overlap

Key: $\omega = 0$ is decentralized and $\omega = |V|$ is centralized

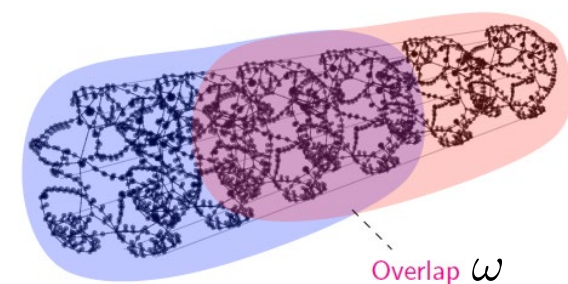
Overlapping Schwarz for QP



Overlapping Schwarz Scheme is:

$$z_k^{\ell+1} = R_k \operatorname{argmin}_{z_k} \frac{1}{2} z_k^T Q_k z_k + (c_k - Q_{-k} z_{V_{-k}}^\ell)^T z_k \quad \text{for } k = 1, \dots, K$$

Overlapping Schwarz for QP



Overlapping Schwarz Scheme is:

$$z_k^{\ell+1} = R_k \operatorname{argmin}_{z_k} \frac{1}{2} z_k^T Q_k z_k + (c_k - Q_{-k} z_{V_{-k}}^{\ell})^T z_k \quad \text{for } k = 1, \dots, K$$

Theorem: The scheme converges linearly:

$$\|z^{\ell} - z^*\|_{\infty} \leq \alpha^{\ell} \|z^0 - z^*\|_{\infty}$$

with convergence rate:

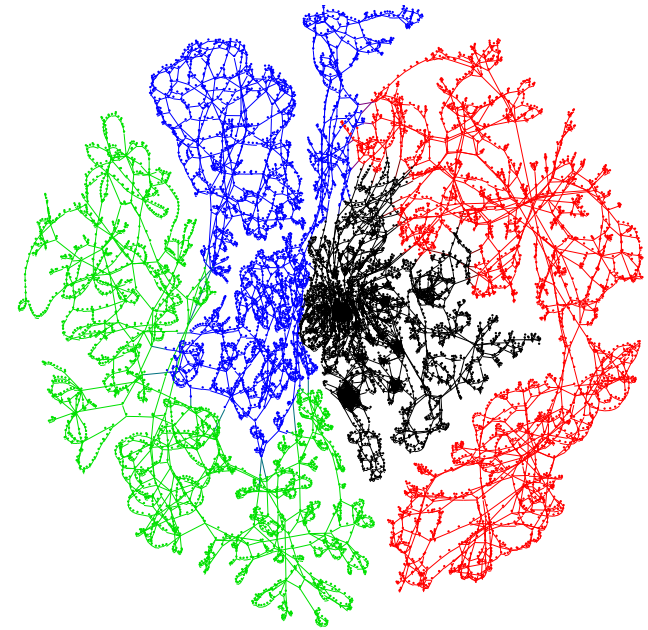
$$0 \leq \alpha \leq \frac{\delta_1}{\lambda_{\min}} \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^{(\omega+1)/\delta_2}$$

Key: Convergence rate improves *exponentially* with ω .

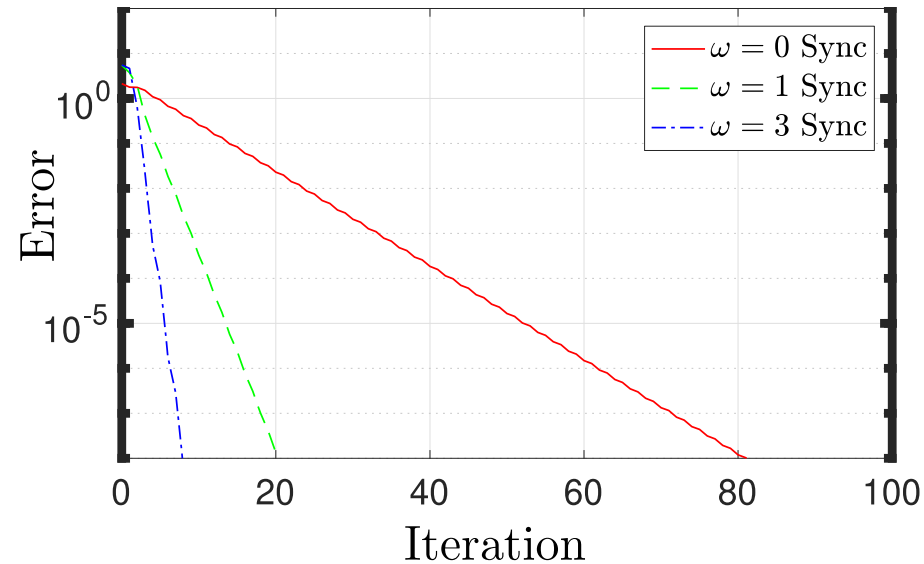
State Estimation

9,241 Node Power Network (Pegasus):

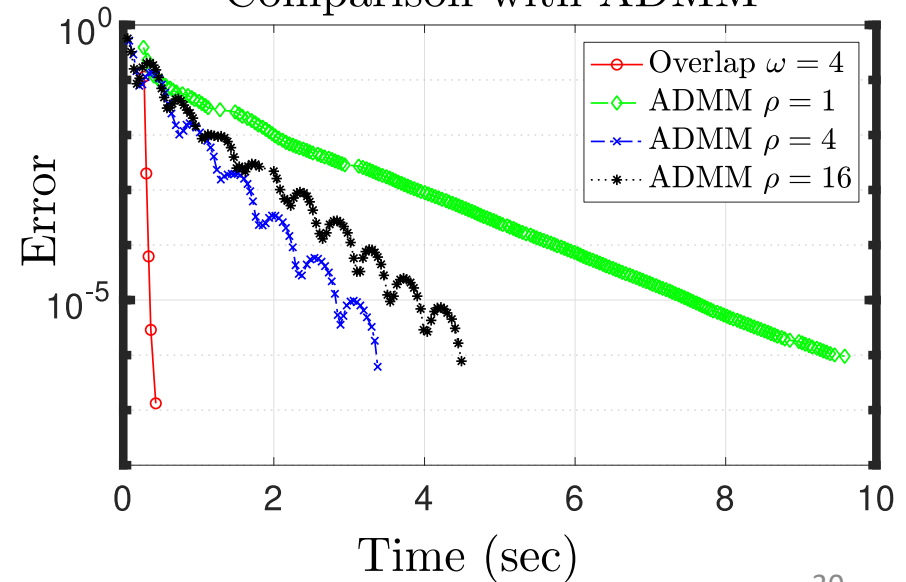
$$\begin{aligned} \min_{\delta, P} \quad & \sum_{i \in V} \left(\frac{\delta_i - \delta_i^m}{\sigma_{\delta_i}} \right)^2 + \sum_{\{i, j\} \in E} \left(\frac{P_{ij} - P_{ij}^m}{\sigma_{P_{ij}}} \right)^2 \\ \text{s.t.} \quad & P_{ij} = y_{ij}(\delta_i - \delta_j), \quad \{i, j\} \in E \end{aligned}$$



Effect of Overlap



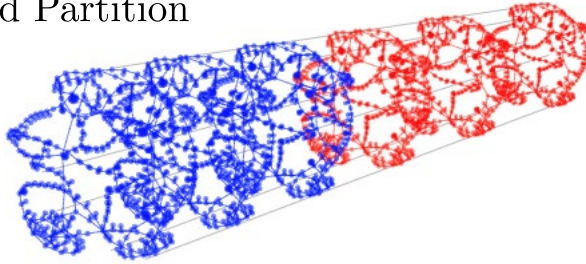
Comparison with ADMM



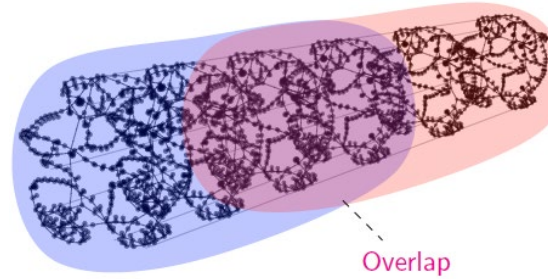
Overlapping Schwarz for NLP

$$\begin{aligned} \min_{\{x_i\}_{i \in V}} \quad & \sum_{i \in V} f_i(\{x_j\}_{j \in N_G[i]}) \\ \text{s.t.} \quad & c_i(\{x_j\}_{j \in N_G[i]}) \geq 0, \quad i \in V \end{aligned}$$

Standard Partition



Overlapping Partition

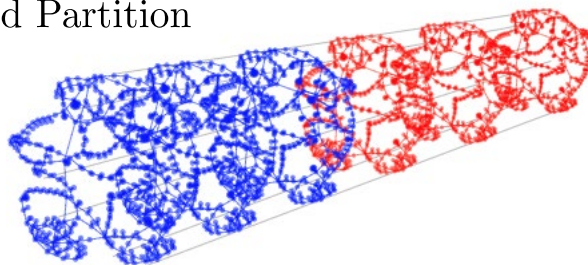


$$\begin{aligned} \{x_i^{(\ell+1)}\}_{i \in V_k} &= R_k \operatorname{argmin} f(\{x_i\}_{i \in V_k^\omega}; \{x_i^{(\ell)}\}_{i \notin V_k^\omega}) \\ \text{s.t.} \quad & c(\{x_i\}_{i \in V_k^\omega}; \{x_i^{(\ell)}\}_{i \notin V_k^\omega}) \geq 0 \end{aligned}$$

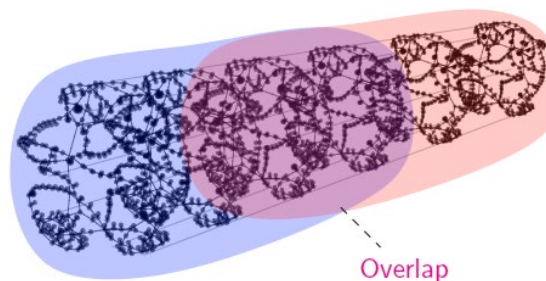
Overlapping Schwarz for NLP

$$\begin{aligned} \min_{\{x_i\}_{i \in V}} \quad & \sum_{i \in V} f_i(\{x_j\}_{j \in N_G[i]}) \\ \text{s.t.} \quad & c_i(\{x_j\}_{j \in N_G[i]}) \geq 0, \quad i \in V \end{aligned}$$

Standard Partition



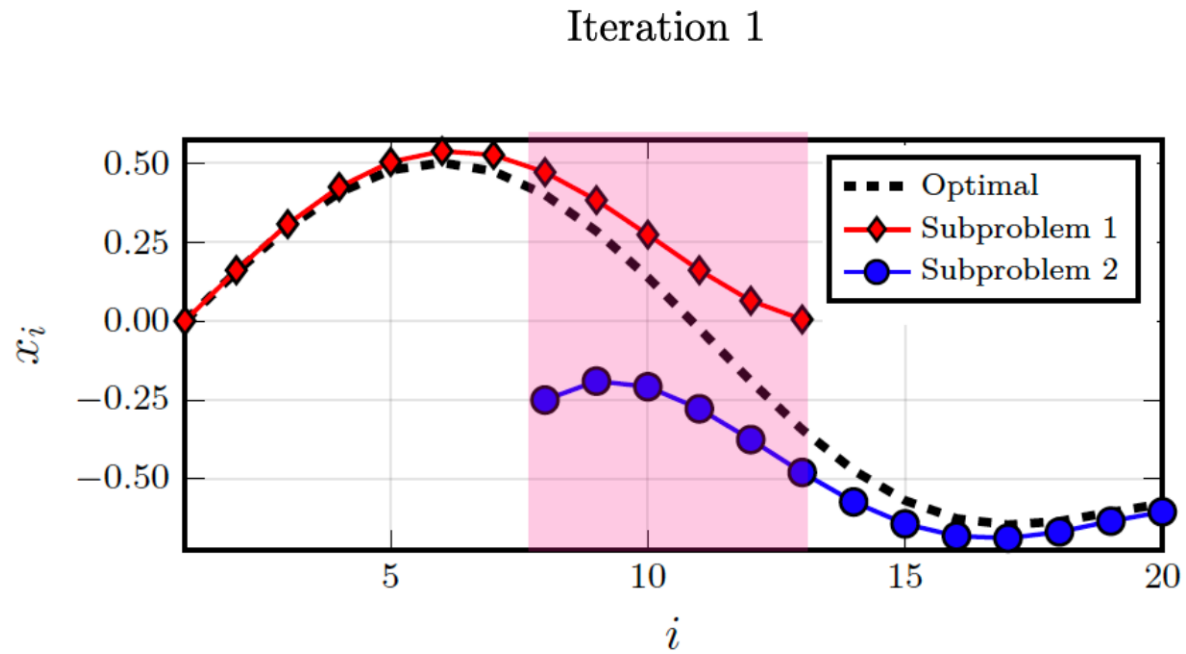
Overlapping Partition



$$\begin{aligned} \{x_i^{(\ell+1)}\}_{i \in V_k} &= R_k \operatorname{argmin} f(\{x_i\}_{i \in V_k^\omega}; \{x_i^{(\ell)}\}_{i \notin V_k^\omega}) \\ \text{s.t.} \quad & c(\{x_i\}_{i \in V_k^\omega}; \{x_i^{(\ell)}\}_{i \notin V_k^\omega}) \geq 0 \end{aligned}$$

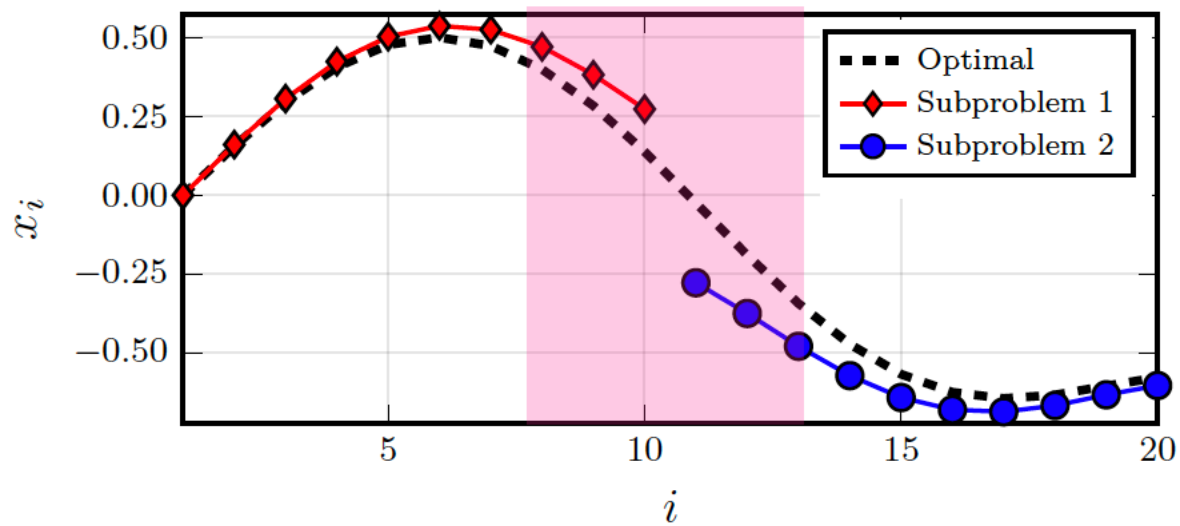
- Key:**
- Linear Local Convergence (Rate Improves *Exponentially* with Overlap)
 - *Exponential Decay of Sensitivity* (EDS) Guarantees Convergence.
 - Schwarz Can be Used Within Interior-Point Solver (as Linear/QP Solver)

EDS Guarantees Convergence



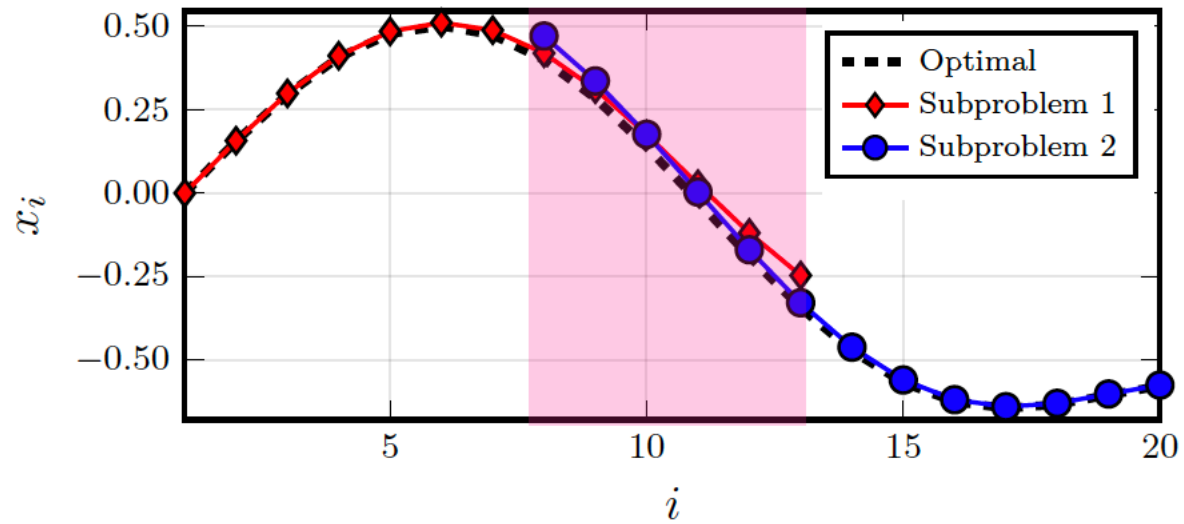
EDS Guarantees Convergence

Iteration 1 (After Restriction)



EDS Guarantees Convergence

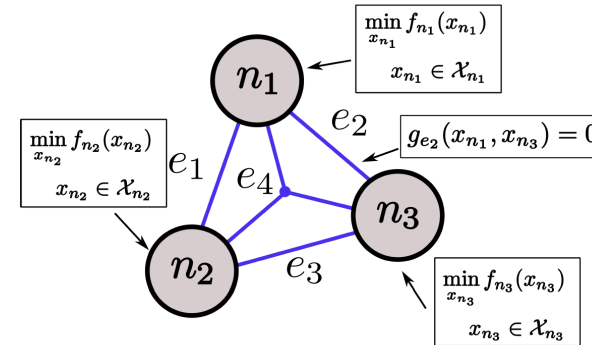
Iteration 2



Software

$$\begin{aligned} \min_{\{x_i\}_{i \in V}} \quad & \sum_{i \in V} f_i(\{x_j\}_{j \in N_G[i]}) \\ \text{s.t.} \quad & c_i(\{x_j\}_{j \in N_G[i]}) \geq 0, \quad i \in V \end{aligned}$$

$\Leftrightarrow$



```
using Plasmo
using Plots
using Ipopt

T = 100 #number of time points
d = sin.(1:T) #disturbance

#Create an OptiGraph
graph = OptiGraph()

#Add nodes for states and controls
@optinode (graph, state[1:T])
@optinode (graph, control[1:T-1])

#Add state variables
for (i,node) in enumerate(state)
    @variable (node,x)
    @constraint (node, x >= 0)
    @objective (node, Min, x^2)
end

#Add control variables
for node in control
    @variable (node,u)
    @constraint (node, u >= -1000)
    @objective (node, Min, u^2)
end

#Initial condition
n1 = state[1]
@constraint (n1, n1[1:x] == 0)

#Dynamic coupling
@linkconstraint (graph, [t = 1:T-1], state[t+1][:x] == state[t][:x] +
    control[t][:u] + d[t])

#Optimize with Ipopt
ipopt = Ipopt.Optimizer
optimize!(graph, ipopt)

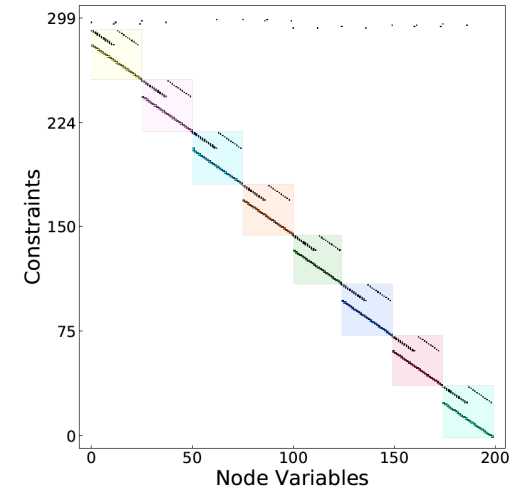
#Plot result structure
plt_graph4 = plot(graph,
    layout_options = Dict(:tol => 0.1, :iterations => 500),
    linealpha = 0.2, markersize = 6)
```

Graph Building

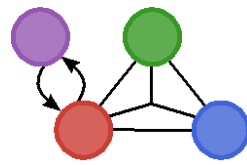
Graph Structure



Jacobian Structure



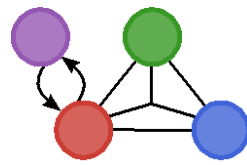
Plasmo.jl



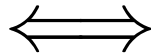
```
1 using Plasmo, Ipopt
```

- Plasmo.jl provides a **user-friendly** syntax similar to JuMP.jl
- Each node embeds a JuMP.jl optimization model
- Node subproblems linked using hyperedges

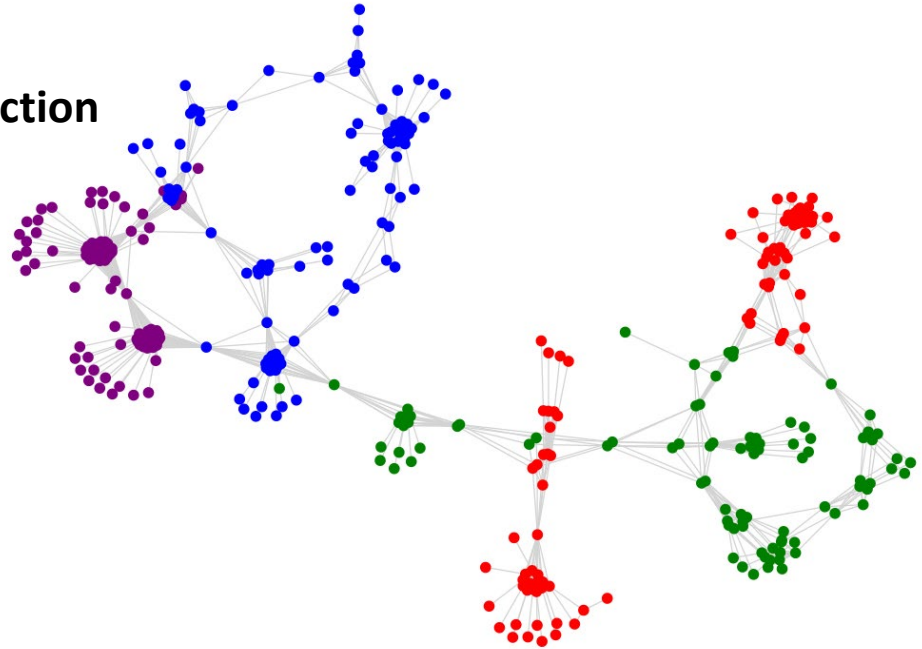
Graph Visualization



System

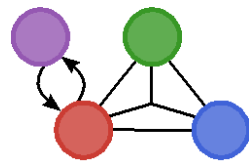


**Graph
Abstraction**

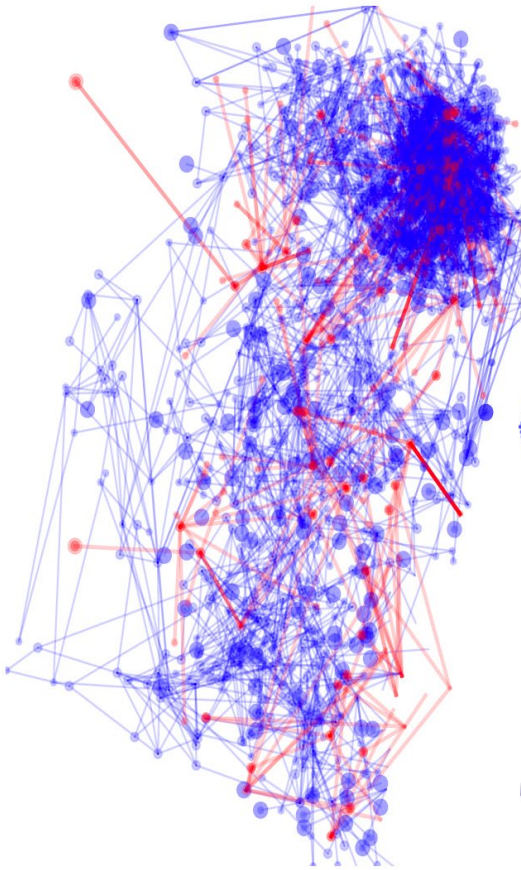


- Graph Abstraction Provides Insights (e.g., Connectivity, Vulnerability)

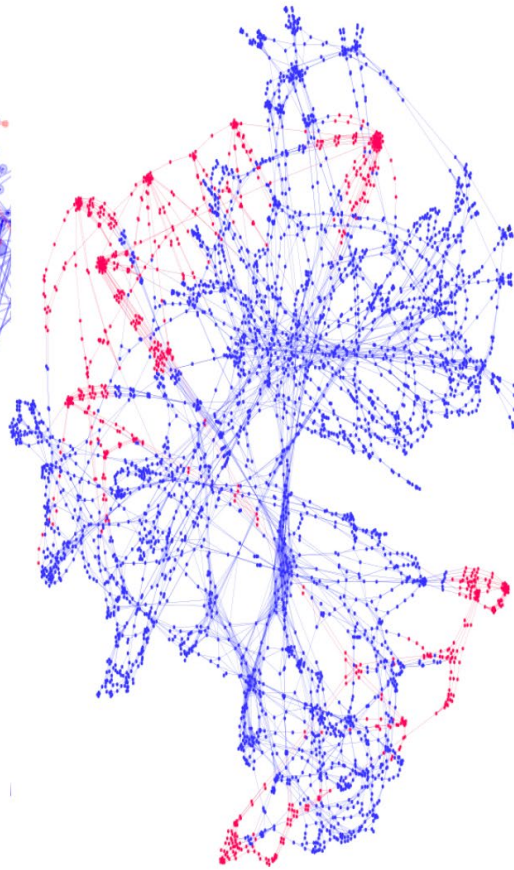
Graph Visualization



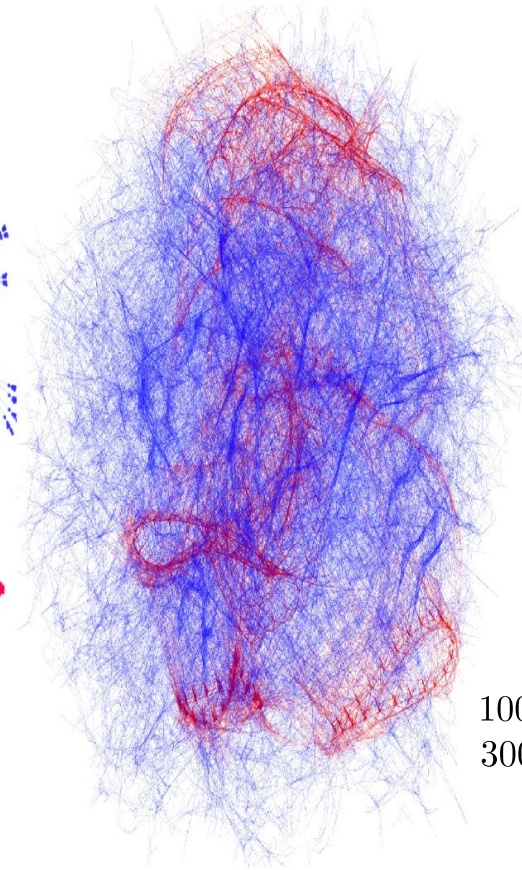
- Plasmo.jl facilitates Graph Manipulation, Visualization, and Decomposition



Gas-Electric Network



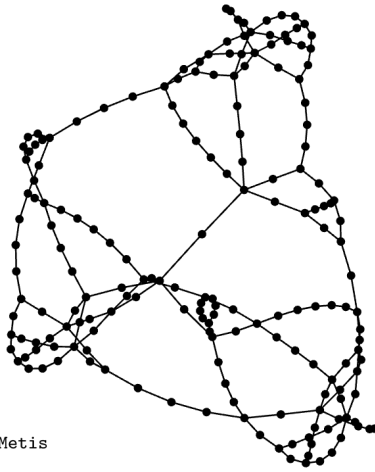
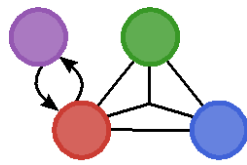
Space Unfolding



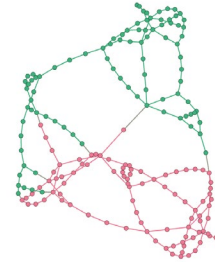
Space-Time Unfolding

100,000 nodes
300,000 edges

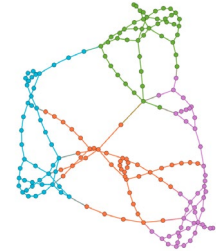
Graph Partitioning



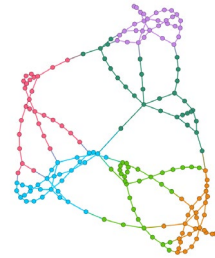
$n_partitions = 2$



$n_partitions = 4$

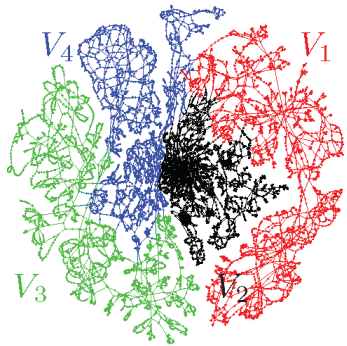


$n_partitions = 6$

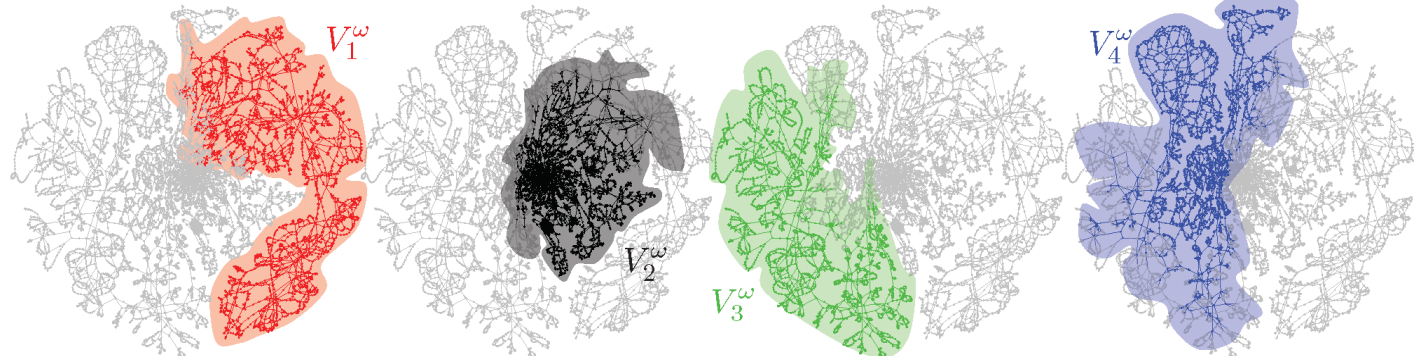


```
1 using Plasm, Metis
2
3 g = OptiGraph()
4 ....
5
6 partition_vector = Metis.partition(
7     simplegraph, n_partitions, alg = :KWAY)
8 ....
9 partition = Partition(hypergraph,
10     partition_vector, hyper_map)
11
12 apply_partition!(g, partition)
```

Standard Partition

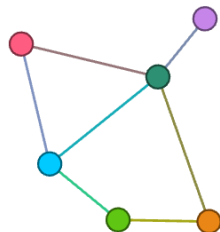


Overlapping Partition

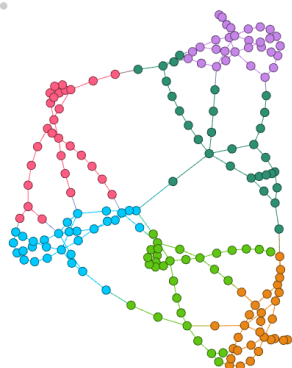


Graph Aggregation/Coarsening

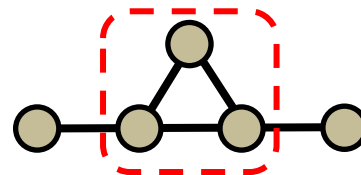
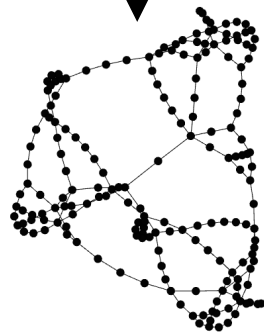
Coarse



Middle



Fine

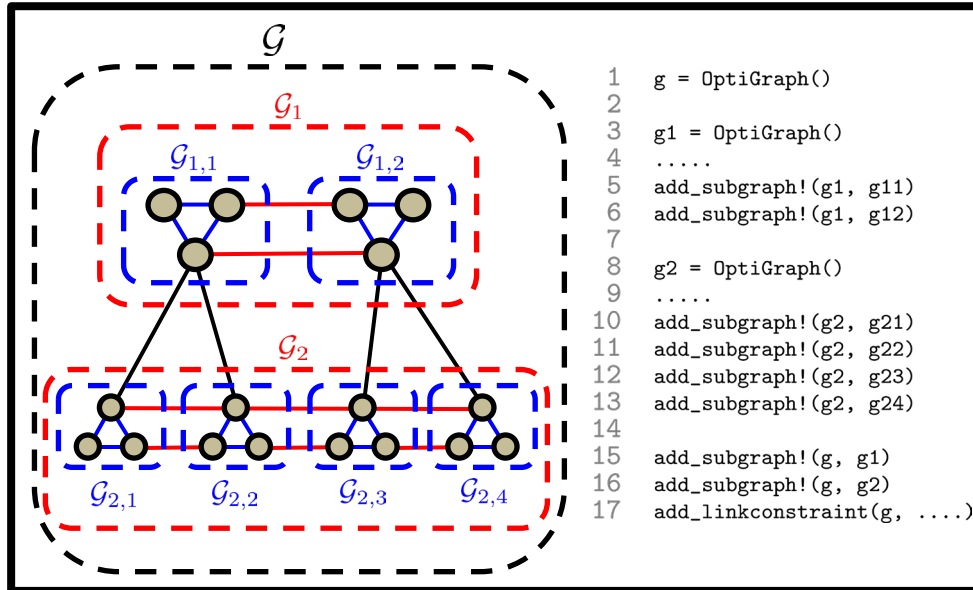
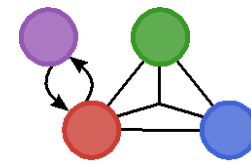


Cyclic Graph



Acyclic Graph

Hierarchical Graphs

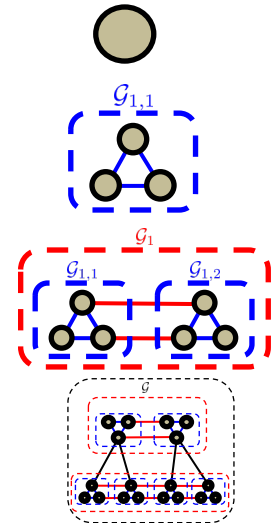


optimize!(g11[:n1]) →

optimize!(g11) →

optimize!(g1) →

optimize!(g) →



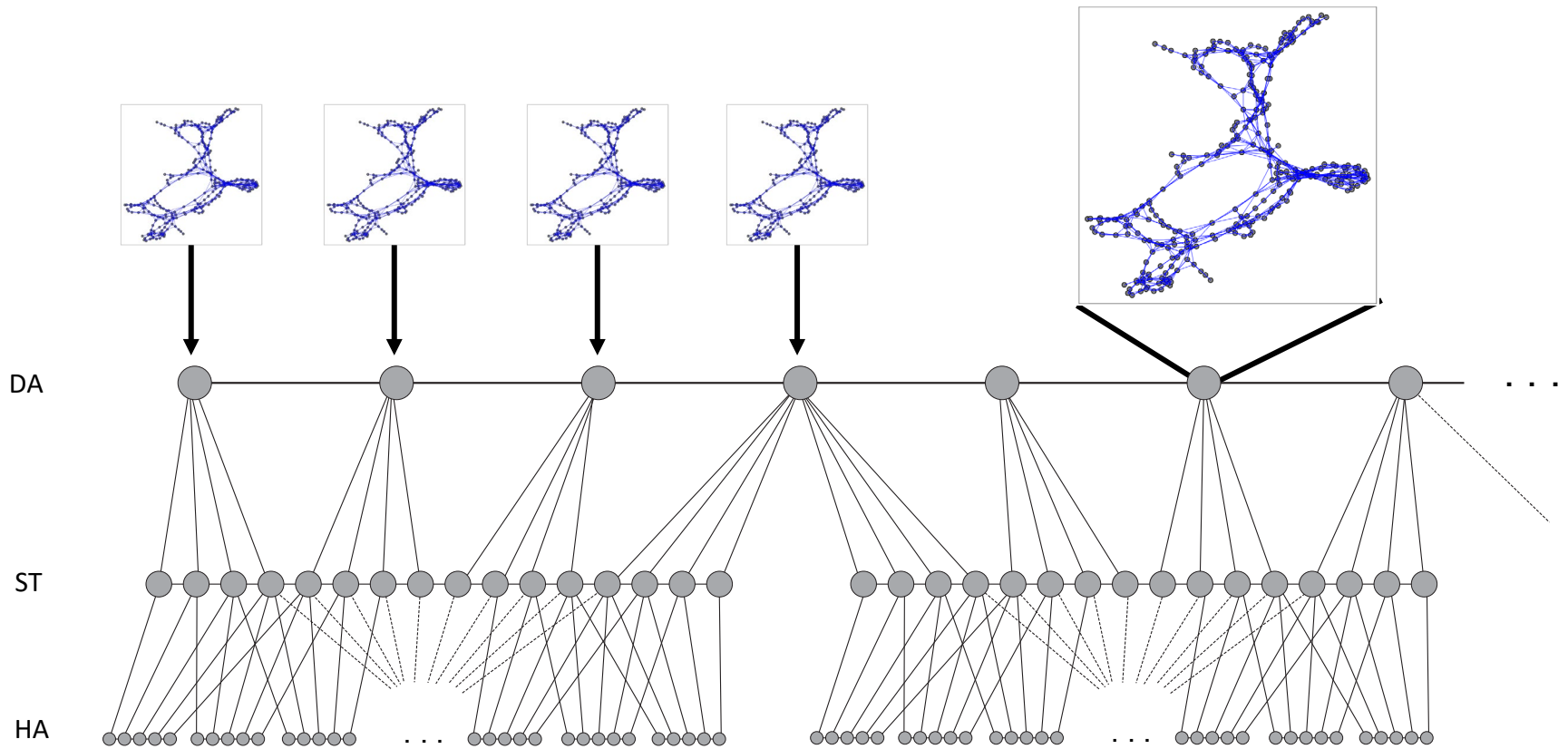
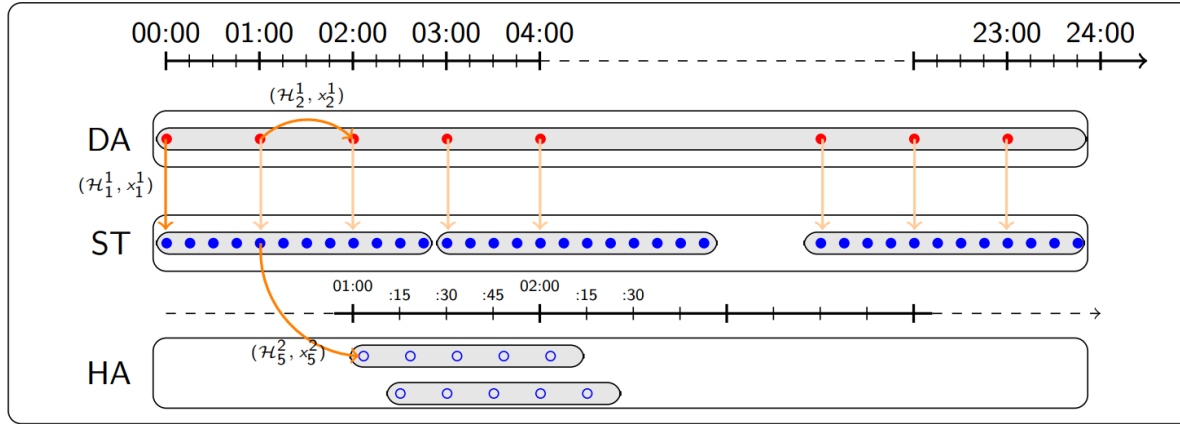
- Nodes can embed full graphs
- Enables **modular & hierarchical** modeling
- Can **solve subgraphs** all-at-once, individually, or as communities/partitions

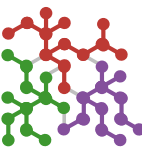
Multi-Scale MPC as Hierarchical Graphs

Day-Ahead
Unit Commitment

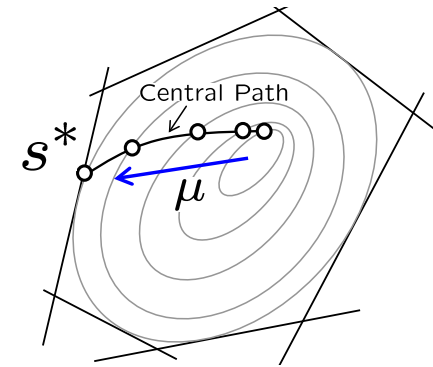
Short-Term
Unit Commitment

Hour-Ahead
Economic Dispatch

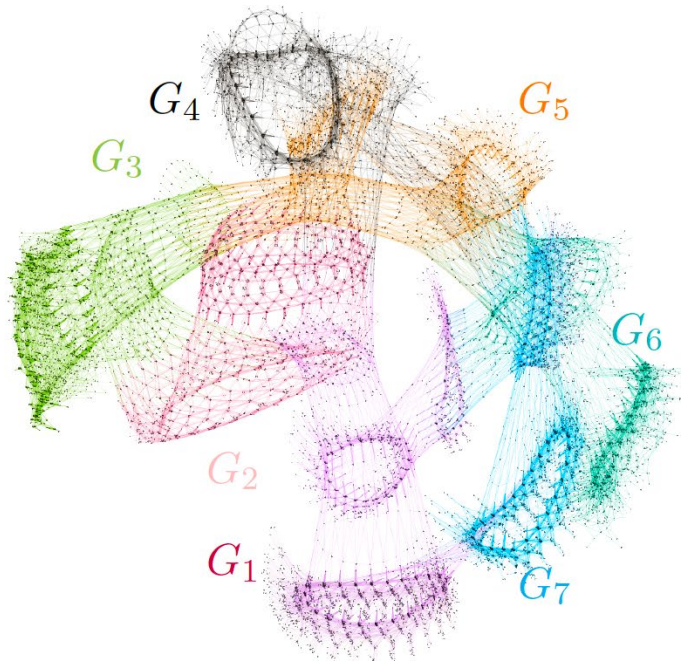




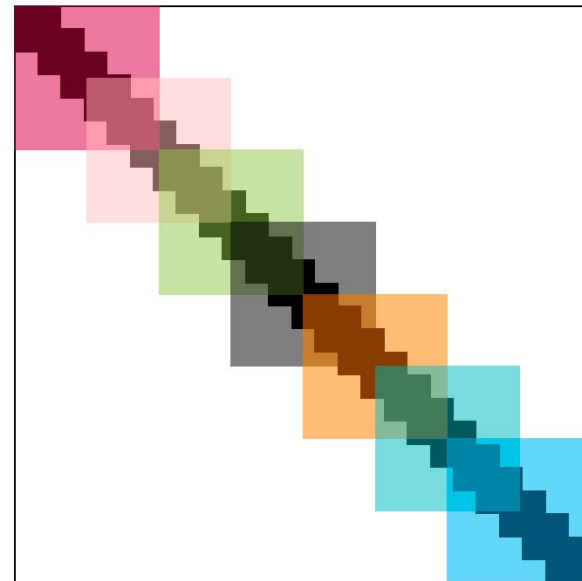
$$\begin{aligned} \min_{\{x_i\}_{i \in V}} \quad & \sum_{i \in V} f_i(\{x_j\}_{j \in N_G[i]}) \\ \text{s.t.} \quad & c_i(\{x_j\}_{j \in N_G[i]}) \geq 0, \quad i \in V \end{aligned}$$



- MadNLP.jl is a Julia-Based Interior-Point Optimizer
- Exploits Graph Structures at Linear Algebra Level (e.g., Schwarz, Schur)

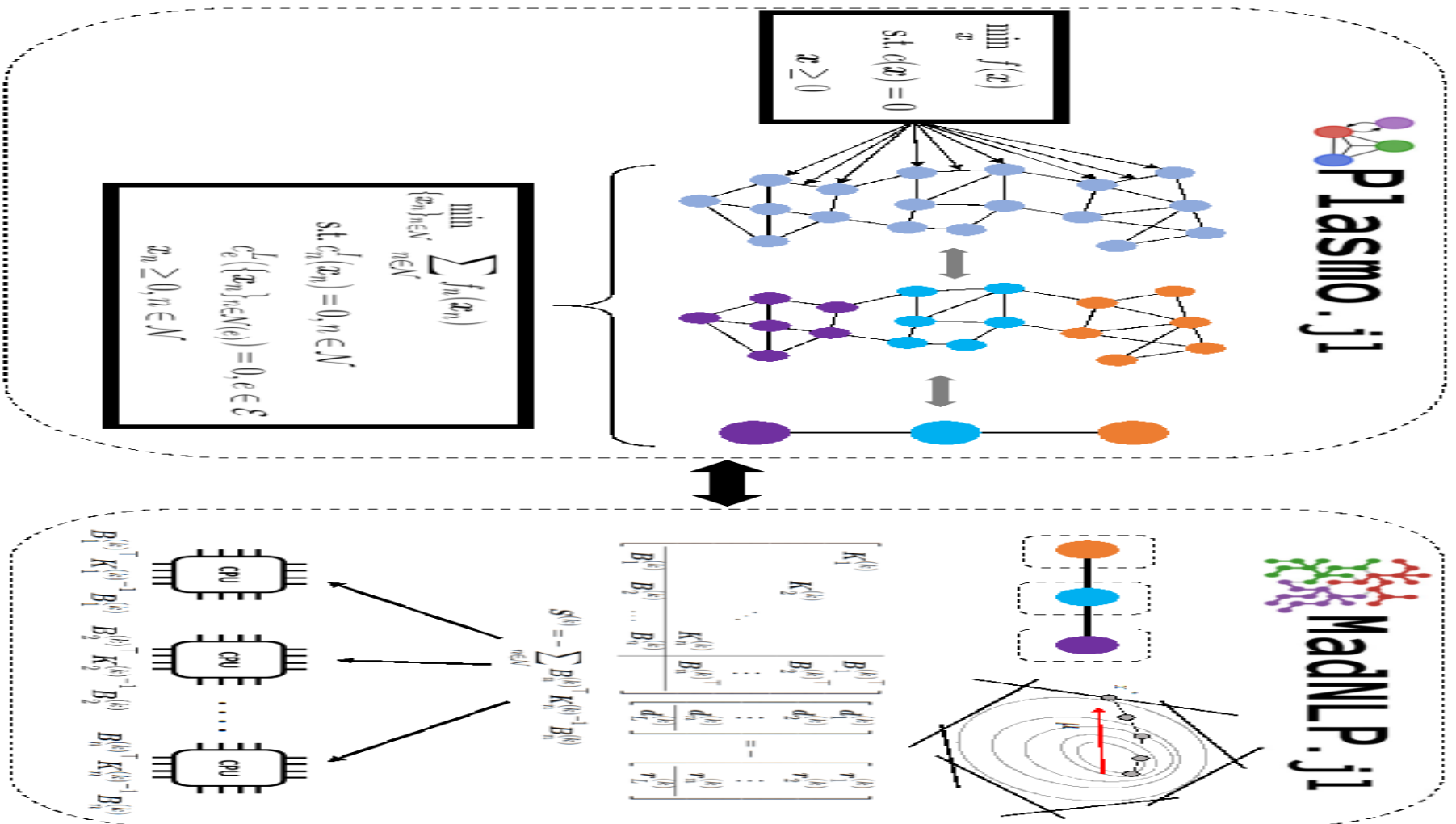


Problem Graph



Linear Algebra (KKT) System

Plasmo.jl + MadNLP.jl

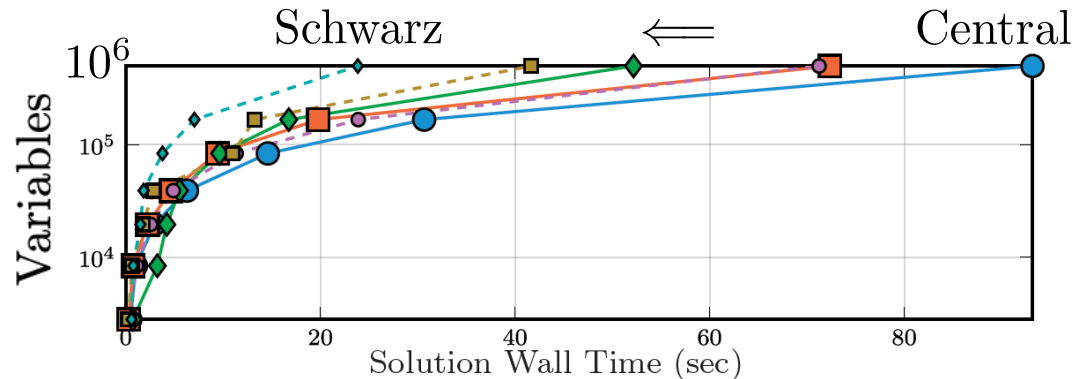


Plasmo.jl + MadNLP.jl

- Optimal Control of Gas Network (NLP with 10^6 Variables)
- Schwarz Decomposition Accelerates Solution by 300%



$$\begin{aligned}
 & \min_{\substack{\rho, \varphi^a, \varphi^-, \\ \alpha, s, d \in \mathbb{R}}} \sum_{t \in \mathcal{T}} \left(\sum_{(i,j) \in \mathcal{C}} \gamma P_{ijt}^a + \sum_{i \in \mathcal{R}} c_{it} s_{it} - \sum_{i \in \mathcal{D}} c_{it} d_{it} \right) \\
 & \text{s.t.} \quad \sum_{j \in \mathcal{N}(i)} f_{ijt}^a = \sum_{j \in \mathcal{R}(i)} s_{jt} - \sum_{j \in \mathcal{D}(i)} d_{jt}, \quad i \in \mathcal{N}, t \in \mathcal{T} \\
 & \quad \rho_i^{\min} \leq \rho_{it} \leq \rho_i^{\max}, \quad i \in \mathcal{N}, t \in \mathcal{T} \\
 & \quad \rho_{it}^2 - \rho_{jt}^2 = -\frac{\lambda L}{D} \varphi_{ijt}^a |\varphi_{ijt}^a|, \quad (i,j) \in \mathcal{P}, t \in \mathcal{T} \\
 & \quad \hat{L}(\dot{\rho}_{jt} + \dot{\rho}_{it}) = -4\varphi_{ijt}^-, \quad (i,j) \in \mathcal{P}, t \in \mathcal{T} \\
 & \quad f_{ijt}^a(\rho_{it} - \rho_{jt}) \leq 0, \quad (i,j) \in \mathcal{C}, t \in \mathcal{T} \\
 & \quad \rho_{jt} = \alpha_{ijt} \rho_{it}, \quad (i,j) \in \mathcal{C}, t \in \mathcal{T} \\
 & \quad P_{ijt}^a \leq P_{ij}^{\max}, \quad (i,j) \in \mathcal{C}, t \in \mathcal{T} \\
 & \quad -f_{ij}^a \leq f_{ijt}^a \leq f_{ij}^a, \quad (i,j) \in \mathcal{C}, t \in \mathcal{T},
 \end{aligned}$$

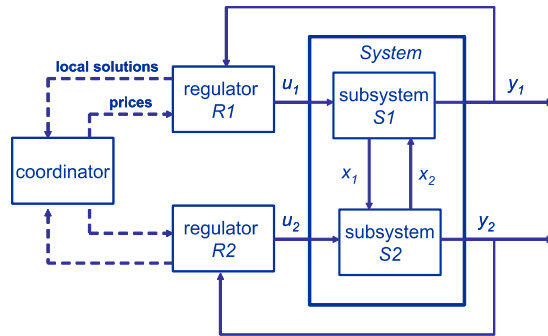


Cyber-Physical Systems

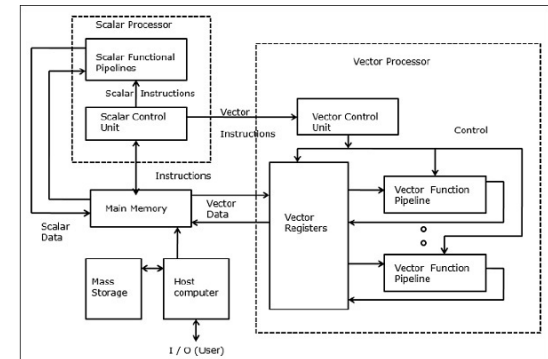
Modeling Cyber-Physical Systems

What is a General Mathematical Abstraction?

Control Architectures



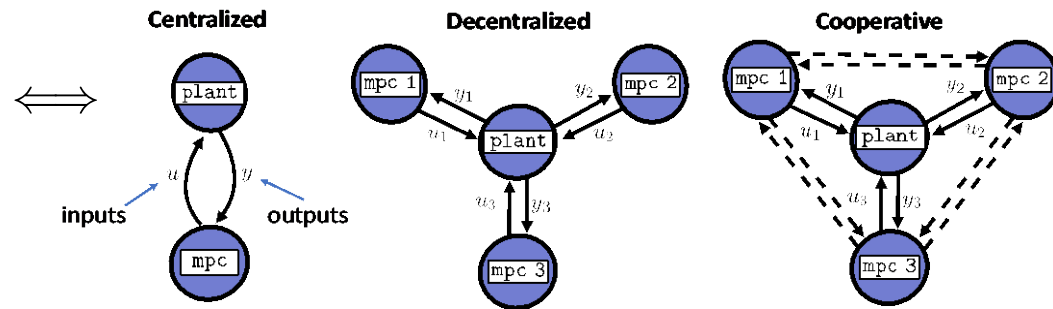
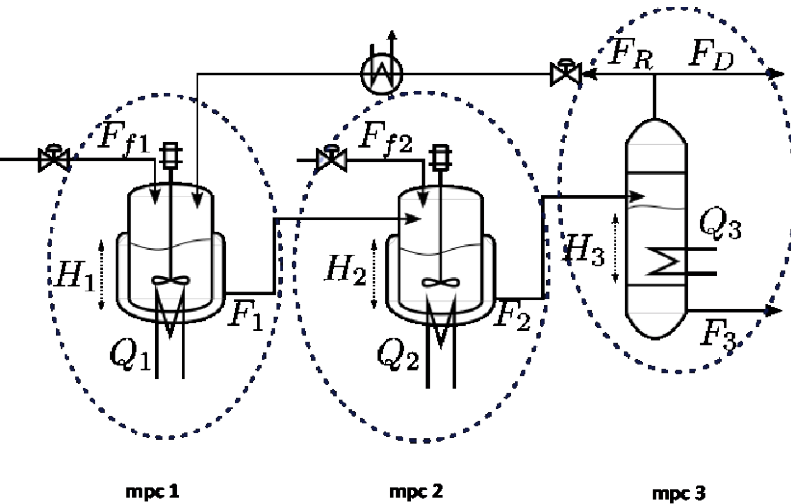
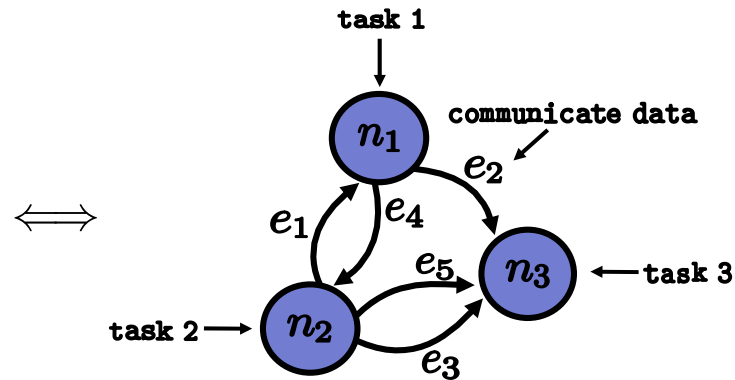
Computing Architectures



- Physical Layer are Unit Operations, Materials
- Cyber Layer are Sensors, Data, Controls, Computers...
- Cyber Layer Makes Decisions that Run Physical Layer
- **Issues:** Memory/Power, Communication, Latency, Security/Privacy, Resilience,...

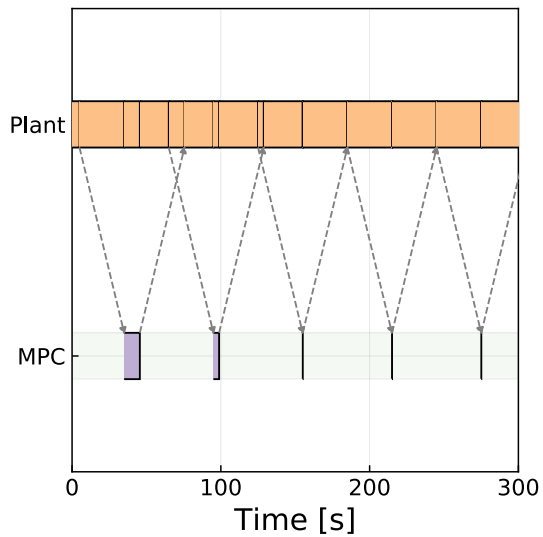
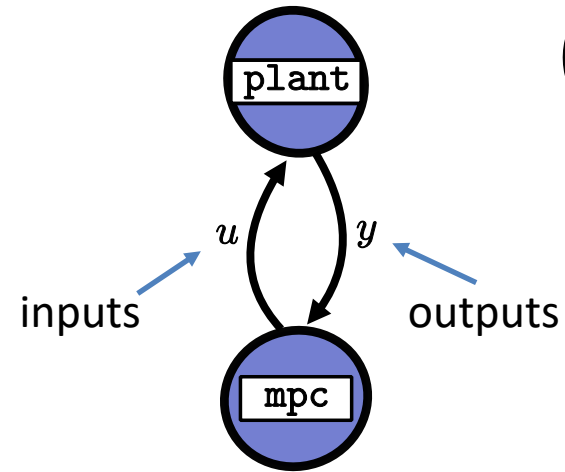
Cyber-Physical Systems as Computing Graphs

- Nodes are Computing Tasks
- Edges are Communication Channels
- Graph Captures Communication Topology

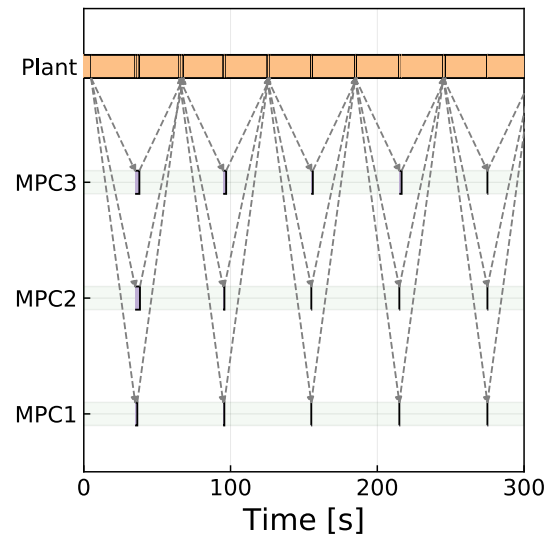
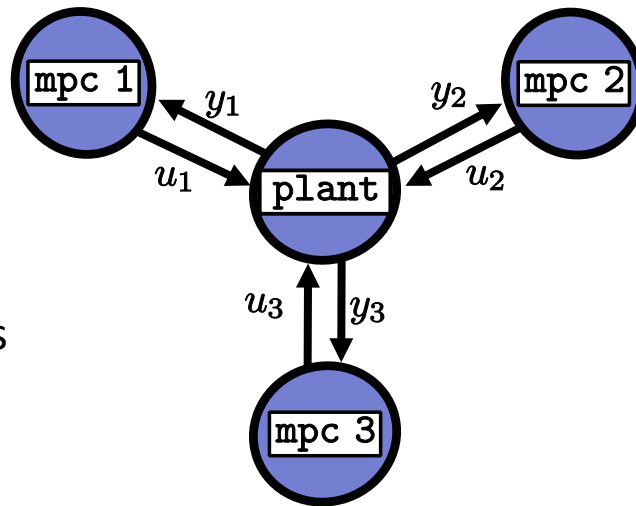


Simulating MPC Architectures

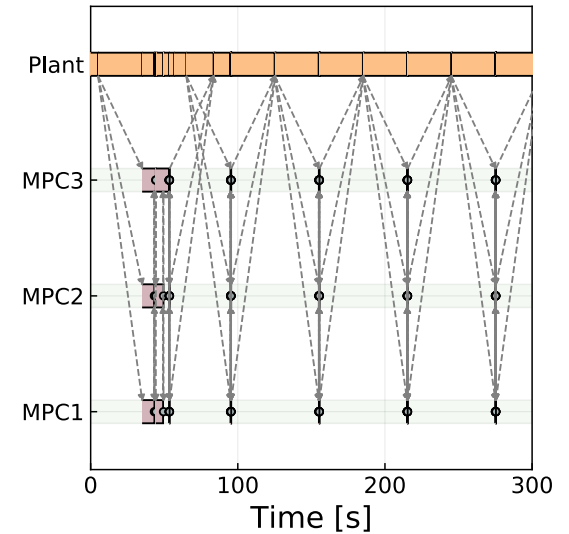
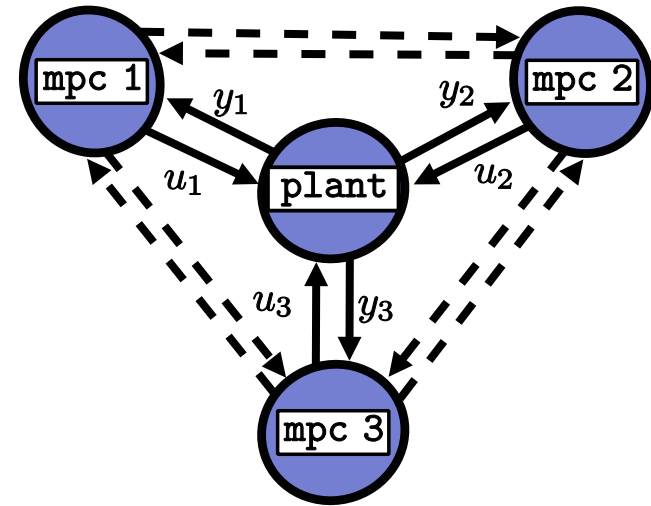
Centralized



Decentralized

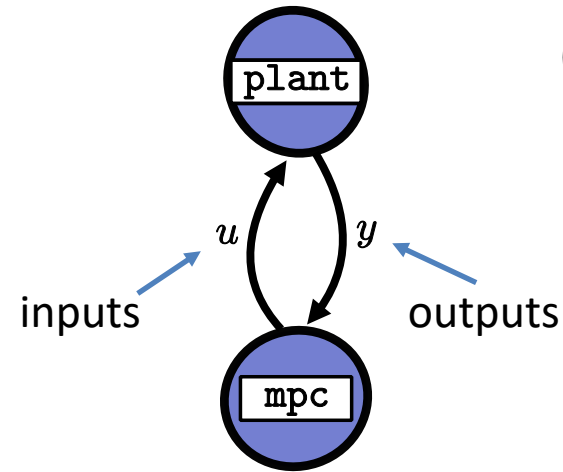


Cooperative

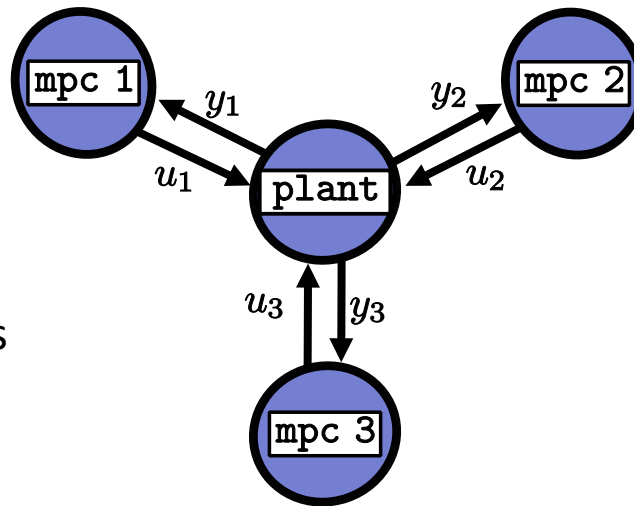


Simulating MPC Architectures

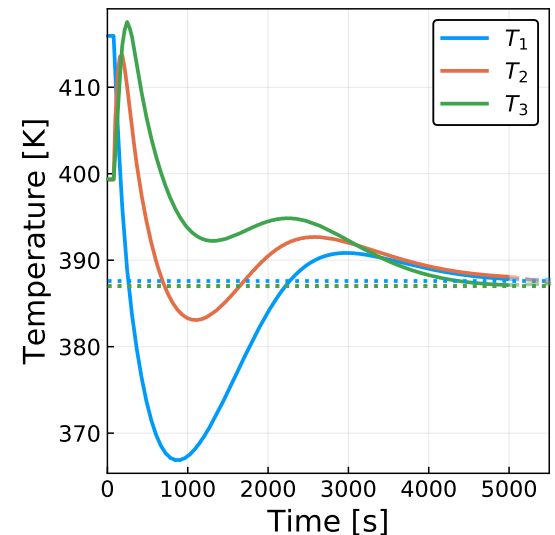
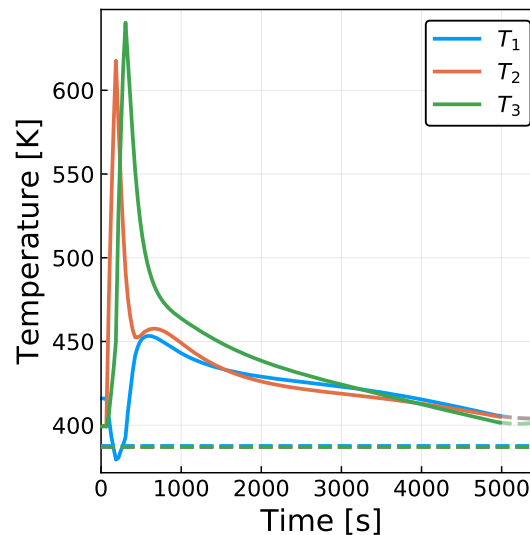
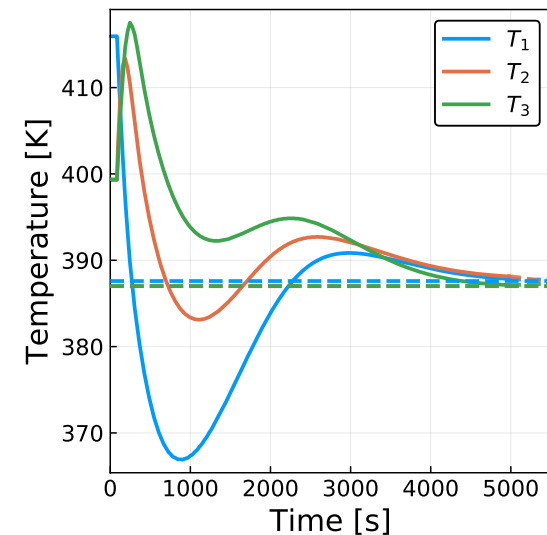
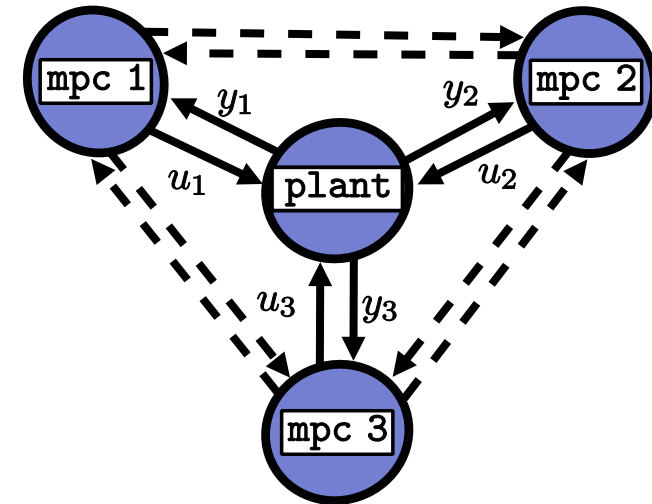
Centralized



Decentralized

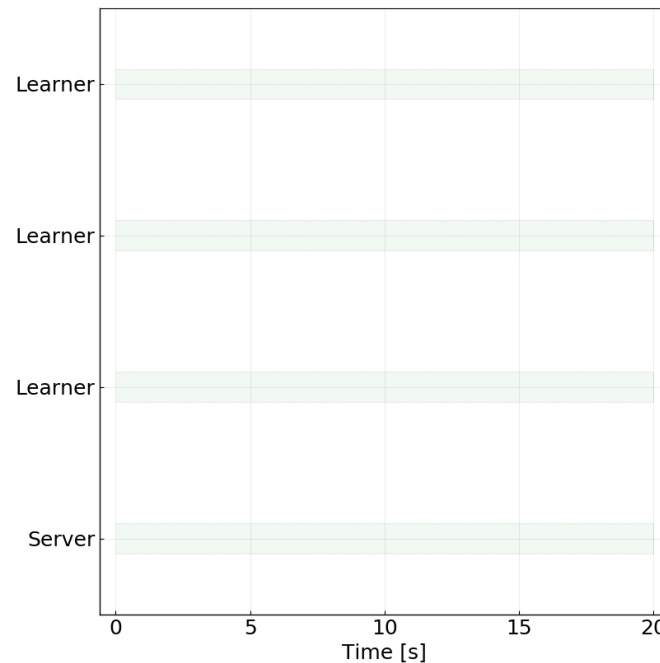
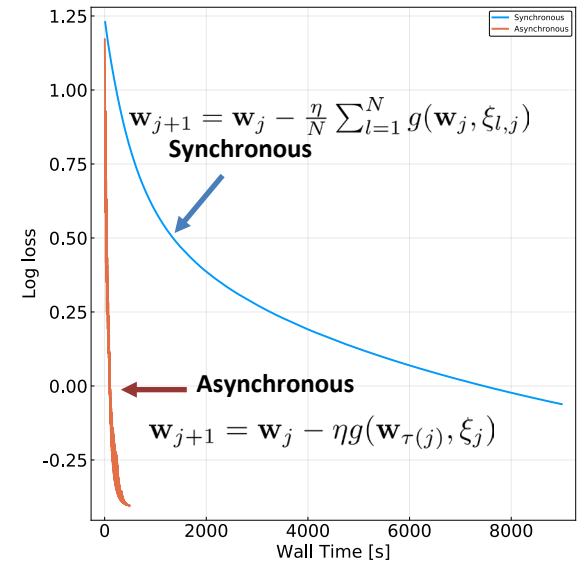
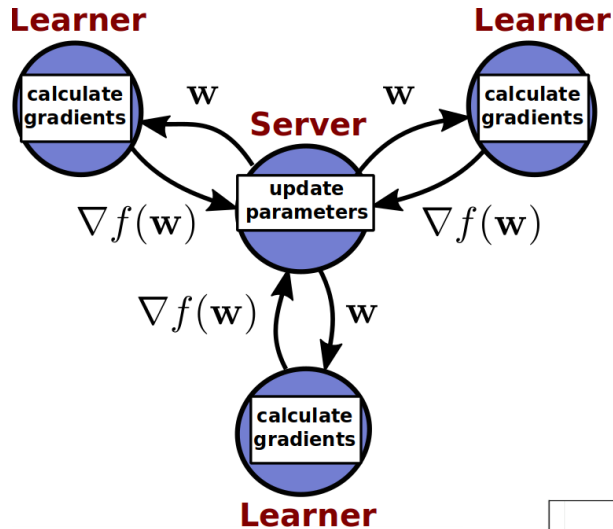


Cooperative

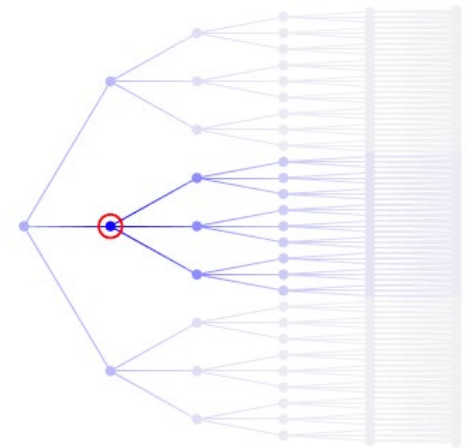


Key: Can simulate communication/computation latency & failures as well as energy usage.

Simulating Distributed Optimization Algorithms



Key: Can simulate behavior of algorithms on specific hardware.

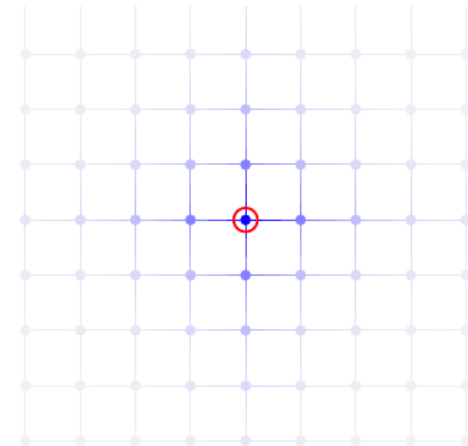
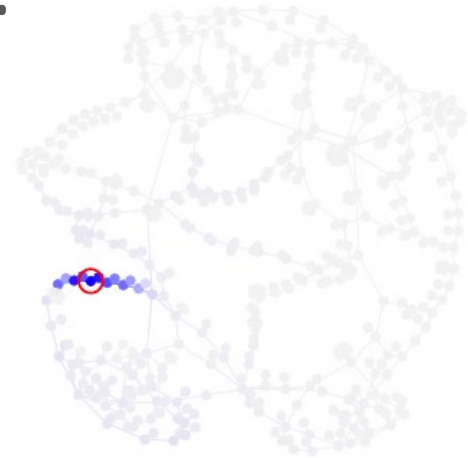


A Graph-Theoretic Perspective on Optimization: Theory, Modeling, Algorithms, and Applications

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University of Wisconsin-Madison

Mathematics and Computer Science Division
Argonne National Laboratory



Work with: Sungho Shin, Mihai Anitescu, Jordan Jalving, David Cole

References

Jalving, J., Cao, Y., & Zavala, V. M. (2019). **Graph-based modeling and simulation of complex systems.** *Computers & Chemical Engineering*, 125, 134-154.

Shin, S., Anitescu, M., & Zavala, V. M. (2022). **Exponential decay of sensitivity in graph-structured nonlinear programs.** *SIAM Journal on Optimization*, 32(2), 1156-1183.

Shin, S., & Zavala, V. M. (2021). **Controllability and observability imply exponential decay of sensitivity in dynamic optimization.** *IFAC-PapersOnLine*, 54(6), 179-184.

Shin, S., Zavala, V. M., & Anitescu, M. (2020). **Decentralized schemes with overlap for solving graph-structured optimization problems.** *IEEE Transactions on Control of Network Systems*, 7(3), 1225-1236.

Shin, S., Coffrin, C., Sundar, K., & Zavala, V. M. (2021). **Graph-based modeling and decomposition of energy infrastructures.** *IFAC-PapersOnLine*, 54(3), 693-698.

Grüne, L., Schaller, M., & Schiela, A. (2020). **Exponential sensitivity and turnpike analysis for linear quadratic optimal control of general evolution equations.** *Journal of Differential Equations*, 268(12), 7311-7341.

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Shin, S., Faulwasser, T., Zanon, M., & Zavala, V. M. (2019). **A parallel decomposition scheme for solving long-horizon optimal control problems.** In *2019 IEEE 58th Conference on Decision and Control (CDC)* (pp. 5264-5271). IEEE.

<https://github.com/zavalab/Plasmo.jl>

<https://github.com/MadNLP/MadNLP.jl>