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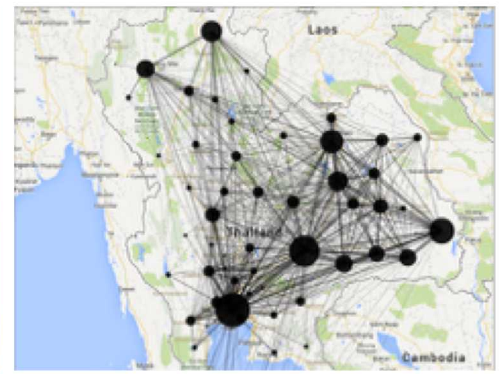

Algorithms, Architectures, and Applications: High-Performance Mathematical Programming Approaches for Improved Safety and Security

Carl D. Laird

PMTS, Discrete Mathematics and Optimization, Center for Computing Research

Associated Professor, Davidson School of Chemical Engineering, Purdue University

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Process Systems Engineering: Computer Aided Decision Making

$$\begin{aligned} \min_{x} \quad & f(x) && \longleftarrow \text{Objective Function} \\ \text{s.t.} \quad & c(x) = 0 && \longleftarrow \text{Equality Constraints} \\ & d^L \le d(x) \le d^U && \longleftarrow \text{Inequality Constraints} \\ & x^L \le x \le x^U && \longleftarrow \text{Variable Bounds} \end{aligned}$$

Mathematical programming (i.e. Optimization)

Problem types classified according to:

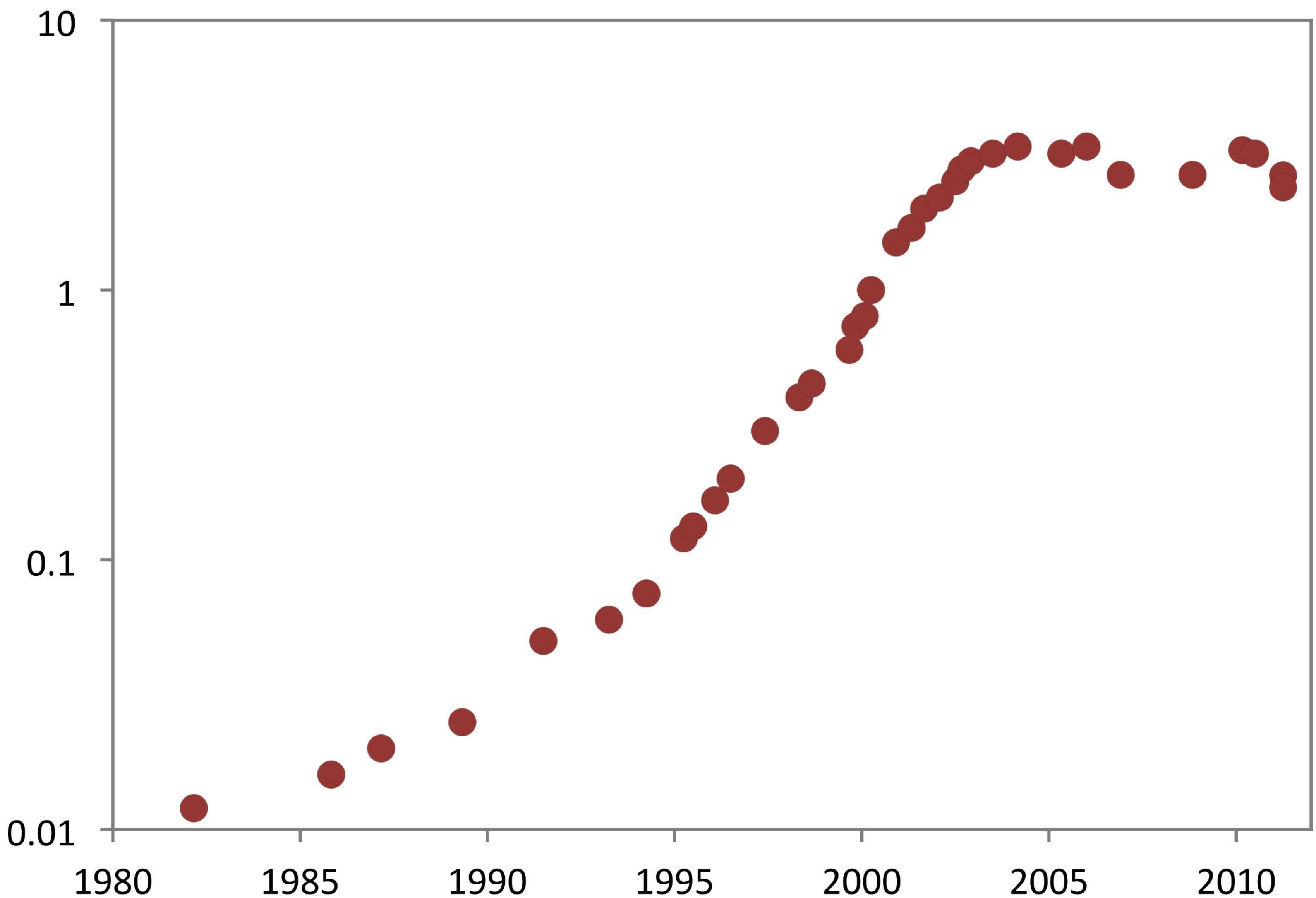
- Linearity/Nonlinearity of objective and constraints
- Continuous/Discrete/Mixed variables

LP, QP, NLP, MILP, MINLP

Useful for much more than… "optimization"

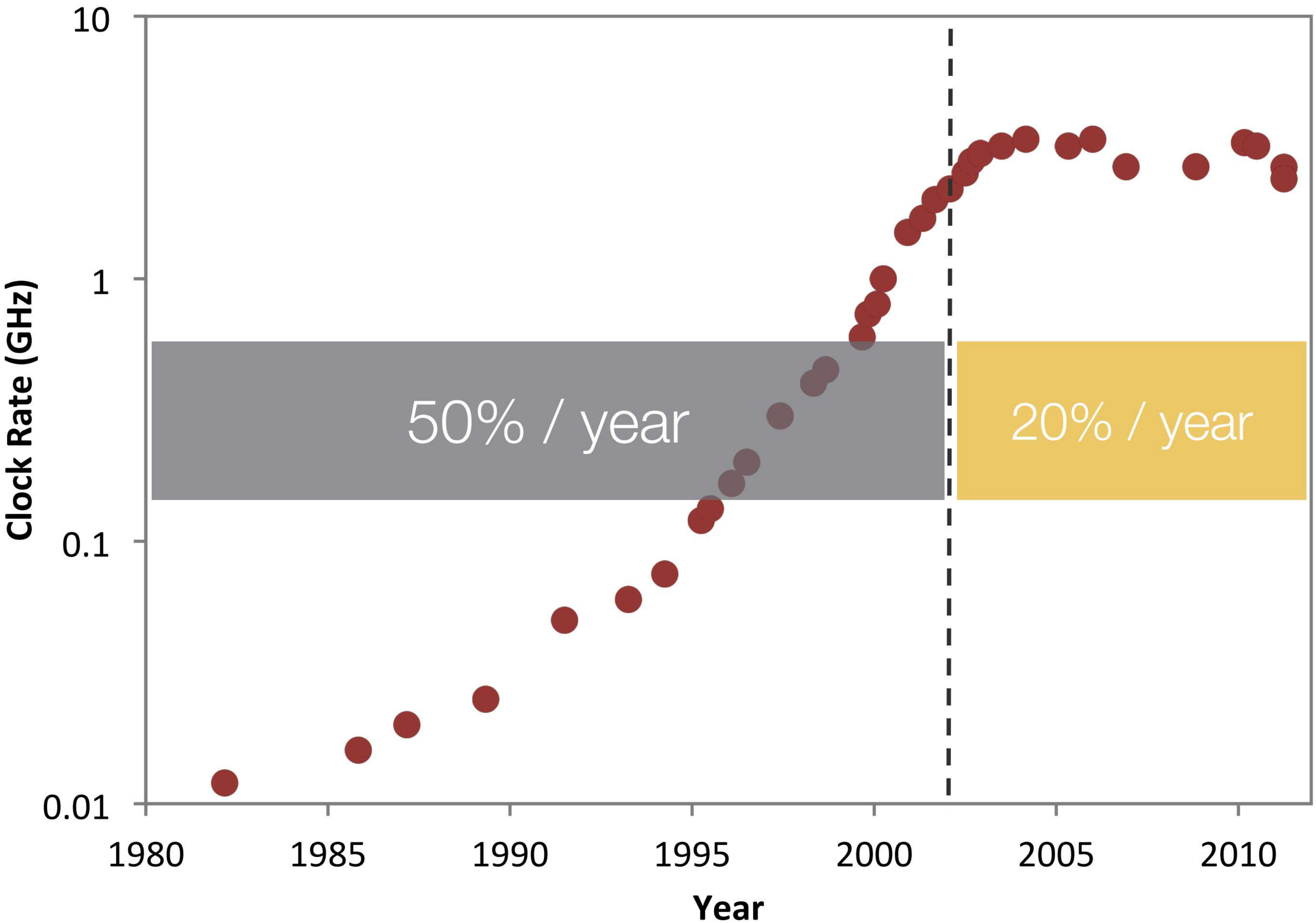
Solve relevant science and engineering problems using advanced modeling, mathematical programming (optimization), and high-performance computing

Landscape of Desktop Scientific Computing



[Steven Edwards, Columbia University]

Landscape of Desktop Scientific Computing



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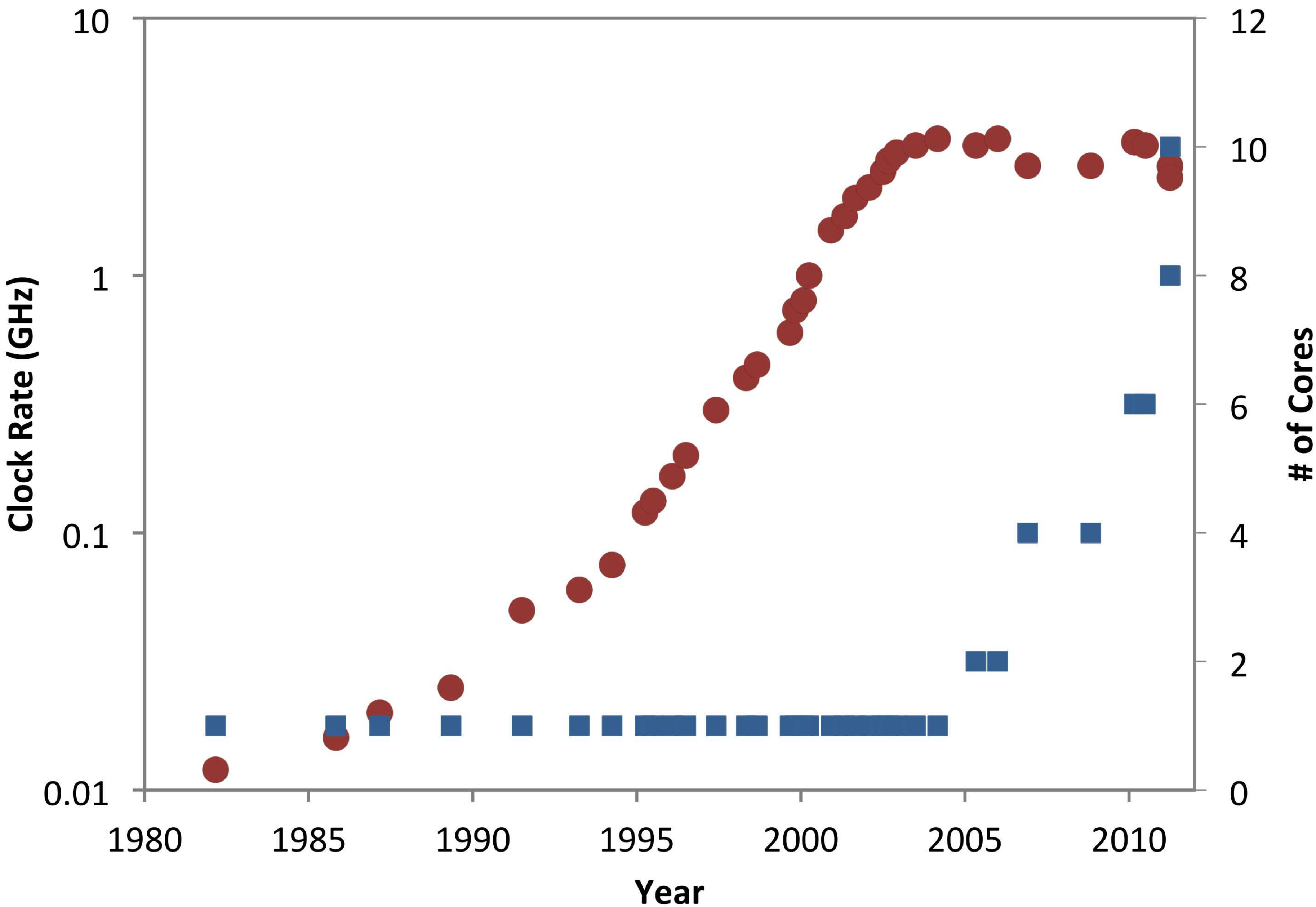


Intel Tick-Tock architecture development model

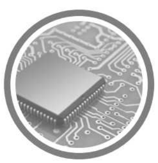
2 designs at each feature size

No more free lunch…
- ½ hardware
- ½ algorithms

65 nm	Tick	Early 2006: Presler
	Tock	Late 2006: Merom
45 nm	Tick	Late 2007: Penryn
	Tock	Late 2008: Nehalem
32 nm	Tick	Early 2010: Westmere
	Tock	Early 2011: Sandy Bridge
22 nm	Process	Early 2012: Ivy Bridge
	Architecture	Mid 2013: Haswell
	Optimization	Mid 2014: Haswell refresh
14 nm	Tick	Late 2014: Broadwell
	Tock	Mid 2015: Skylake
		Early 2017: Kaby Lake
		Late 2017: Coffee Lake


Applications

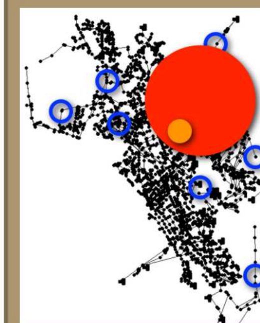

Adoption


Architectures


Algorithms

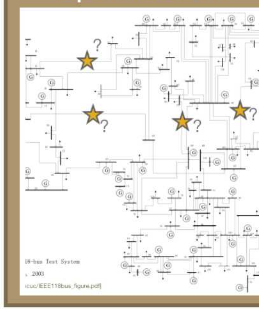
EPA, Sandia

Water Security



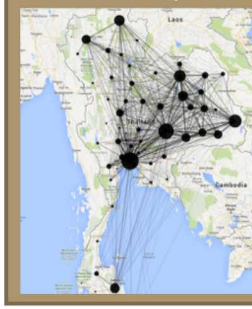
FERC, Sandia

Powergrid Optimization



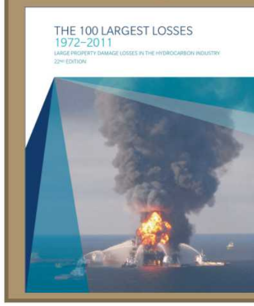
U. Florida, Hopkins

Infectious Disease Spread



P2SAC, MKOPSC

Safety Systems Design



High-level modeling languages and open-source software (Pyomo, IPOPT, WST, WNTR, CHAMA, EGRET)

Optimization algorithms (NLP, MINLP, SP), Numerical analysis, Problem formulation

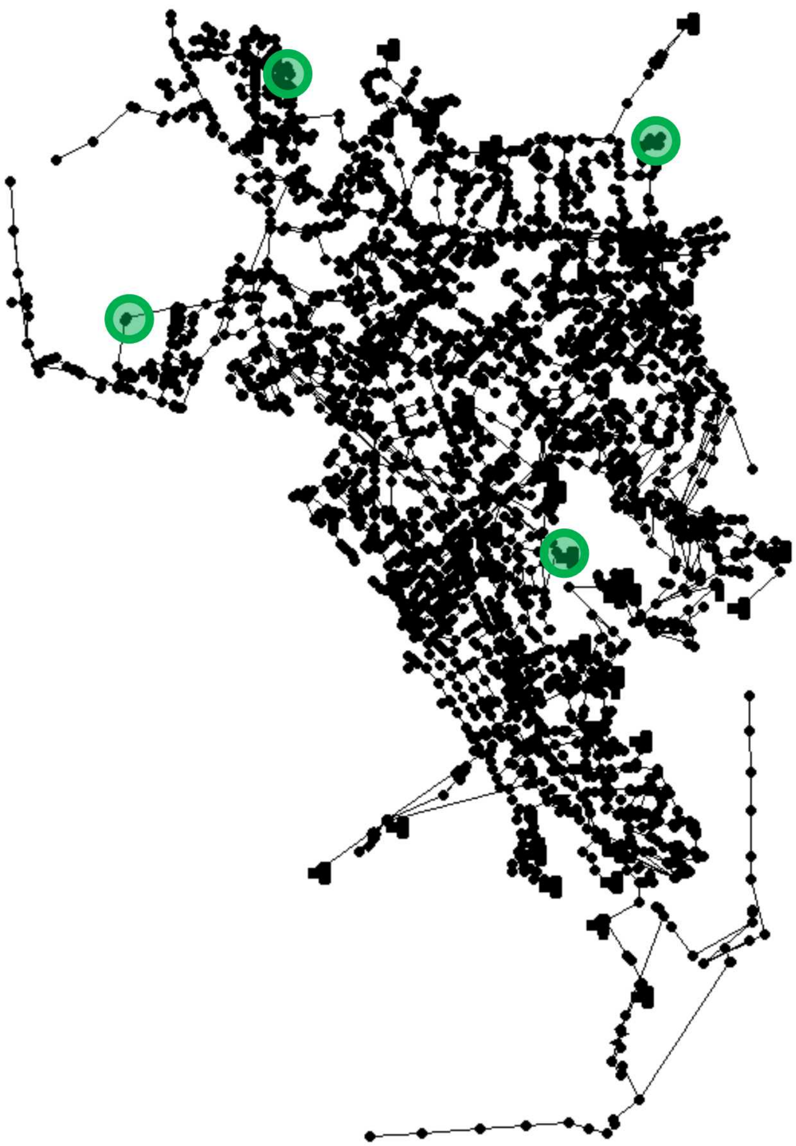
Scientific computing, parallel computing, software development

Protecting Drinking Water Infrastructure

Water distribution systems

- Large networks of junctions and pipes
- Vulnerable to chemical and biological contamination

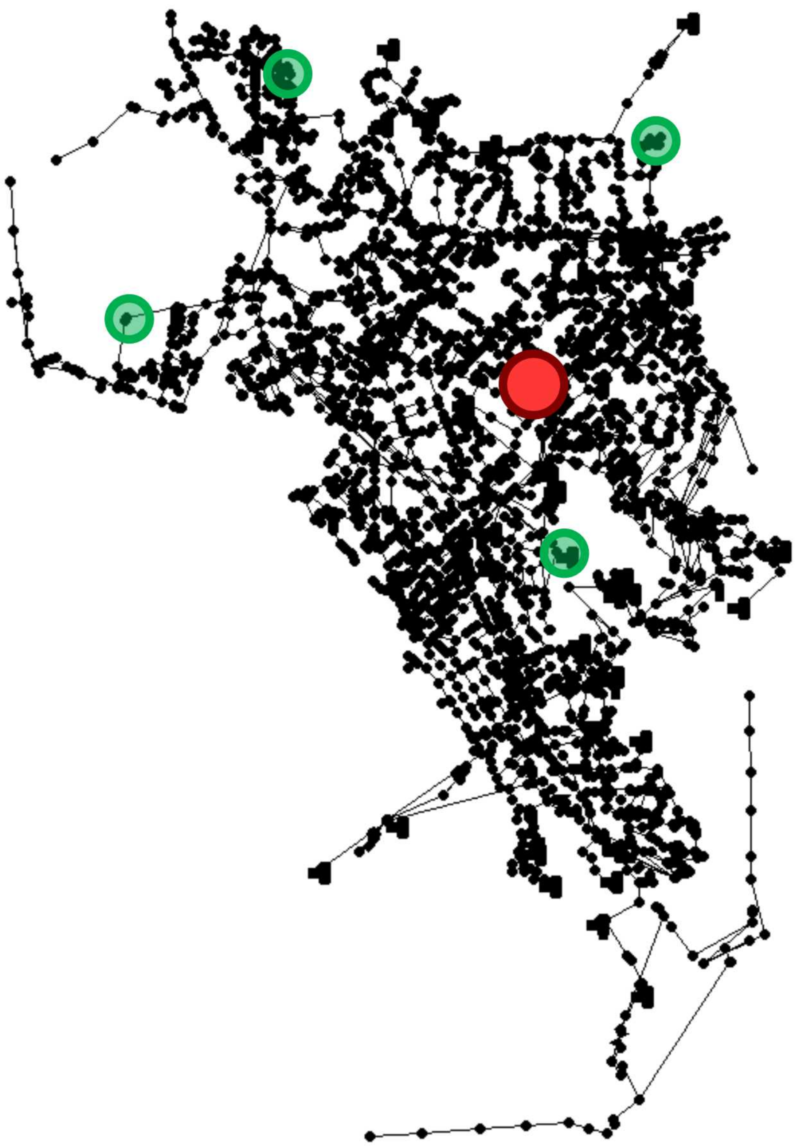
Early Warning and Response System



Fixed set of sensors

- What technology?
- Where will they be placed? How many?

Early Warning and Response System



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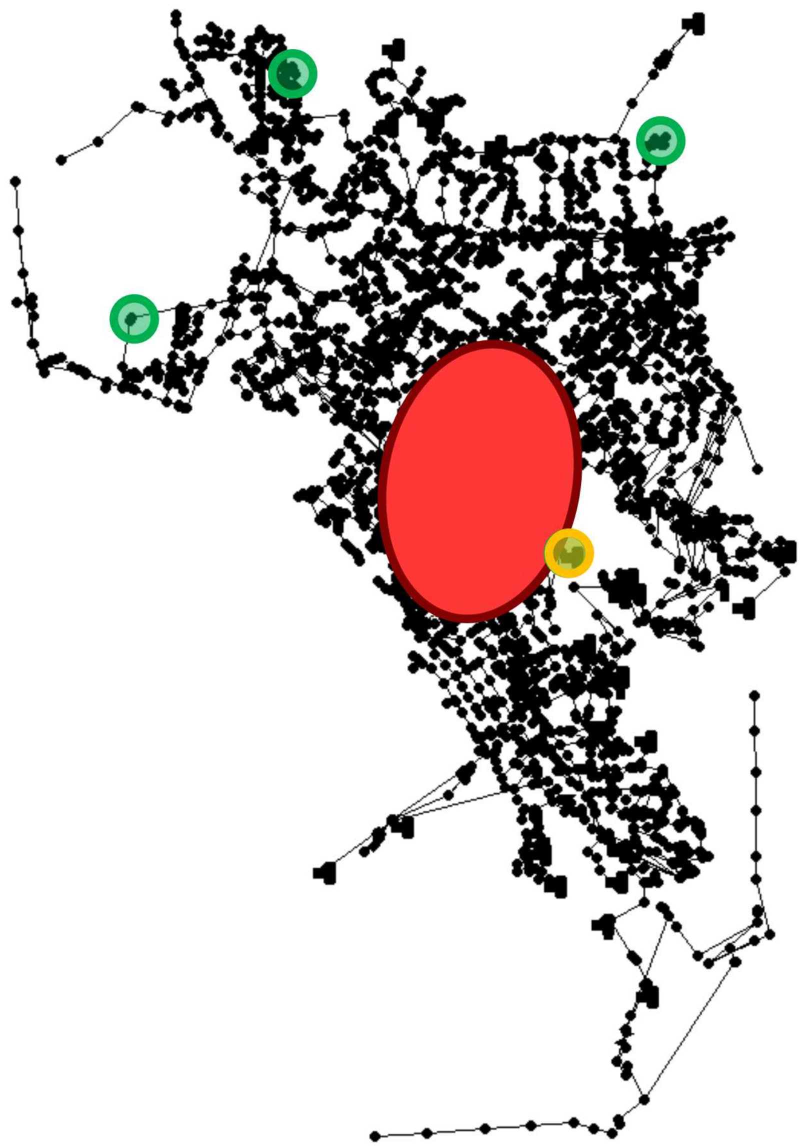

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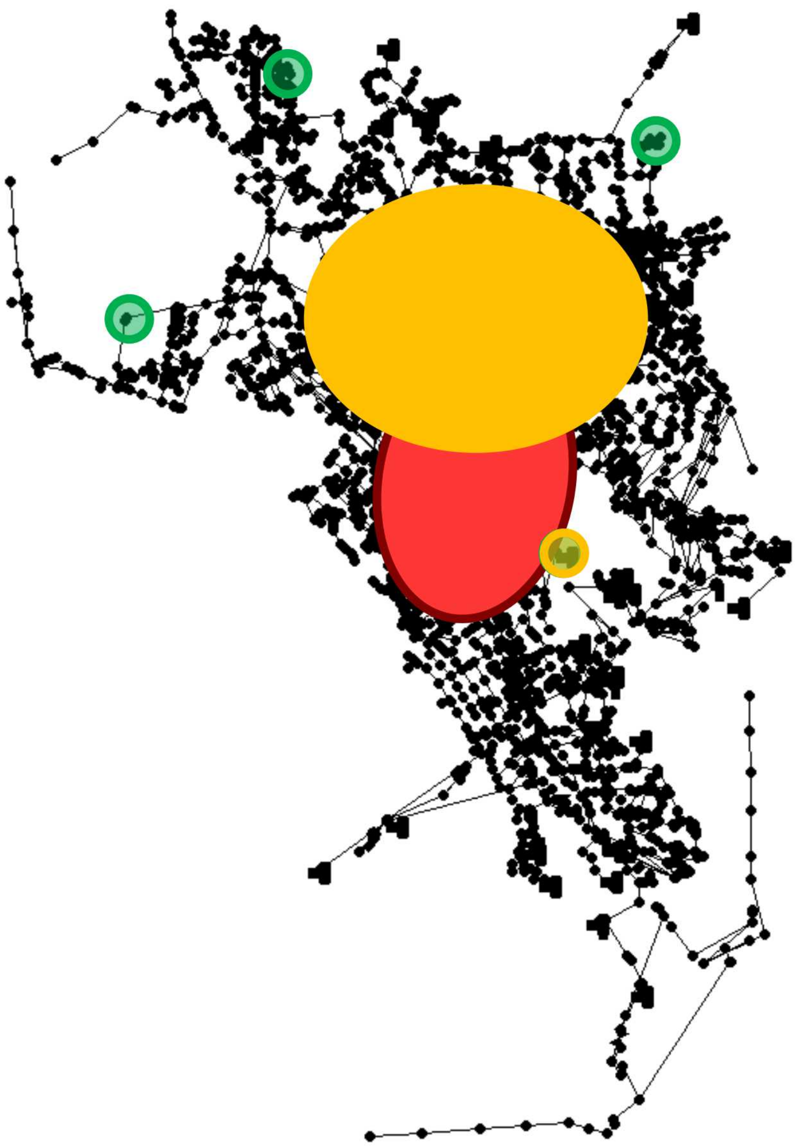
Early Warning and Response System



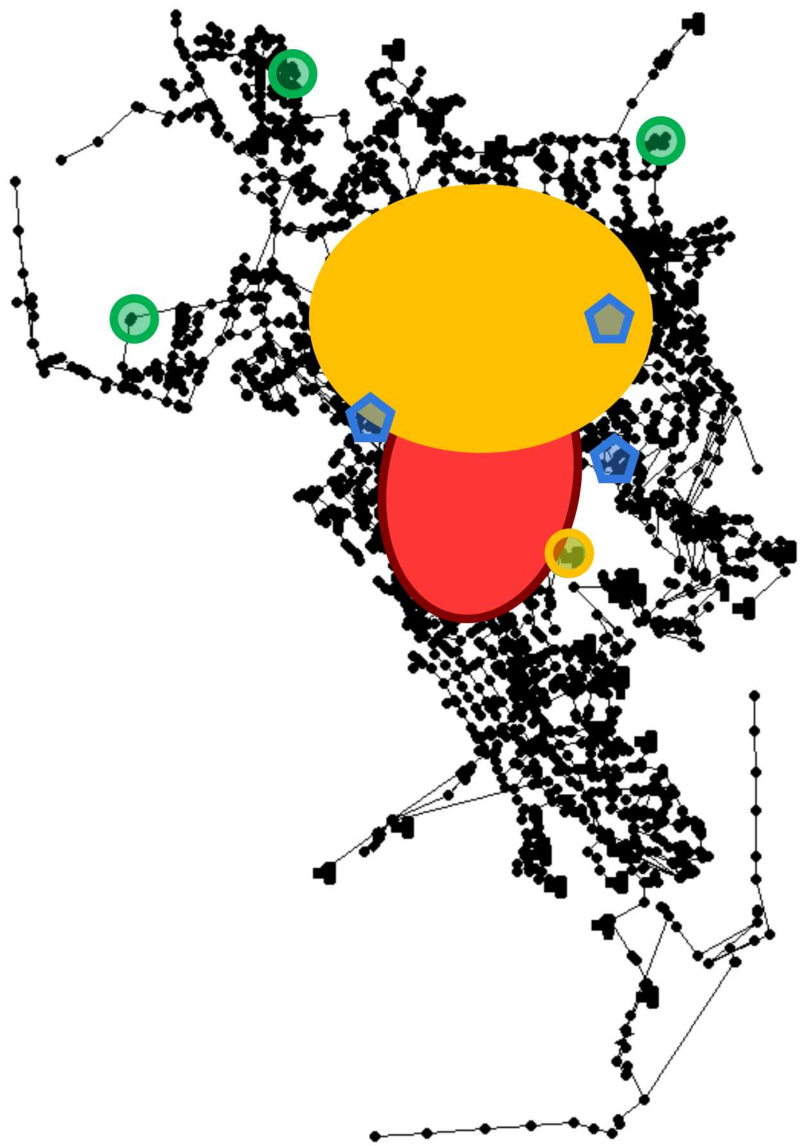
Fixed set of sensors

- What technology?
- Where will they be placed? How many?

Real-time response

- Where is the contaminant?
- Where is the source?
- What is the best action?

Early Warning and Response System



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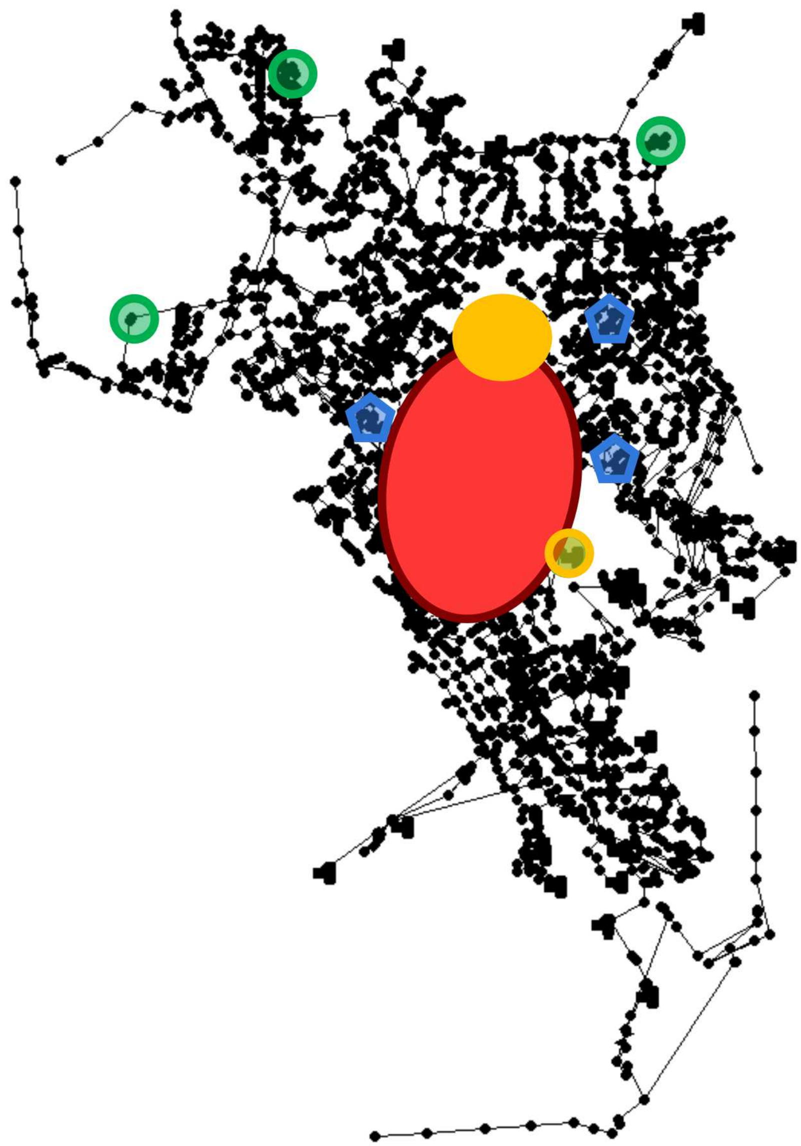

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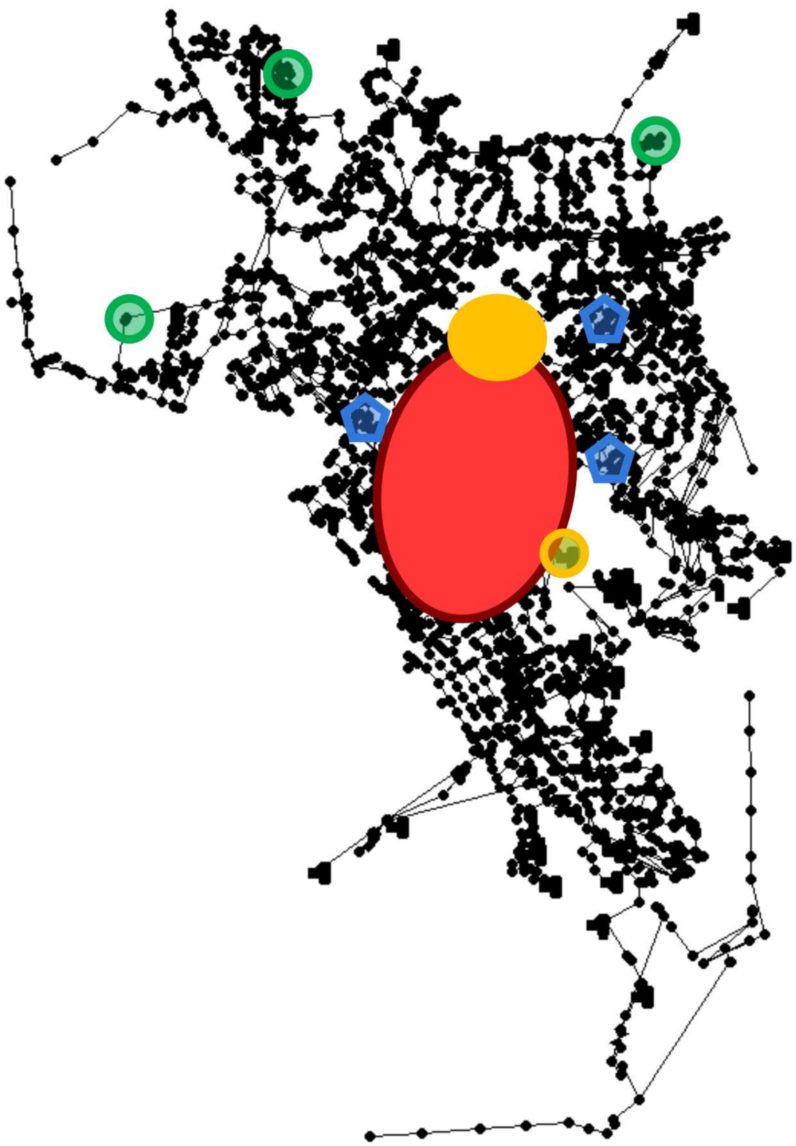


Vulnerability assessment

- Millions of WQ simulations

Detection hardware

- Chemistry/Signal analysis

Mitigation System Design

Huge uncertainty space
(contamination location, hydraulics, rxns)

Optimal Real-time response

Very large-scale models (10,000s nodes)

Real-time performance required

Our work in Water Security

Santiago-Rodriguez, J., Bynum, M., Hart, D., Laird, C.D., Klise, K.A., Haxton, T., "Optimal sampling locations to reduce uncertainty in contamination extent in water distribution systems", (Under EPA pre-publication review)

Seth, A., Hackebiel, G.A., Klise, K.A., Haxton, T., Murray, R., and Laird, C.D., "A Stochastic Programming Formulation for Disinfectant Booster Station Placement in Water Distribution Systems", submitted.

Seth, Arpan, et al. "Testing Contamination Source Identification Methods for Water Distribution Networks." Journal of Water Resources Planning and Management 142.4 (2016): 04016001.

Mann, A.V., Hackebeil, G., Laird, C.D., "Explicit Water Quality Model Generation and Rapid Multi-Scenario Simulation", Journal of Water Resources Planning and Management, Volume 14, May 2014, Pages 666-677.

Mann, A.V., McKenna, S.A., Hart, W.E., and Laird, C.D., "Real-Time Inversion in Large-Scale Water Networks Using Discrete Measurements", Computers & Chemical Engineering, Volume 37, February 2012, Pages 143-151.

Berry, J., Hart W., Laird, C.D., and Uber, J., "A Morphing Technique to Disguise Water Networks", Proceedings of, EWRI World Environmental and Water Resources Congress 2007, May, 2007.

Laird, C.D., Biegler, L.T. and van Bloemen Waanders, B.G., "Real-Time, large scale optimization of water network systems using a subdomain approach", In: L.T. Biegler, O. Ghattas, M. Heinkenschloss, D. Keyes, and B. van Bloemen Waanders, Eds., SIAM Series in Computational Science and Engineering #3, SIAM, 2007, Real-Time PDE-Constrained Optimization, Pages 291-308.

Laird, C.D., Biegler, L.T. and van Bloemen Waanders, B.G., "Mixed-integer approach for obtaining unique solutions in source inversion of water networks", A.S.C.E. Journal of Water Resources Planning and Management, Volume 132, June 2006, Pages 242-251.

Laird, C.D., Biegler, L.T., van Bloemen Waanders, B.G. and Bartlett, R., "Contamination source determination for water networks", A.S.C.E. Journal of Water Resources Planning and Management, Volume 131, March 2005, Pages 125-134

Optimal Real-time Sampling Approach

Given a contamination event

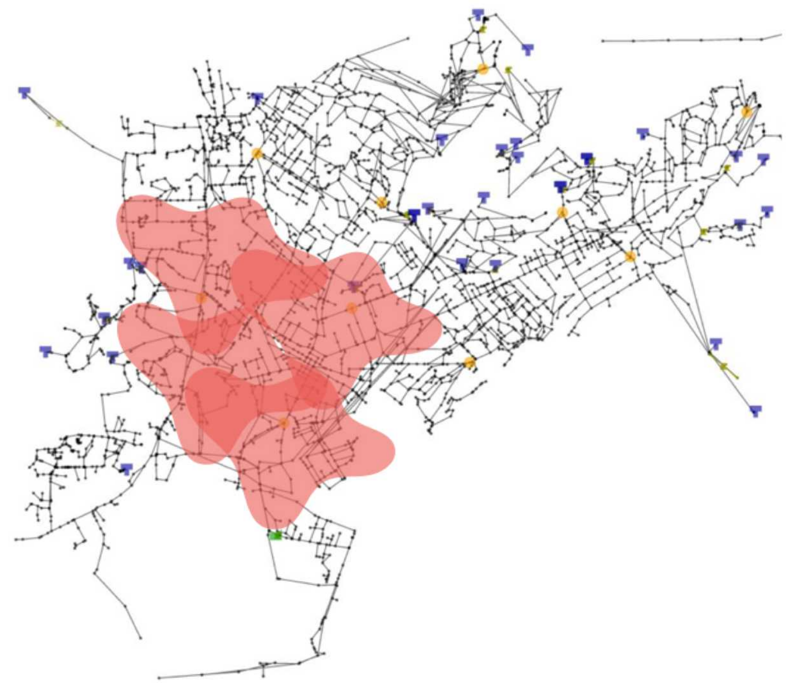
- Determine the best estimate of extent of contamination plume (probabilistic)

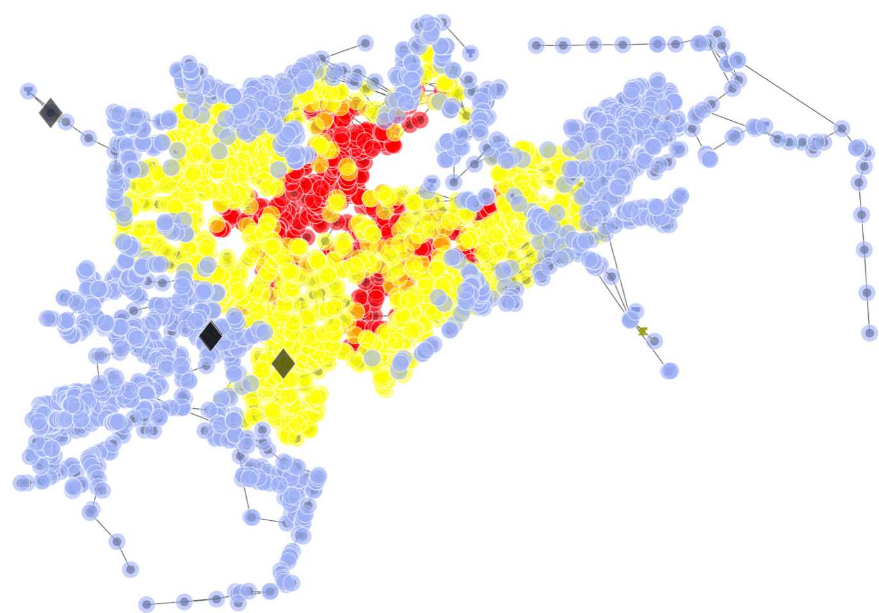
Account for uncertainty in

- Contamination source location/time
- Poorly characterized hydraulics
- Reaction dynamics

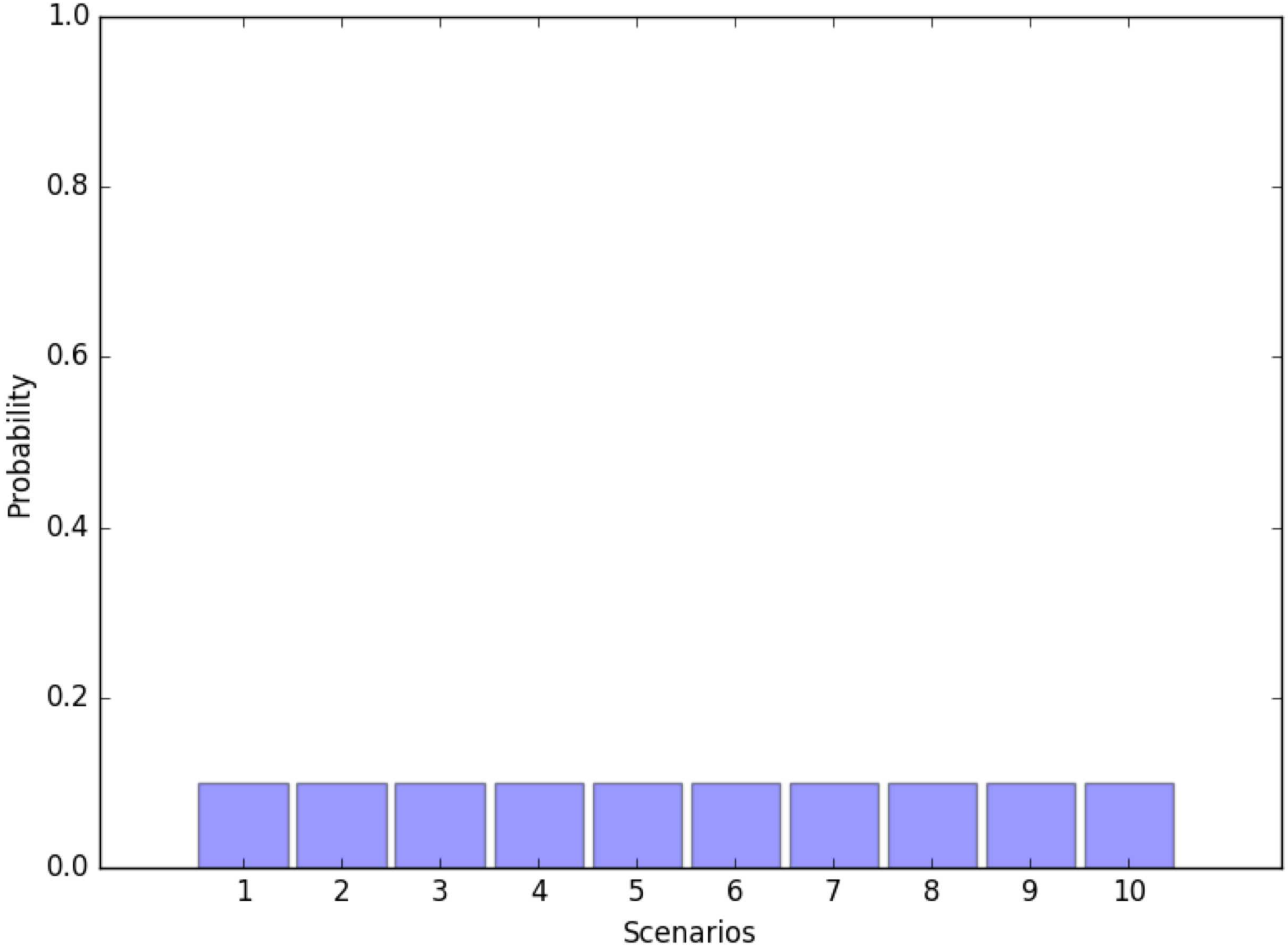
Computational approach

- Pre-compute contamination scenarios
- Propagate scenario probability to contamination probability
- Bayesian updates to scenario probability based on sample measurements
- Optimization approach to determine the best sampling locations





Quickly Shape Scenario Probability Distribution



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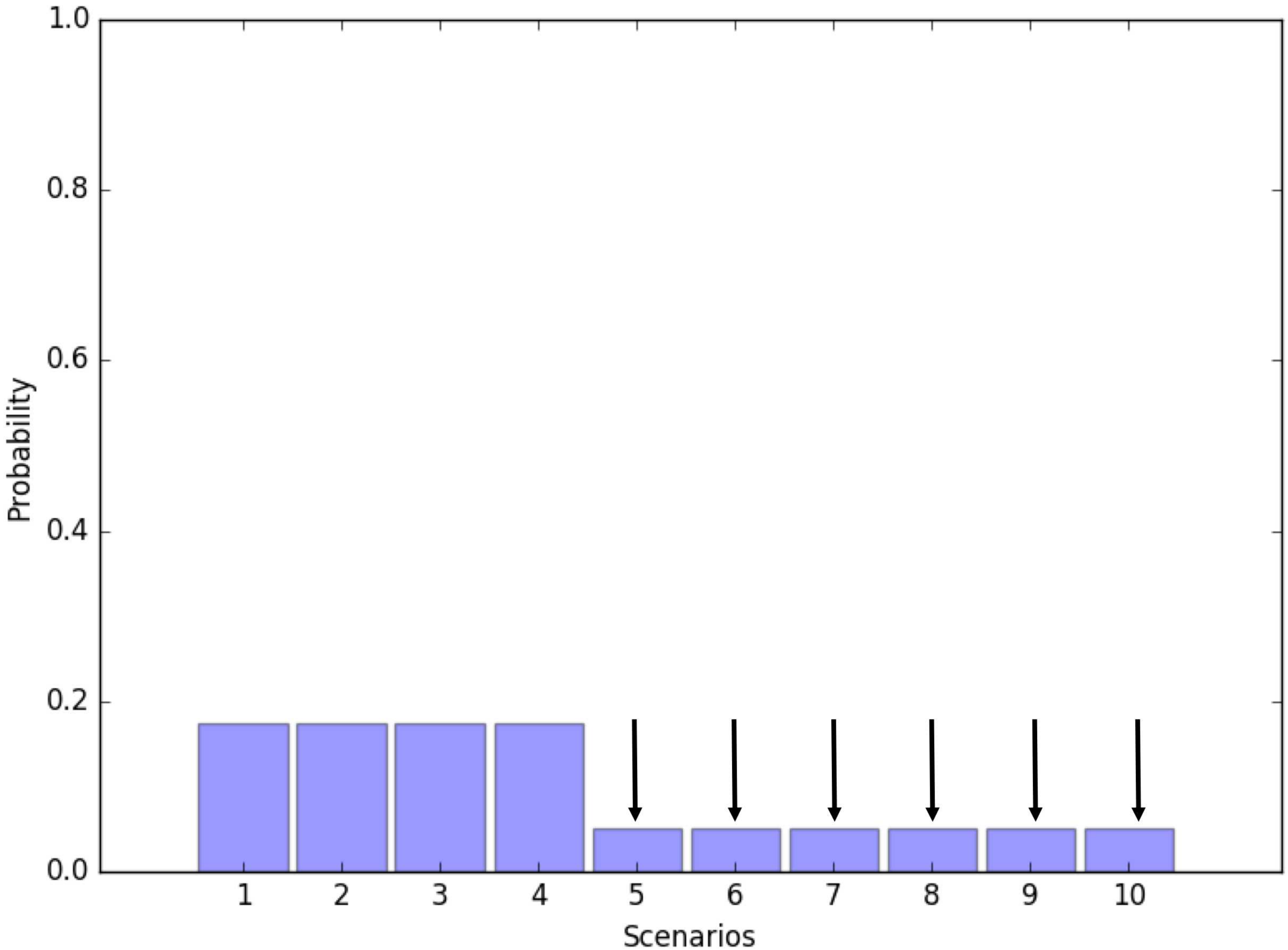
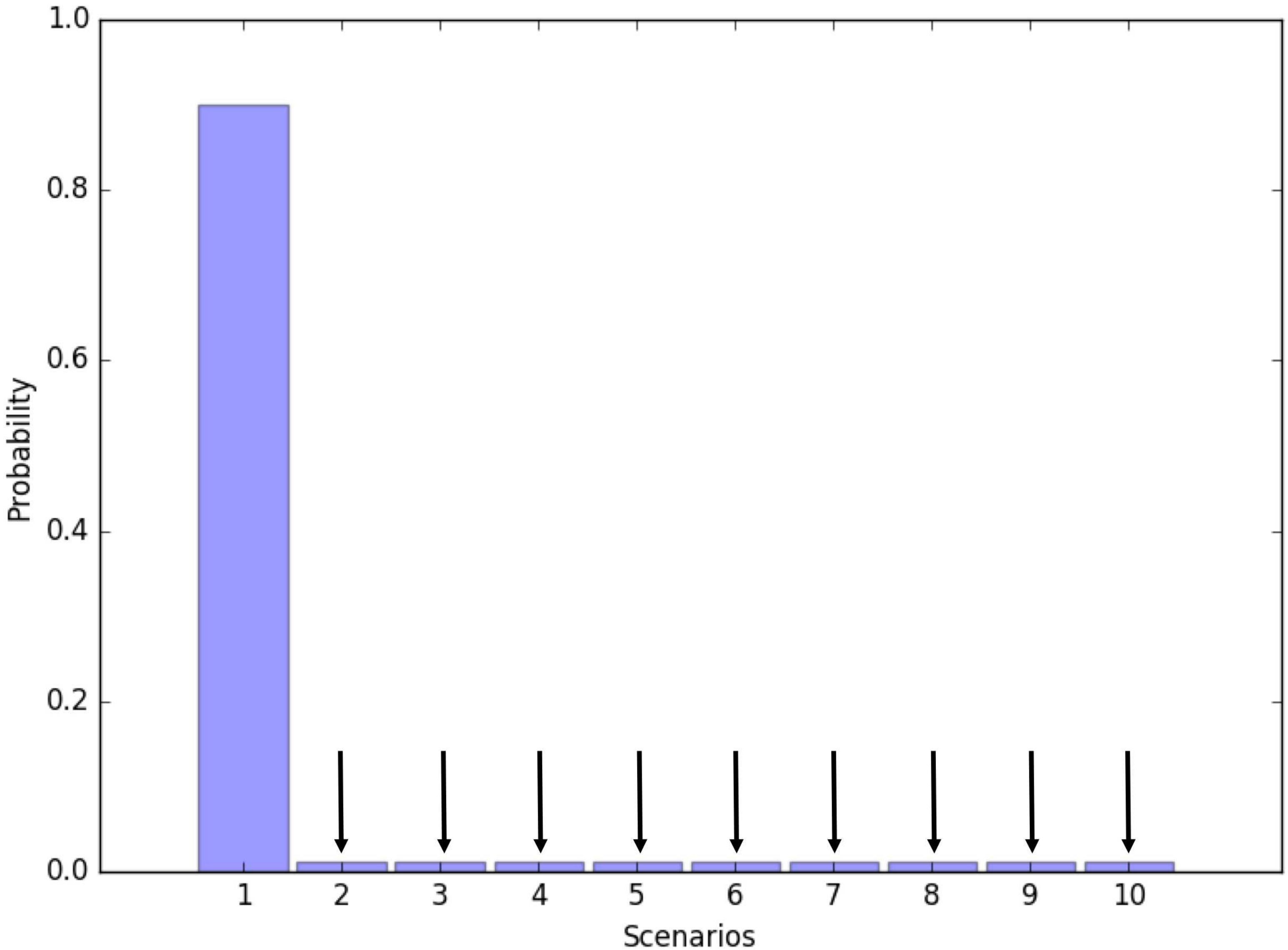


Quickly Shape Scenario Probability Distribution



Optimization formulation

$$\max_x \sum_{s \in S} P_s^{\text{miss}}$$

Maximize expected value of mismatch probability across all scenarios

$$\text{s.t.} \quad P_s^{\text{miss}} = 1 - P_s^{\text{match}} \qquad \forall\, s \in S$$

Probability that scenario s mismatches on at least one

$$P_s^{\text{match}} = \prod_{n \in N} \alpha_{s,n}^{x_n} \qquad \forall\, s \in S$$

Probability that scenario s matches all measurements

$$\sum_{n \in N} x_n \leq S_{\text{max}}$$

Maximum number of sample locations

$$x_n \in \{0, 1\} \qquad \forall\, n \in N$$

Variable: which nodes will be sampled

Optimization formulation

$$\max_x \sum_{s \in S} P_s^{\text{miss}}$$

$$\text{s.t.} \quad P_s^{\text{miss}} = 1 - P_s^{\text{match}} \qquad \forall\, s \in S$$

$$P_s^{\text{match}} = \prod_{n \in N} \alpha_{s,n}^{x_n} \qquad \forall\, s \in S$$

$$\sum_{n \in N} x_n \leq S_{\text{max}}$$

$$x_n \in \{0, 1\} \qquad \forall\; n \in N$$

Optimization formulation

$$\max \sum_{s \in S} P_s^{\text{miss}}$$

$$\text{s.t.} \quad P_s^{\text{miss}} = 1 - P_s^{\text{match}} \qquad \forall\, s \in S$$

$$\sout{P_s^{\text{match}} = \prod_{n \in N} \alpha_{s,n}^{x_n}} \qquad \forall\, s \in S$$

$$\tilde{P}_s = \sum_{n \in N} x_n \ln\left(\alpha_{s,n}\right) \qquad \forall\, s \in S$$

$$P_s^{\text{match}} = \exp\left(\tilde{P}_s\right) \qquad \forall\, s \in S$$

$$\sum_{n \in N} x_n \leq S_{\max}$$

$$x_n \in \{0, 1\} \qquad \forall\, n \in N$$

Optimization formulation

$$\max \quad \sum_{s \in S} P_s^{\text{miss}}$$

$$\text{s.t.} \quad P_s^{\text{miss}} = 1 - P_s^{\text{match}}$$

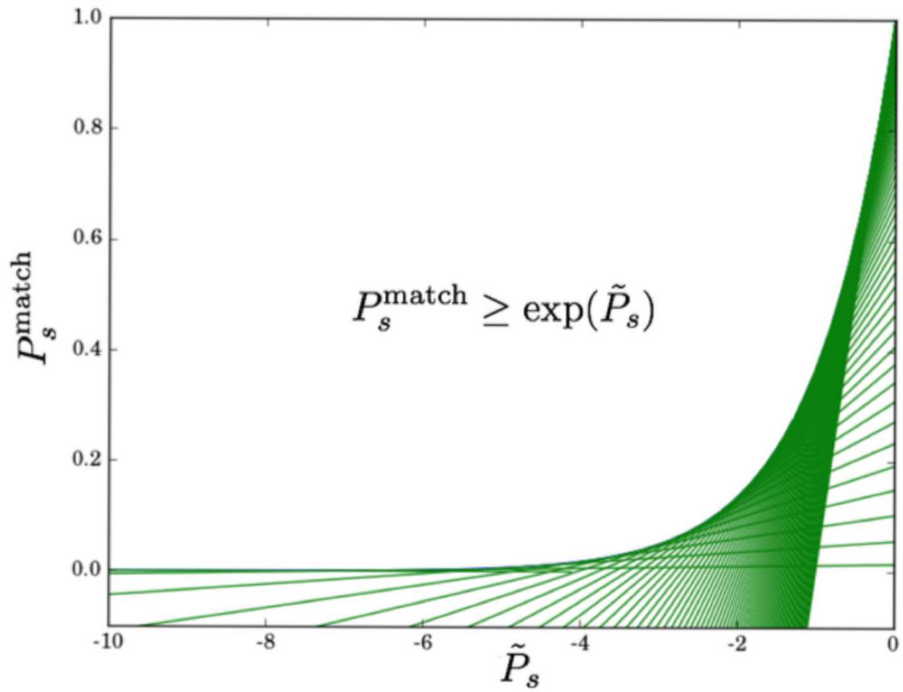
~~$$P_s^{\text{match}} = \prod_{n \in N} \alpha_{s,n}^{x_n}$$~~

$$\tilde{P}_s = \sum_{n \in N} x_n \ln\left(\alpha_{s,n}\right)$$

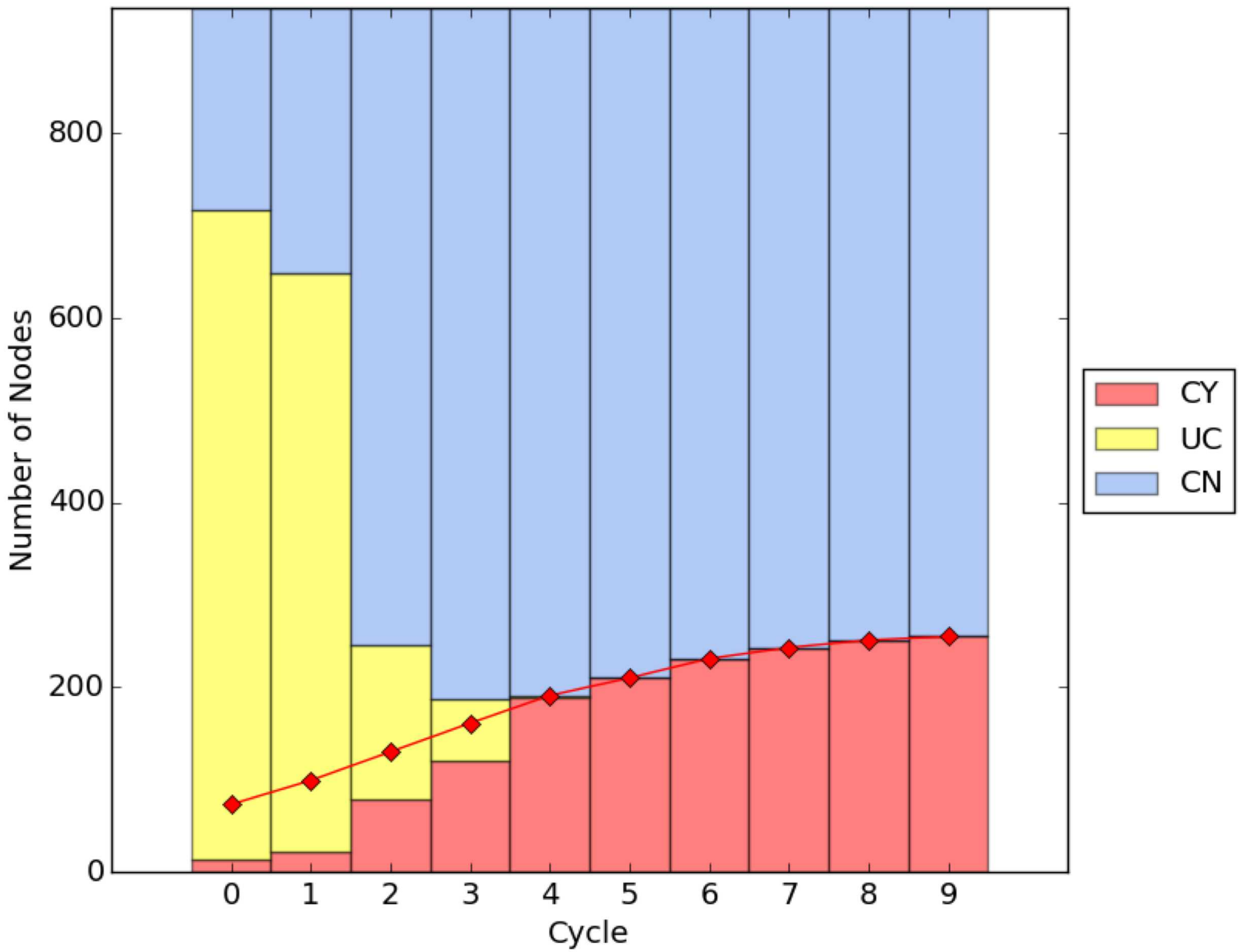
$$P_s^{\text{match}} \geq \exp\left(\tilde{P}_s\right) \qquad \forall\ s \in S$$

$$\sum_{n \in N} x_n \leq S_{\max}$$

$$x_n \in \{0, 1\} \qquad \forall\ n \in N$$



Reduction in Uncertainty of Contaminant Plume



Summary: Protecting Water Distribution Systems

Water distribution systems are vulnerable to chemical or biological contamination (accidental or intentional)

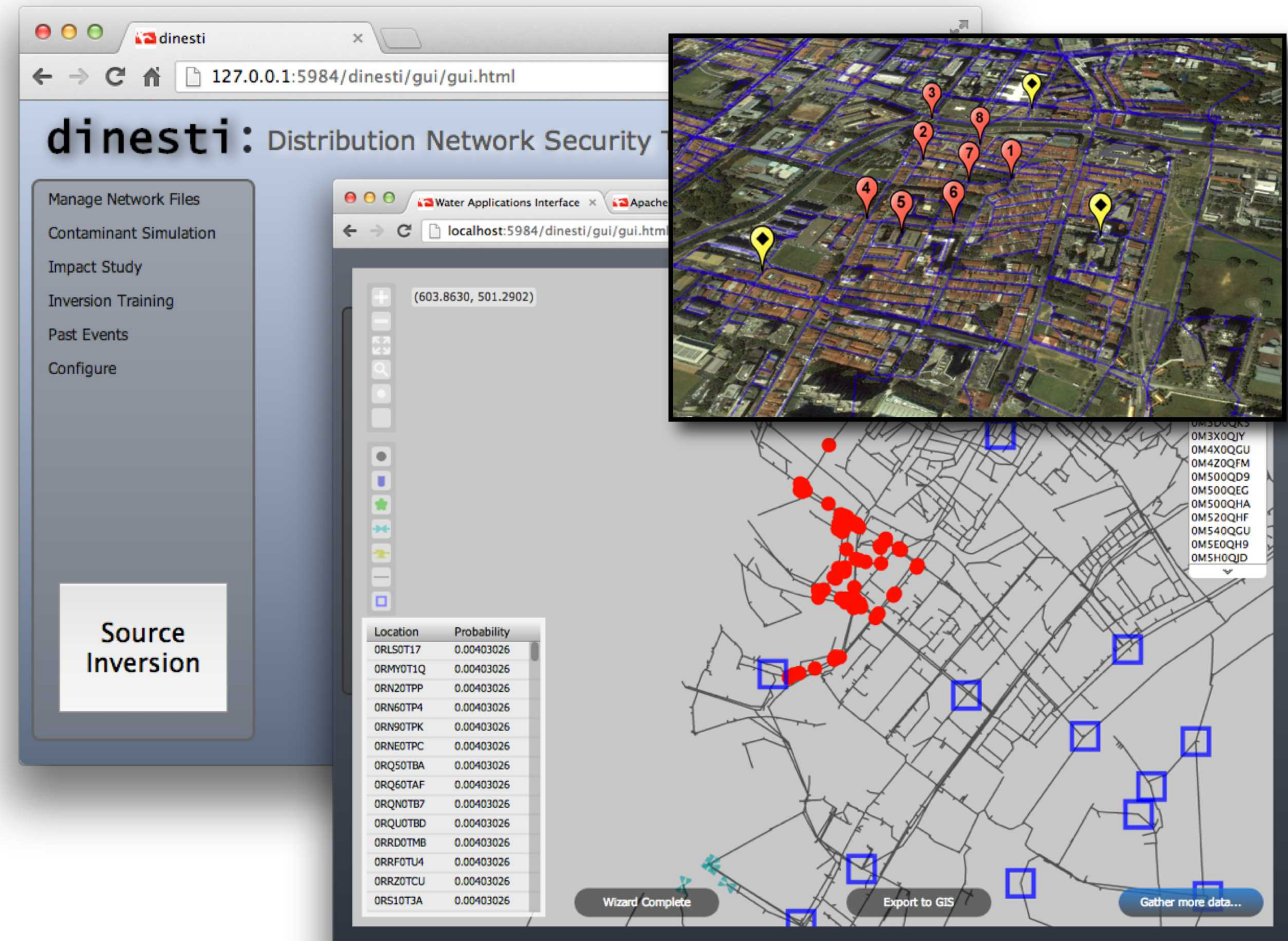
Significant research into optimal design of mitigation systems

- Sensor / Booster placement (TEVA-SPOT, WST)
- Current research:
  - Confidence intervals as function of # of scenarios
  - Optimization considering sensor failure probabilities

Optimal real-time response more challenging

- Large models embedded into optimization
- Real-time performance is required
- Source inversion solved for large networks (continuous only)
- Optimal sampling solved for large networks (hydraulics input)
- Remarkably few sampling cycles (and teams) required for inversion and plume extent
- Flushing and recovery open problem (hydraulics part of solution)

Installed sampling and source inversion system



Optimal gas detector placement in process facilities

Marsh (2012). The 100 largest losses 1972-2011. London, United Kingdom.

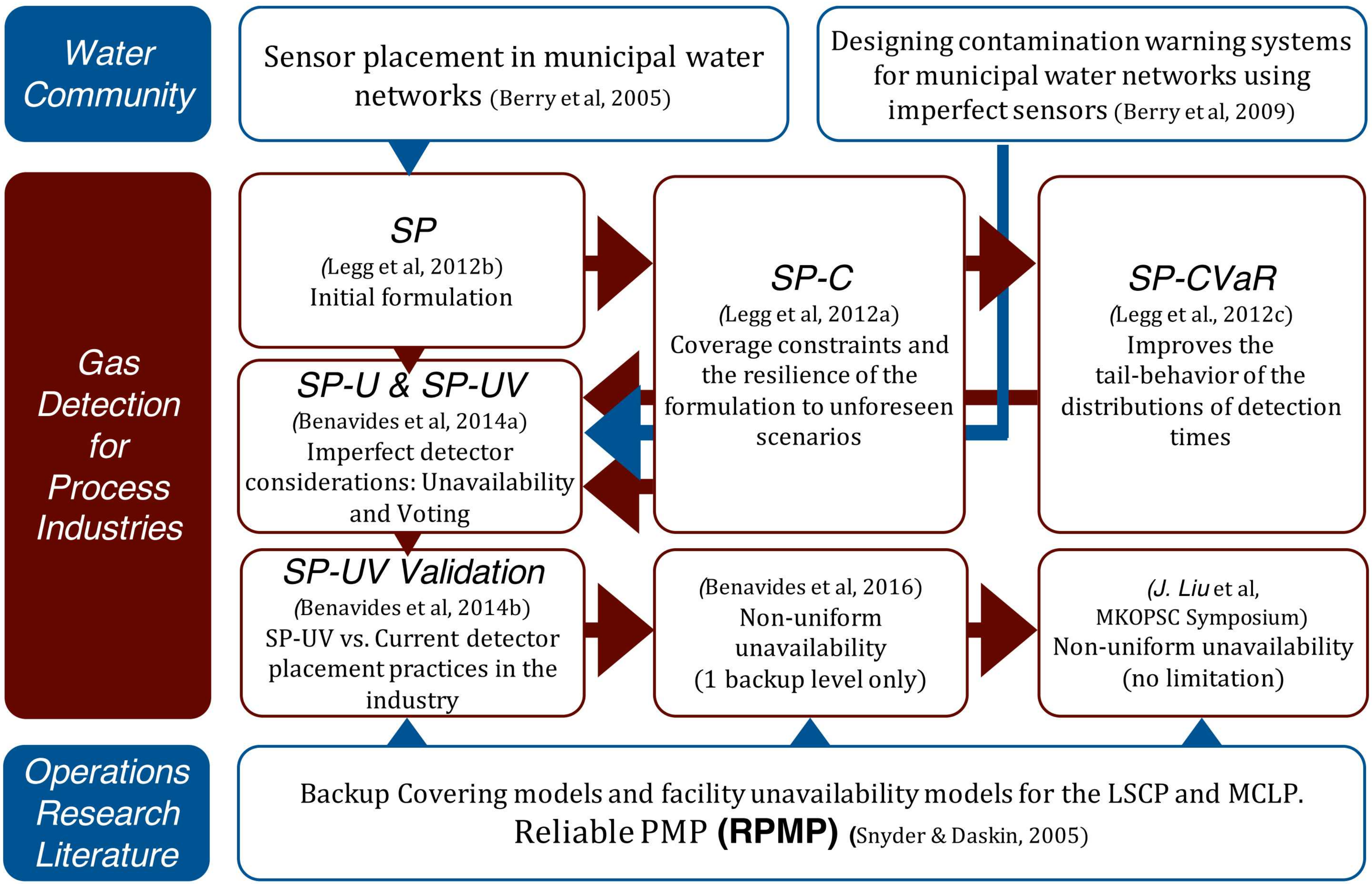
Less than 50% of all known gas released are detected (HSE 1997 & 2003)

Design of gas detector systems: rule-of-thumb and semi-quantitative methods

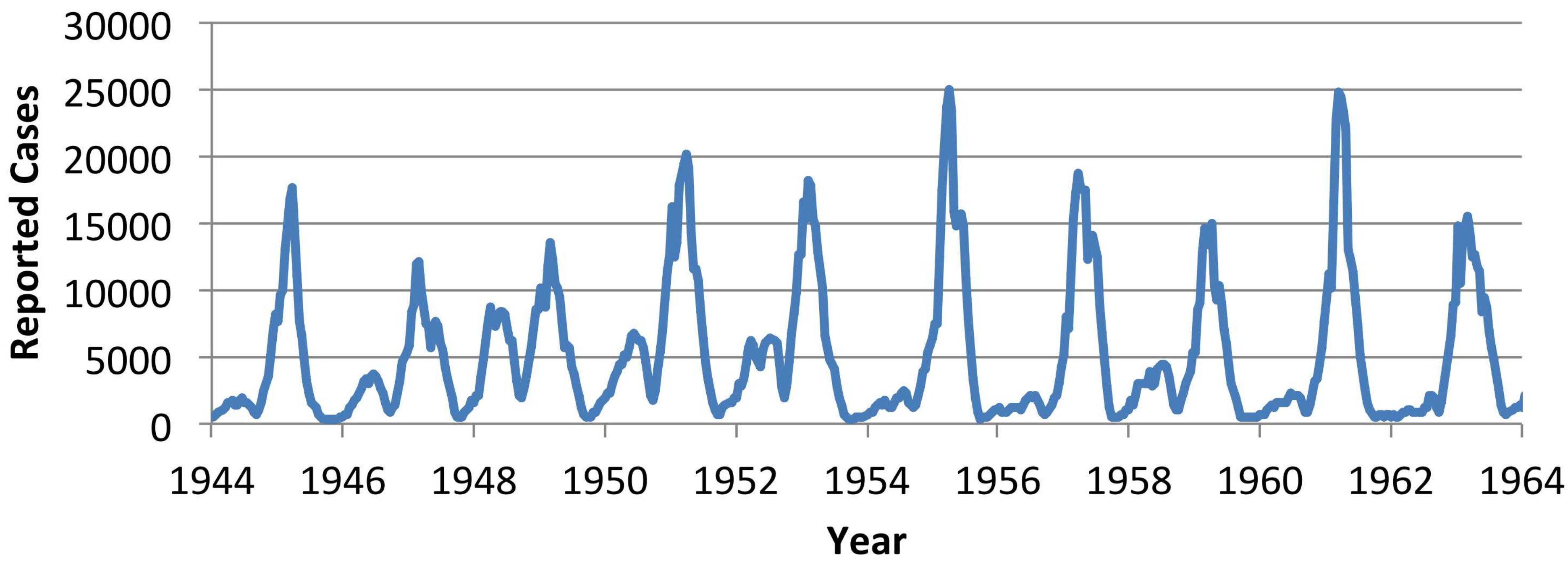
Optimal gas detector placement

- 100's of leak dispersion simulations (location, weather)
- Solve for sensor placement that minimizes expected impact
- Handles voting / sensor failure
- Outperforms existing guidelines
- Most used (volumetric coverage) was worse than random

Publications in Gas Detector Placement



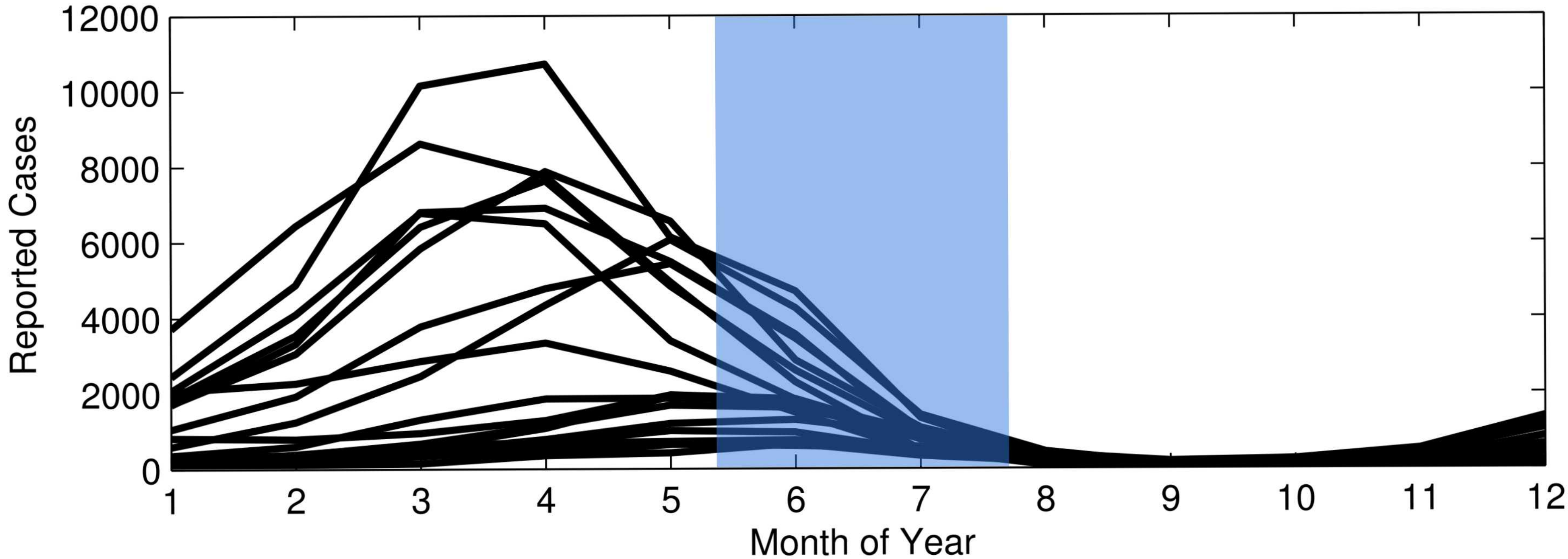
Estimating drivers of infectious disease dynamics



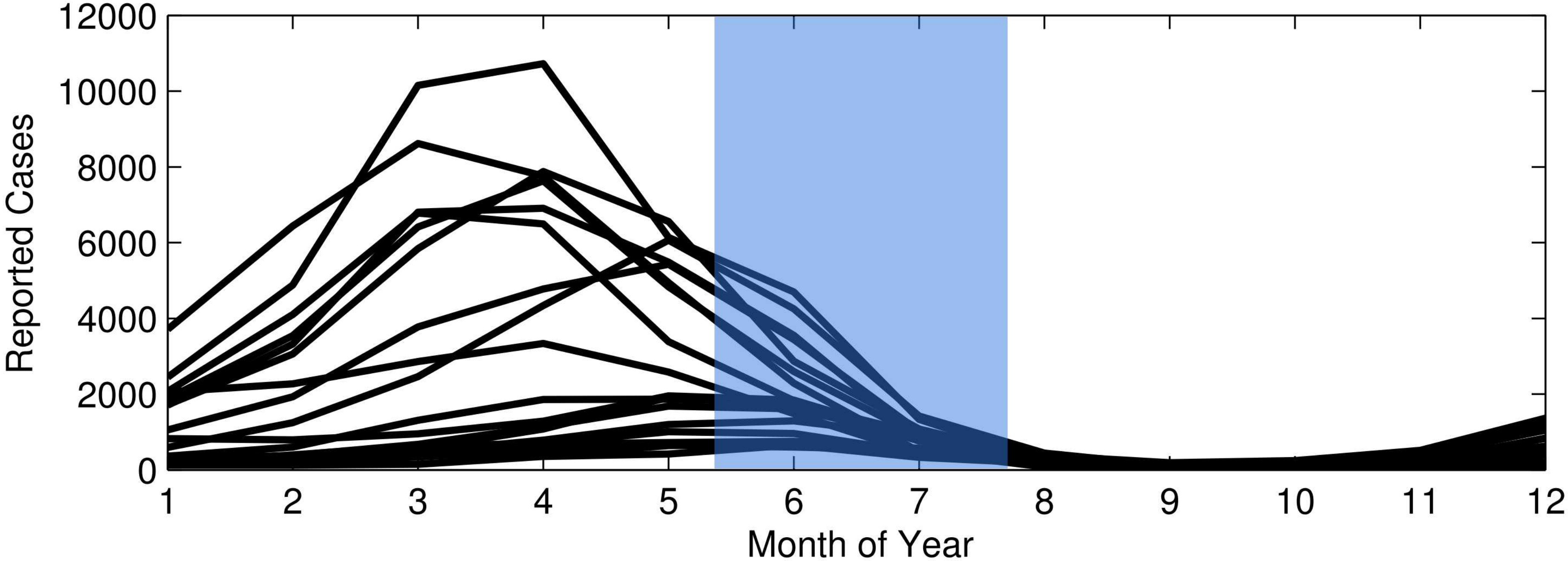
Can we use this data to better understand the fundamental drivers of infectious disease dynamics? (transmission vector? Seasonal mixing?)

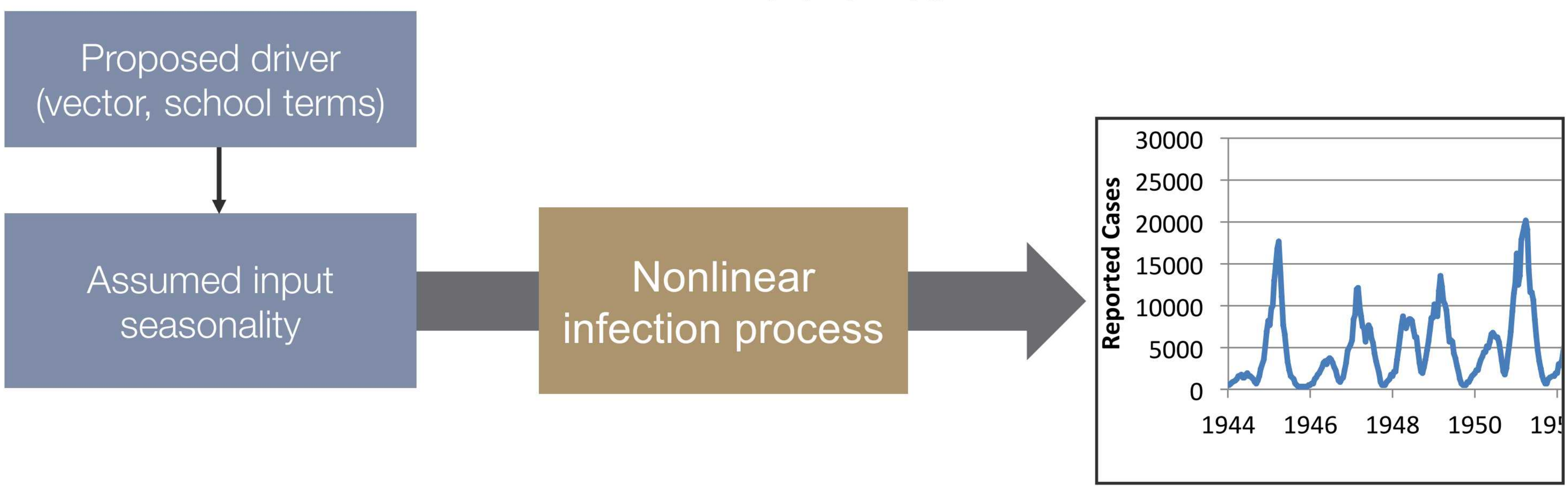
How can we use this data for improved intervention in emerging childhood respiratory illness?

Estimating Seasonality in Input Drivers

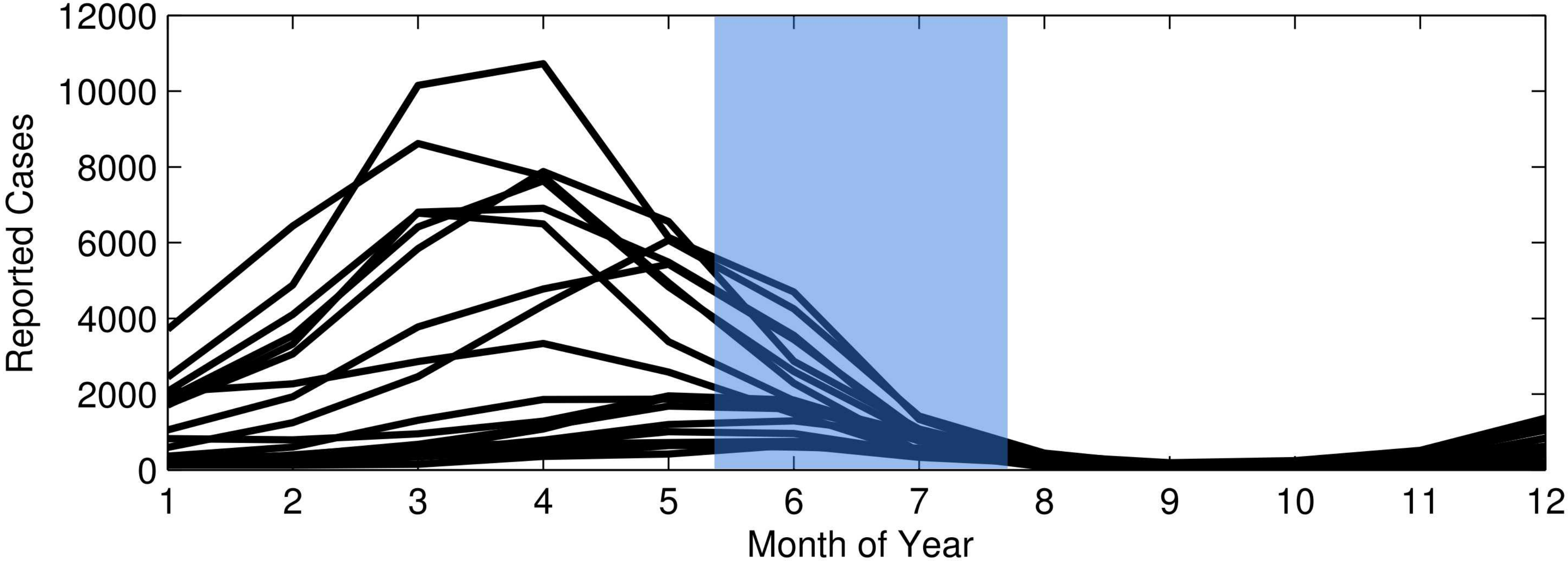


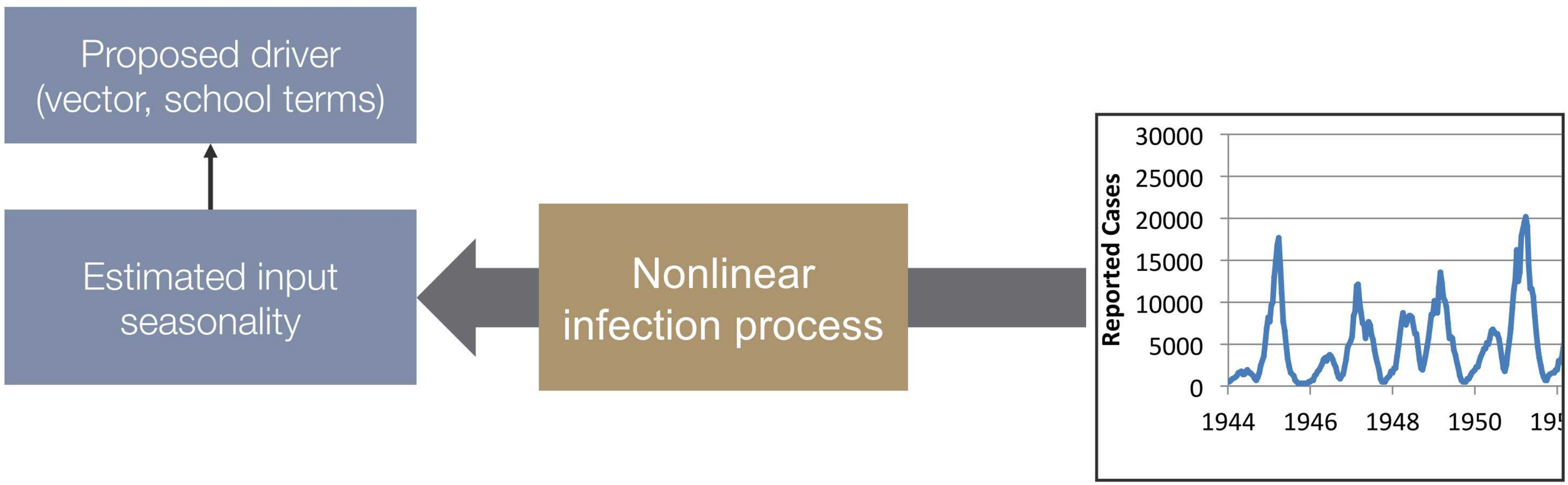
Estimating Seasonality in Input Drivers





Estimating Seasonality in Input Drivers





Estimating Seasonal Drivers in Childhood Infectious Diseases

Childhood Infectious Diseases (e.g., measles, chickenpox)

- Seasonality induced by school holidays
- Pre-vaccination era: Everyone contracts the disease
- Still a significant problem in developing countries (easy ID)

Estimation challenges

- Long time horizons (20-30 years)
- Historical aggregated monthly or biweekly
- No susceptible information
- Severe under reporting of cases (1/2 for UK, 1/100 for Thailand)
- Missing data (1974, 1979), substantial noise, time-varying reporting fraction

Data used:

- England & Wales: 60 and 900 city datasets (1944-1963)
- US: New York City, Baltimore, TYCO Data
- Thailand: 76 Provinces (1972-1998)

Estimating Seasonal Drivers in Childhood Infectious Disease

Compartment models based on status w.r.t. the disease (SIR)

Formulated as discrete-time or continuous time dynamic optimization problem

Estimate unknown seasonal transmission parameter from case data

Time-varying, restricted to be yearly periodic

$$
\begin{aligned}
\min \quad & \mathcal{L}(\varepsilon_M(t), \varepsilon_Q) \\
\text{s.t.} \quad & \\
& \frac{dI}{dt} = \frac{\beta(y(t))S(t)I(t)}{N(t)} \cdot \varepsilon_M(t) - \gamma I(t) \\
& \frac{dS}{dt} = \frac{-\beta(y(t))S(t)I(t)}{N(t)} \cdot \varepsilon_M(t) + B(t) \\
& \frac{dQ}{dt} = \frac{\beta(y(t))S(t)I(t)}{N(t)} \cdot \varepsilon_M(t) \\
& R_k^\star = \eta_k \left(Q(t_k) - Q(t_{k-1})\right) + \varepsilon_{Q_k} \quad \forall k \in \mathcal{T} \\
& 0 \leq I(t), S(t) \leq N(t) \\
& 0 \leq \beta(y(t)), Q(t)
\end{aligned}
$$

Efficient Optimization of Discretized Systems

$$\min_u \int_{t_0}^{t_f} L(x, y, u) \, dt$$

$$\text{s.t.} \quad F(\dot{x}, x, y, u) = 0$$

$$x(t_0) = x_0$$

Optimize-then-discretize
Variational Approach (Pontryagin, 1962)

Discretize-then-optimize
Apply NLP Solver

Sequential Approach

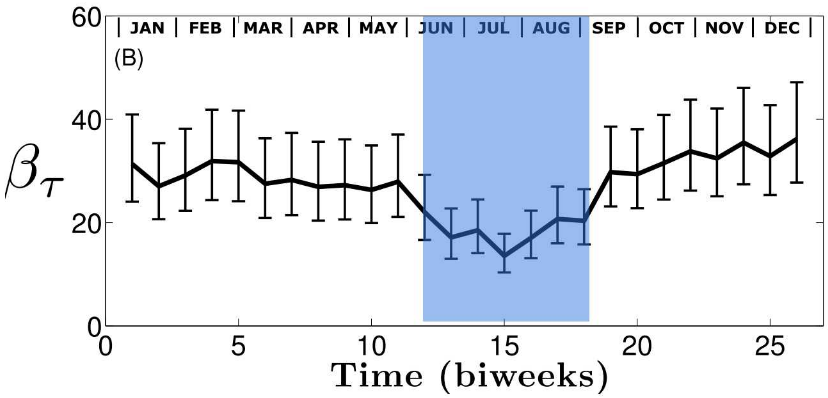
- Discretize controls only
- Small NLP Problem
- Sensitivities or adjoints for derivatives
- Converge simulation in each iteration

. . .

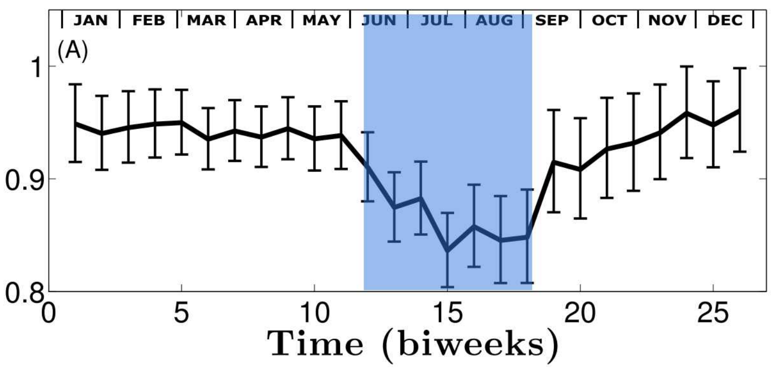
Simultaneous Approach

- Discretize entire problem (states and controls - OCFE)
- Converge simulation only once with optimization
- Very large-scale NLP
- Structured NLP

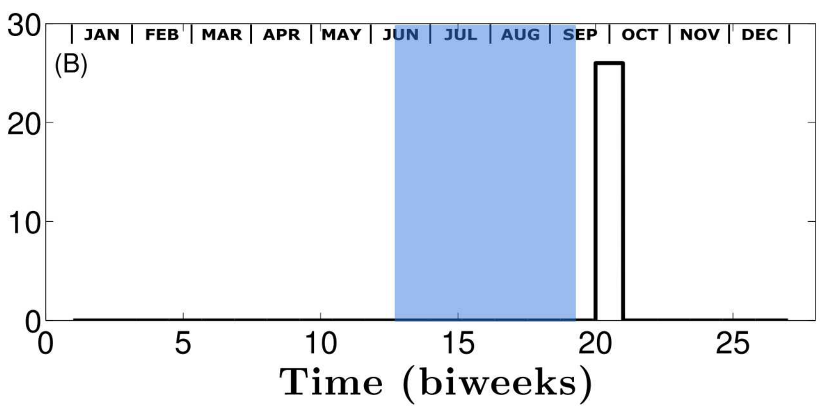
Estimated Seasonal Patterns for NYC



Seasonality in transmission parameter



Seasonality in mixing coefficient



Seasonality in birth rate only

Our work in infectious disease modeling

- Zhen, T., Cummings, D., and Laird, C.D., "A Nonlinear Optimization Approach to the Estimation of Spatial Transmission Parameters in Infectious Disease Spread", in progress

- Liu, J., Cummings, D., and Laird, C.D., “MINLP Approaches for Parameter Estimation in Deterministic and Stochastic Disease Models”, in progress.

- Word, D.P., Young, J.K., Cummings, D.A.T., Iamsirithaworn, S., and Laird, C.D., "Interior-Point Methods for Estimating Seasonal Parameters in Discrete-Time Infectious Disease Models", PLOS One, Volume 8-10, October 2013, Pages 1-13.

- Word, D.P., Cummings, D.A.T., Burke, D.S., Iamsirithaworn, S., and Laird, C.D., "A Nonlinear Programming Approach for Estimation of Transmission Parameters in Childhood Infectious Disease Using a Continuous Time Model", Journal of the Royal Society Interface, Volume 9, August 2012, Pages 1983-1997

- Word, D.P., Abbott III, G.H., Cummings, D, and Laird, C.D., "Estimating Seasonal Drivers in Childhood Infectious Diseases with Continuous Time and Discrete-Time Models", Proceedings of, American Control Conference (ACC) 2010, Baltimore, MD, June 30 - July 2, 2010, Pages 5137-5142.

- Word, D.P., Young, J., Cummings, D., and Laird, C.D., "Estimation of seasonal transmission parameters in childhood infectious disease using a stochastic continuous time model", In: S. Pierucci and G. Buzi Ferraris, Eds., Computer Aided Chemical Engineering, Volume 28, Elsevier, 2010, 20th European Symposium on Computer Aided Process Engineering, Pages 229-234.

Summary: Estimation of Infectious Disease Models

Pioneering work estimating seasonal transmission with TSIR model

- Grenfell, Bjornstadt (2000): Two-stage linear estimation

Recent approaches:

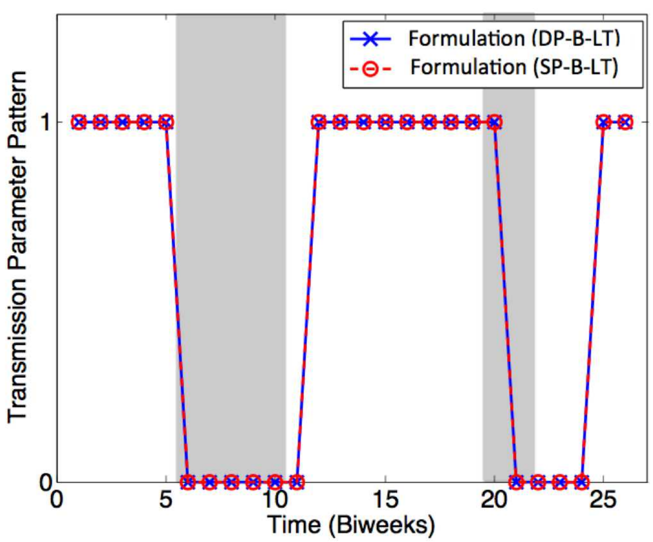
- Cauchemez & Ferguson (2008): Sampling-based approach (single-city: 20 hrs)
- Hooker et. al (2010): Sequential dyn. Optimization (single-city: over 2 hours)

Nonlinear Programming Approaches Provide Fast, Reliable Estimation

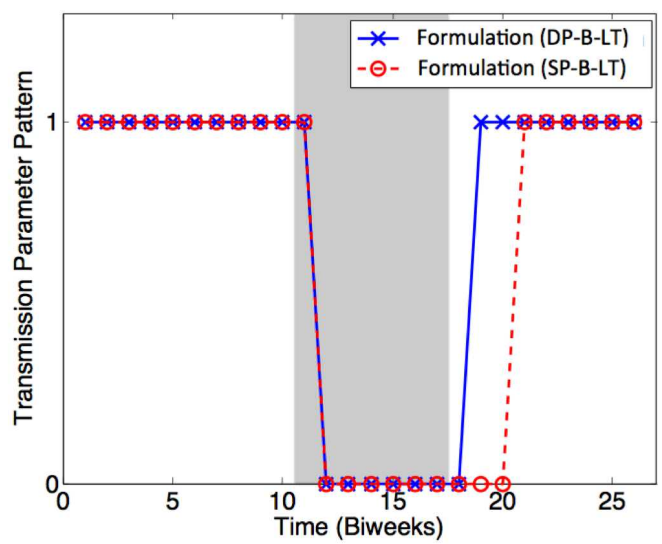
- Discrete-time / Continuous time models
- Very fast, (20 hours —> under 30 seconds) Changes the science

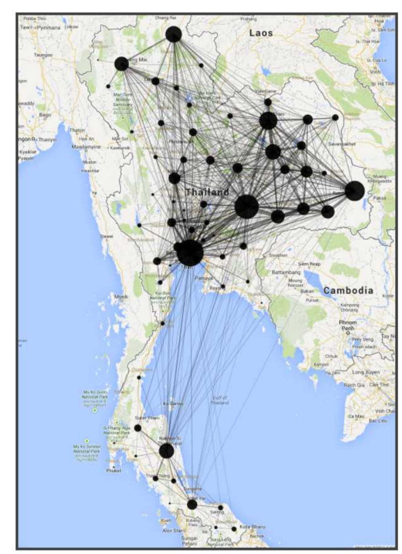
Results show strong correlation with school-term holidays over different environments

Bangkok:
Time Horizon: 1980-1987
Reporting Fraction: 3.2 %



New York City:
Time Horizon: 1947-1962
Reporting Fraction: 10.7 %





Parallel Computing Architectures

	Single Data	Multiple Data
Single Instruction	SISD	SIMD
Multiple Instruction	MISD	MIMD

Alternative architectures (e.g, Graphics Processing Unit)

- Affordable -- 1000's cores
- Specialized compilers and tools (CUDA, OpenCL)
- Several complexities and limitations

Desktop Multi-core (MIMD)

- Affordable hardware
- Standard tools (threads/openMP)
- Fast communication (no network)

- Low # of cores (relatively)
- Bottleneck: Memory access/# CPU

HPC Cluster (MIMD)

- Distributed computing (networked)
- Standard tools (MPI)
- Scalable: 100-1000s of cores

- Bottlenecks: communication

Nonlinear Interior-Point Methods

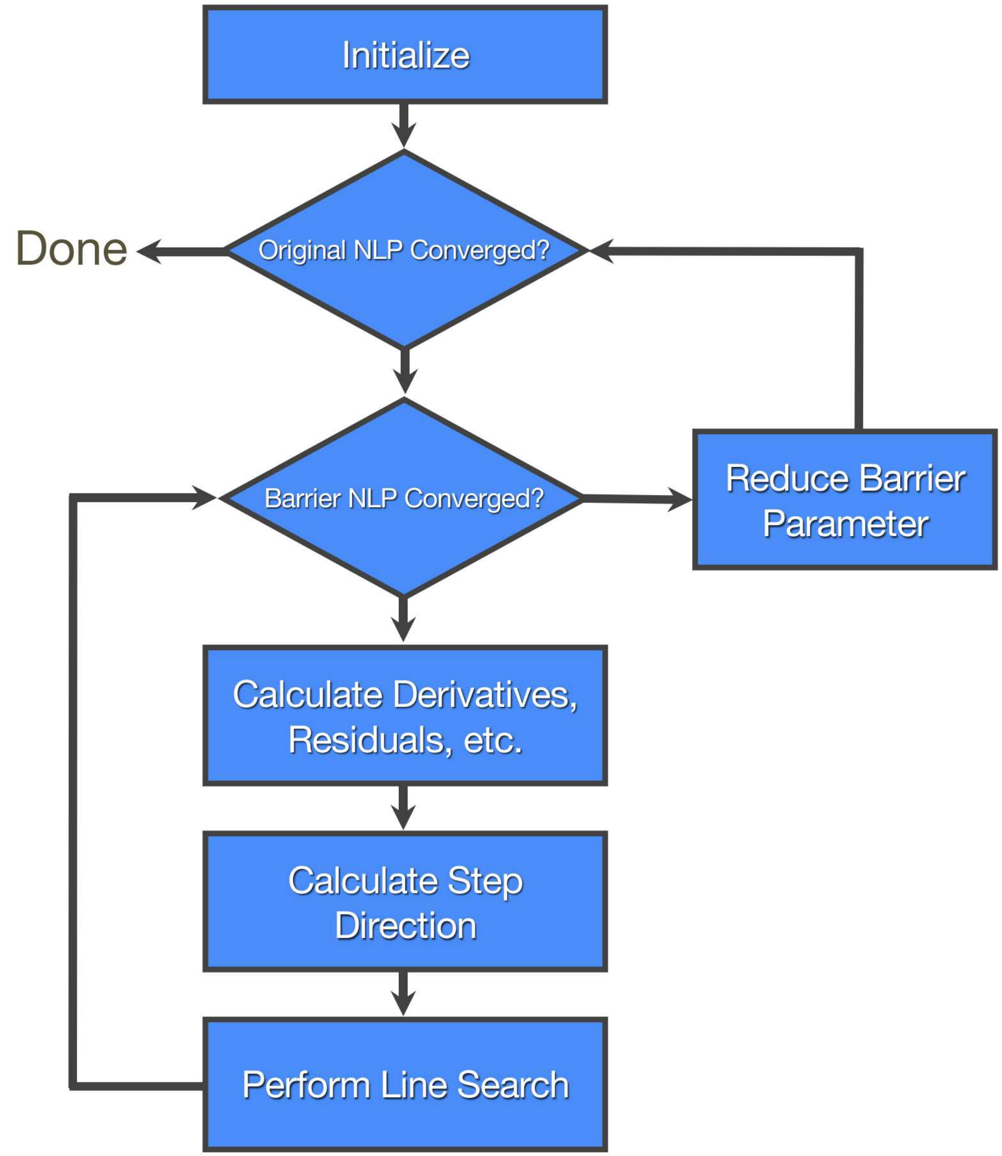
Original NLP

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & c(x) = 0 \\ & x \geq 0 \end{aligned}$$

Barrier NLP

$$\begin{aligned} \min_x \quad & f(x) - \mu \cdot \sum_i ln(x_i) \\ \text{s.t.} \quad & c(x) = 0 \end{aligned}$$

KNITRO (Byrd, Nocedal, Hribar, Waltz)
LOQO (Benson, Vanderbei, Shanno)
IPOPT (Wachter, Laird, Biegler)



Nonlinear Interior-Point Methods

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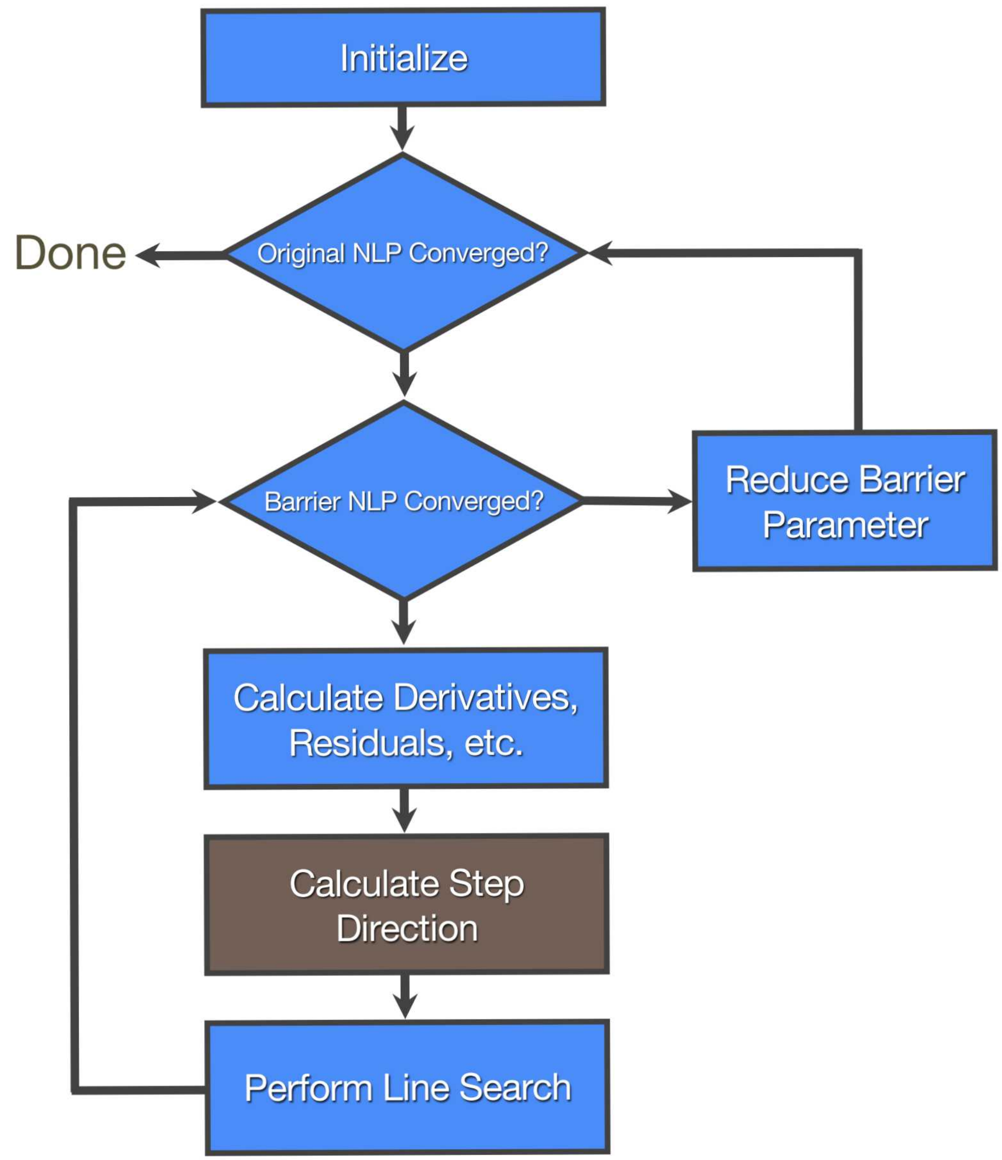


Nonlinear Primal-Dual Interior-Point Step

$$\min_x \; f(x) \quad \text{s.t} \quad c(x)=0, \quad x \geq 0$$

$$\min_x \; f(x) - \mu \sum_i \ln(x_i) \quad \text{s.t} \quad c(x)=0$$

$$\nabla f(x) + \nabla c(x)^T \lambda - \mu X^{-1} e = 0$$
$$c(x) = 0$$
$$(x > 0)$$

$$z=\mu X^{-1} e$$

$$\nabla f(x) + \nabla \quad \lambda - z = 0$$
$$c(x) = 0$$
$$Xz = \mu e$$
$$> 0, z > 0)$$

$$\begin{bmatrix} W_k + \Sigma_k + \delta_w I & \nabla c(x_k) \\ \nabla c(x_k)^T & -\delta_c I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} \nabla \psi_\mu(x_k) + \nabla c(x_k)^T \lambda_k \\ c(x_k) \end{bmatrix}$$

$$(W_k = \nabla^2_{xx} \mathcal{L}, \; \Sigma_k = Z_k X_k^{-1})$$

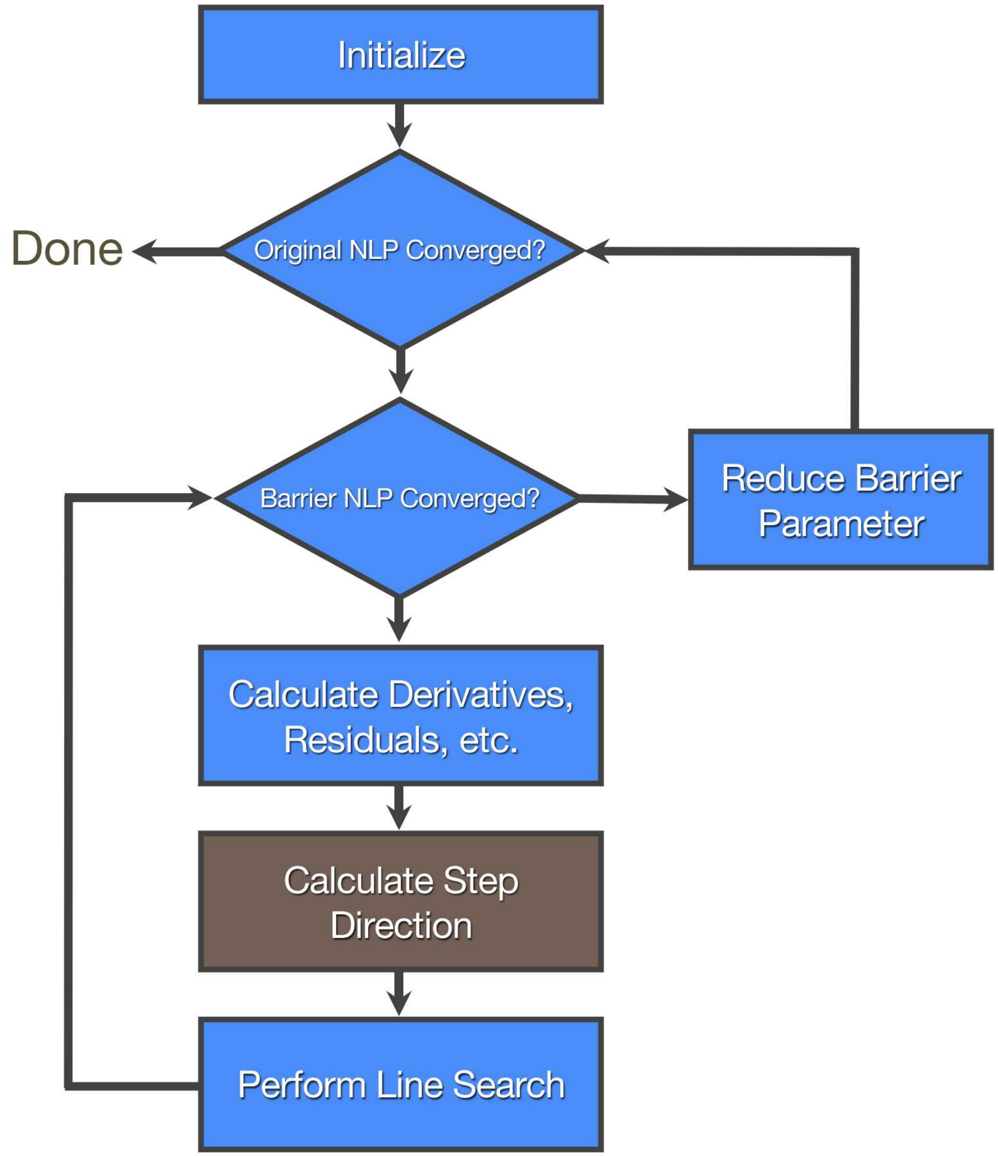
Nonlinear Interior-Point Methods

Structure in the optimization problem induces structure in the linear algebra

Parallelize all scale-dependent operations
- Vector and matrix operations
- Model evaluation

Compared with problem-level decomposition, implementation is time consuming

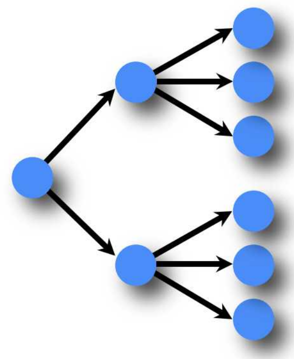
Retain convergence properties of serial algorithm

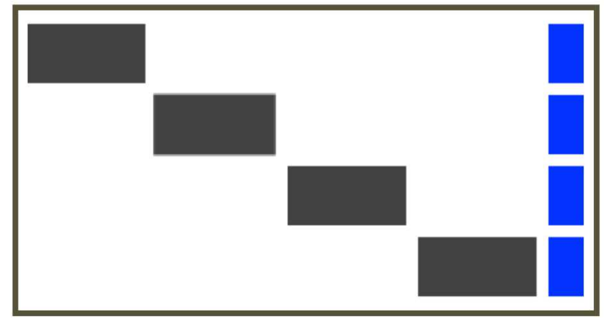


Exploiting Problem Structure

Optimization Under Uncertainty

- block structure because of coupled scenarios
- common structure of many applications



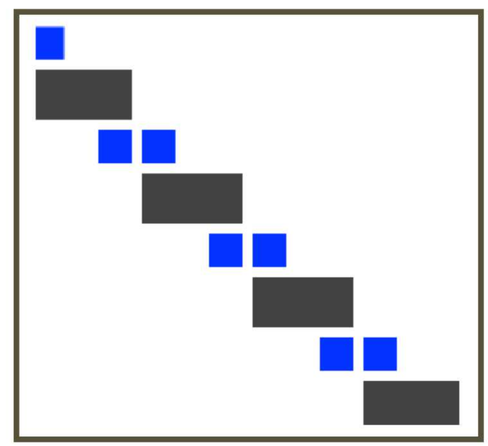


Kang, J., Word, D.P., and Laird, C.D., "An interior-point method for efficient solution of block-structured NLP problems using an implicit Schur-complement decomposition", Computers and Chemical Engineering, 2014.

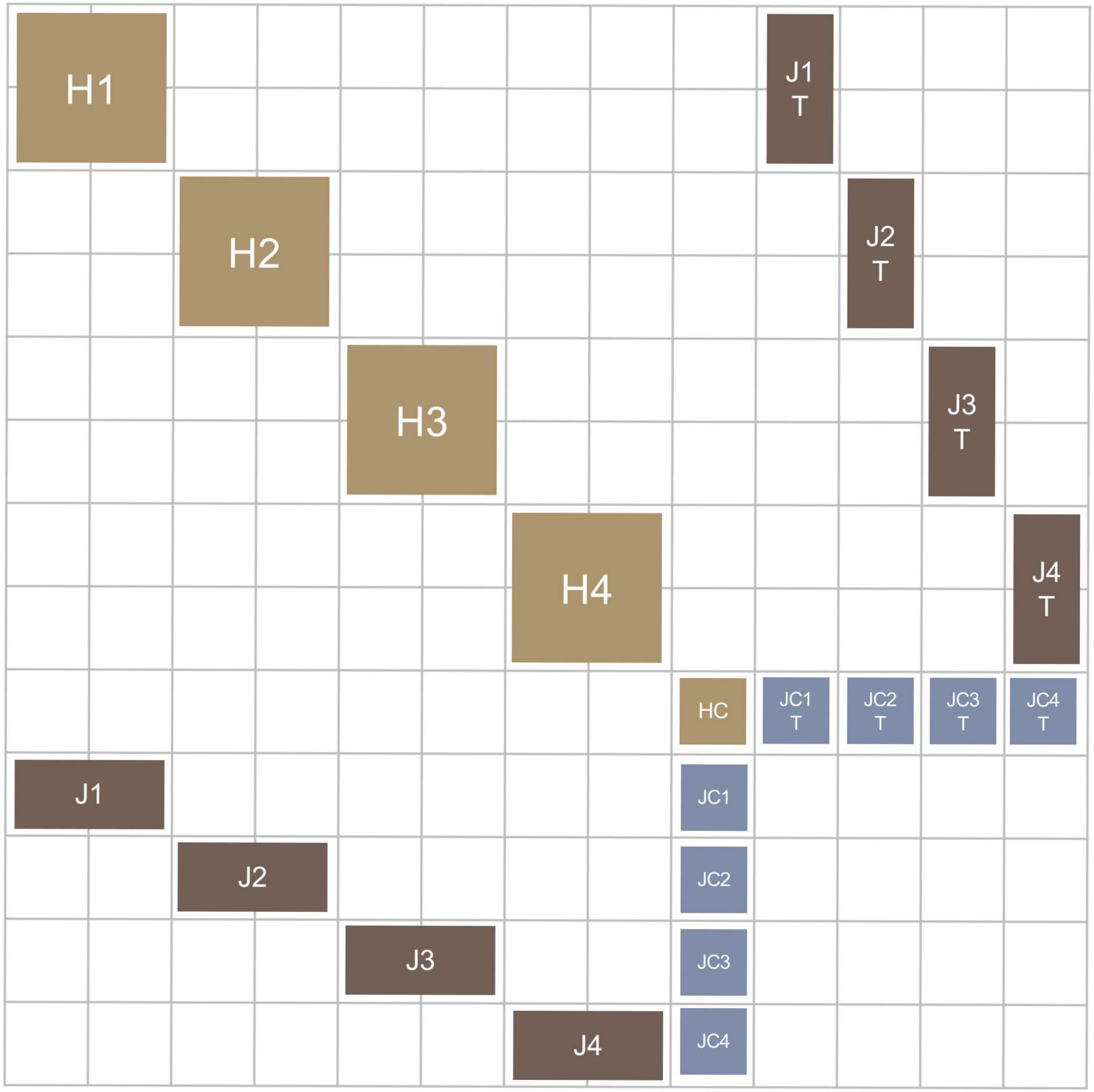
Dynamic Optimization

- block structure because of finite element discretization

$$\begin{aligned} \min_{u} \int_{t_0}^{t_f} & L(x, y, u)\, dt \\ \text{s.t.}\;\; & F(\dot{x}, x, y, u) = 0 \\ & x(t_0) = x_0 \\ (x, y, u)^L \leq & (x, y, u) \leq (x, y, u)^U \end{aligned}$$



Word, D.P., Kang, J., Akesson, J., and Laird, C.D., "Efficient Parallel Solution of Large-Scale Nonlinear Dynamic Optimization Problems", Computational Optimization and Applications, 2014.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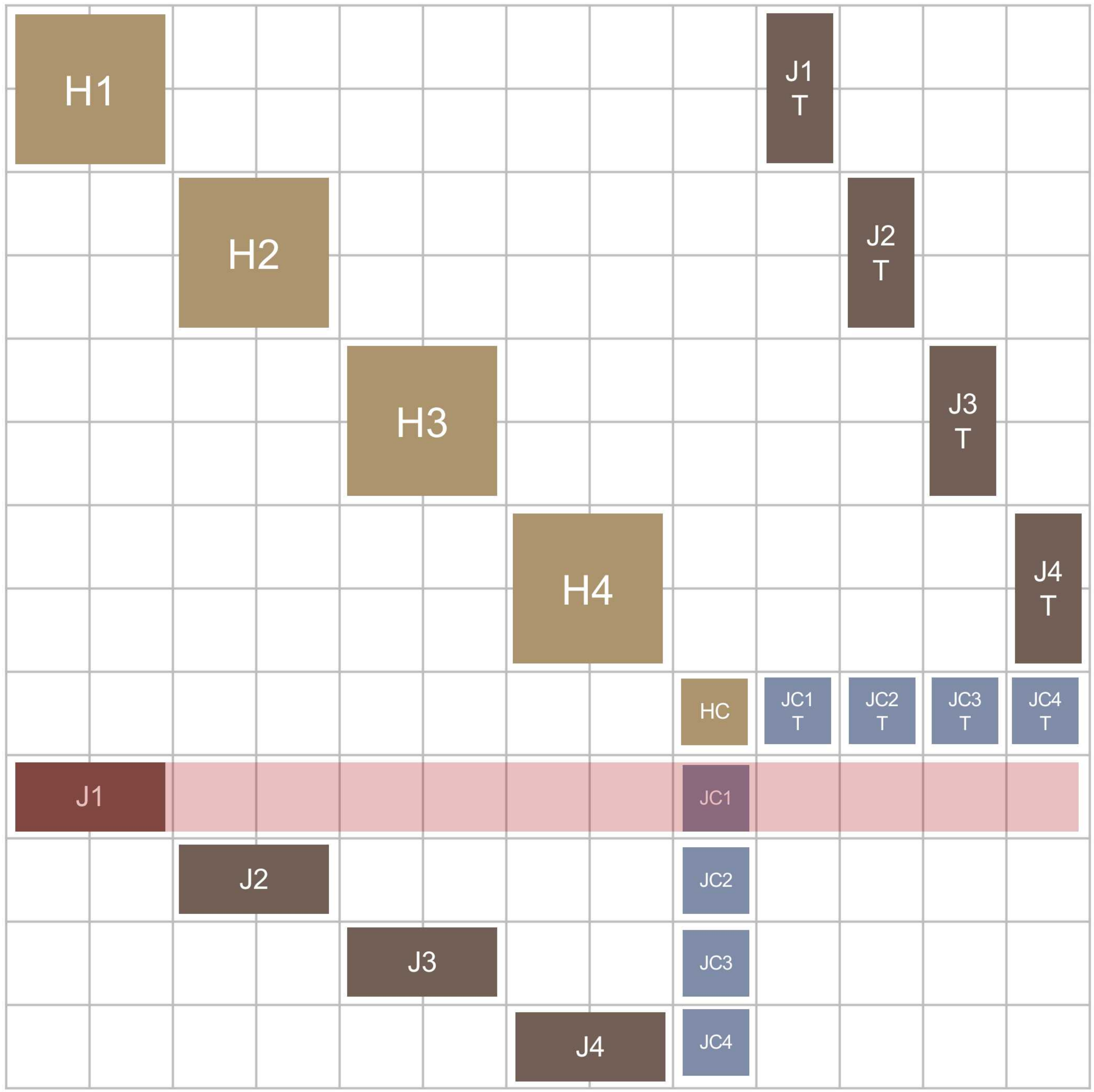
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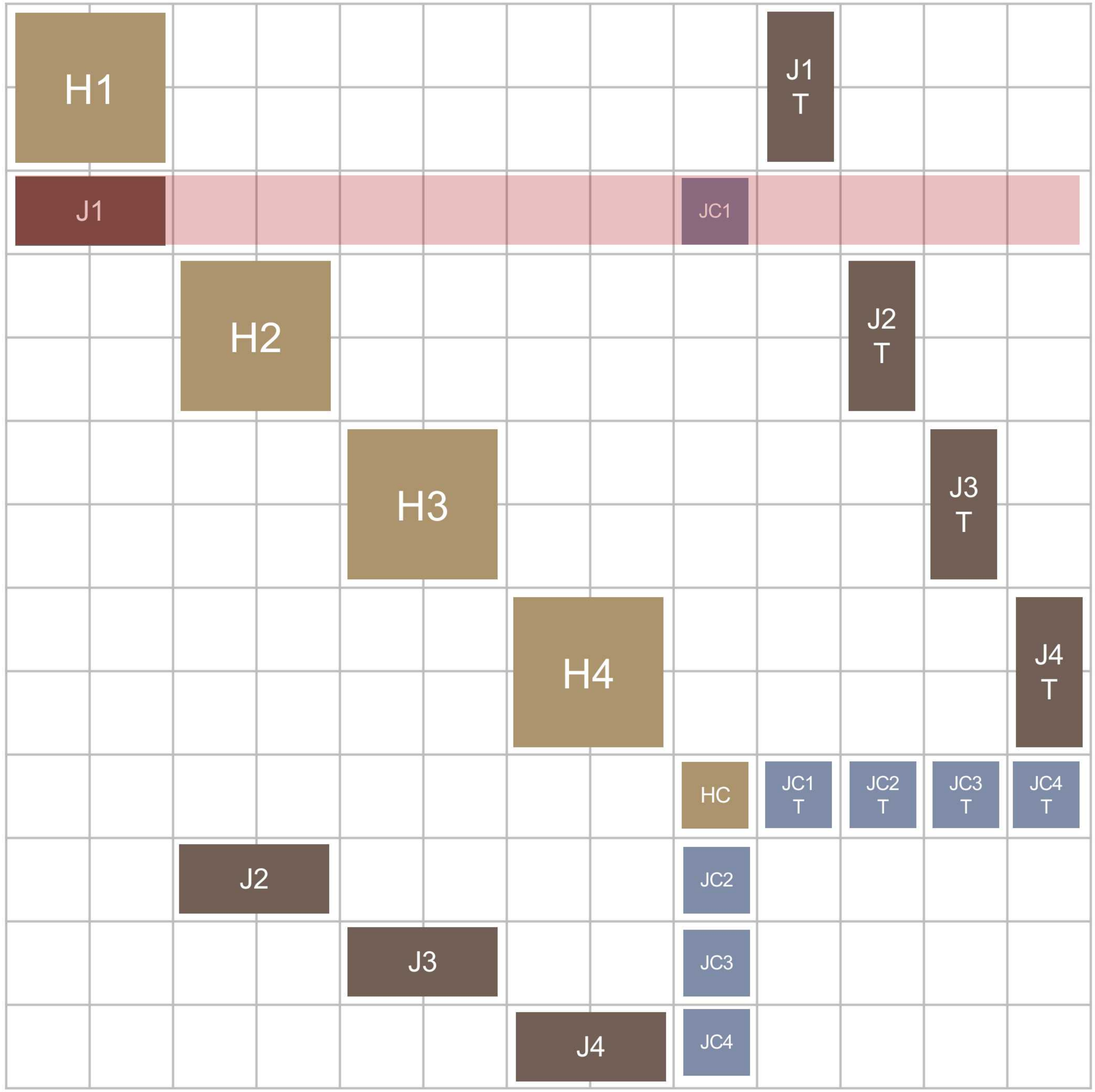
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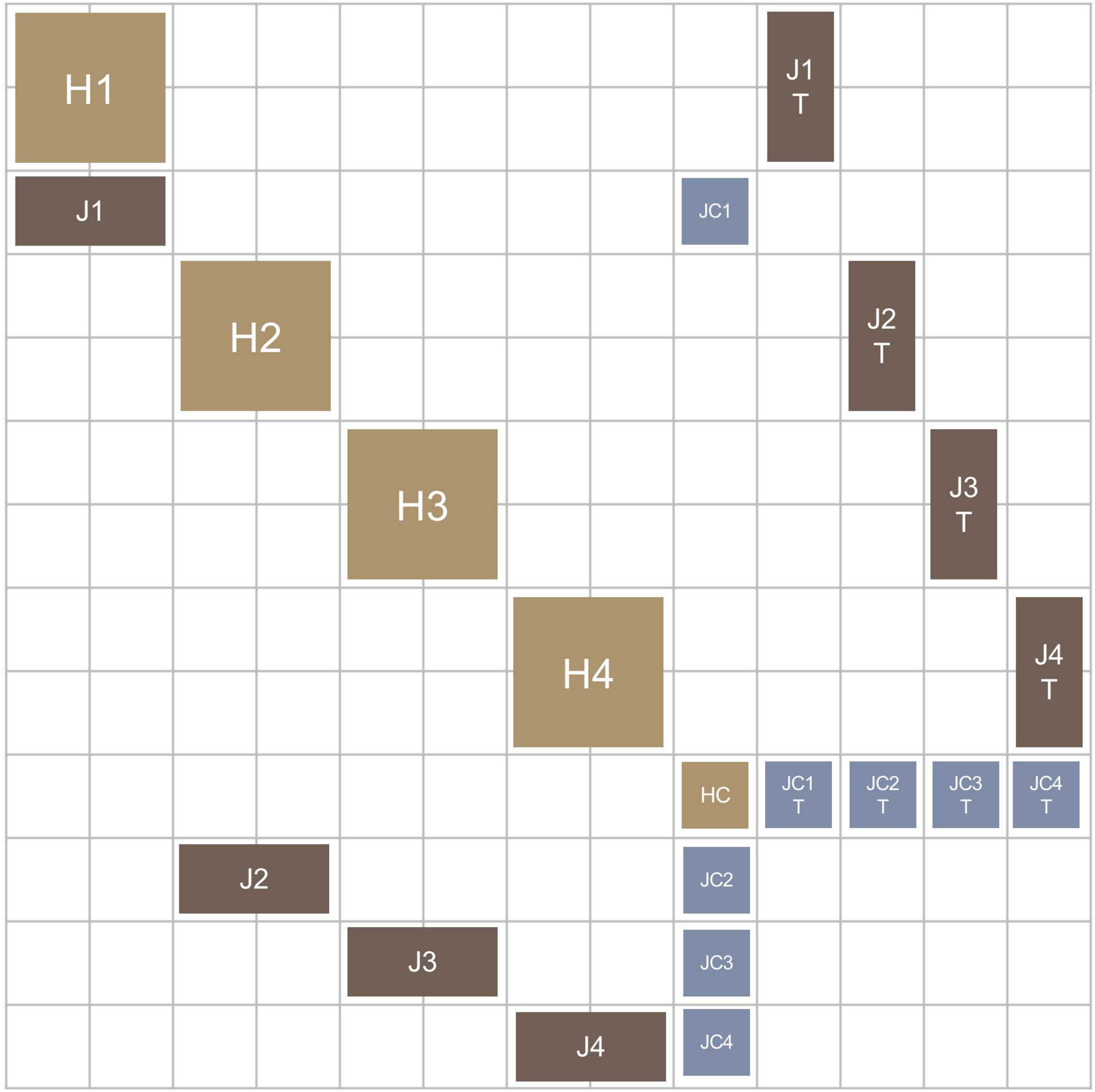
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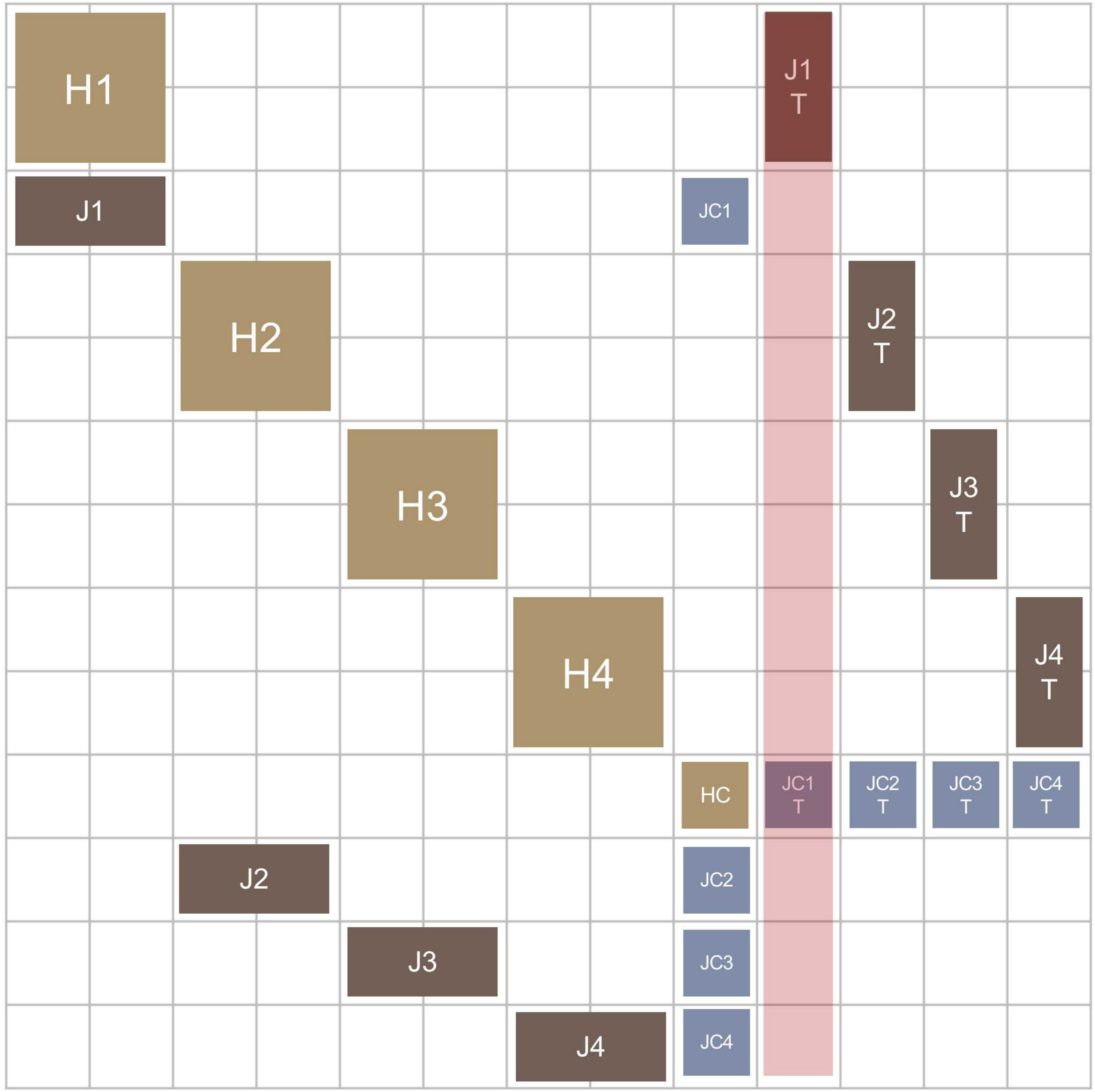
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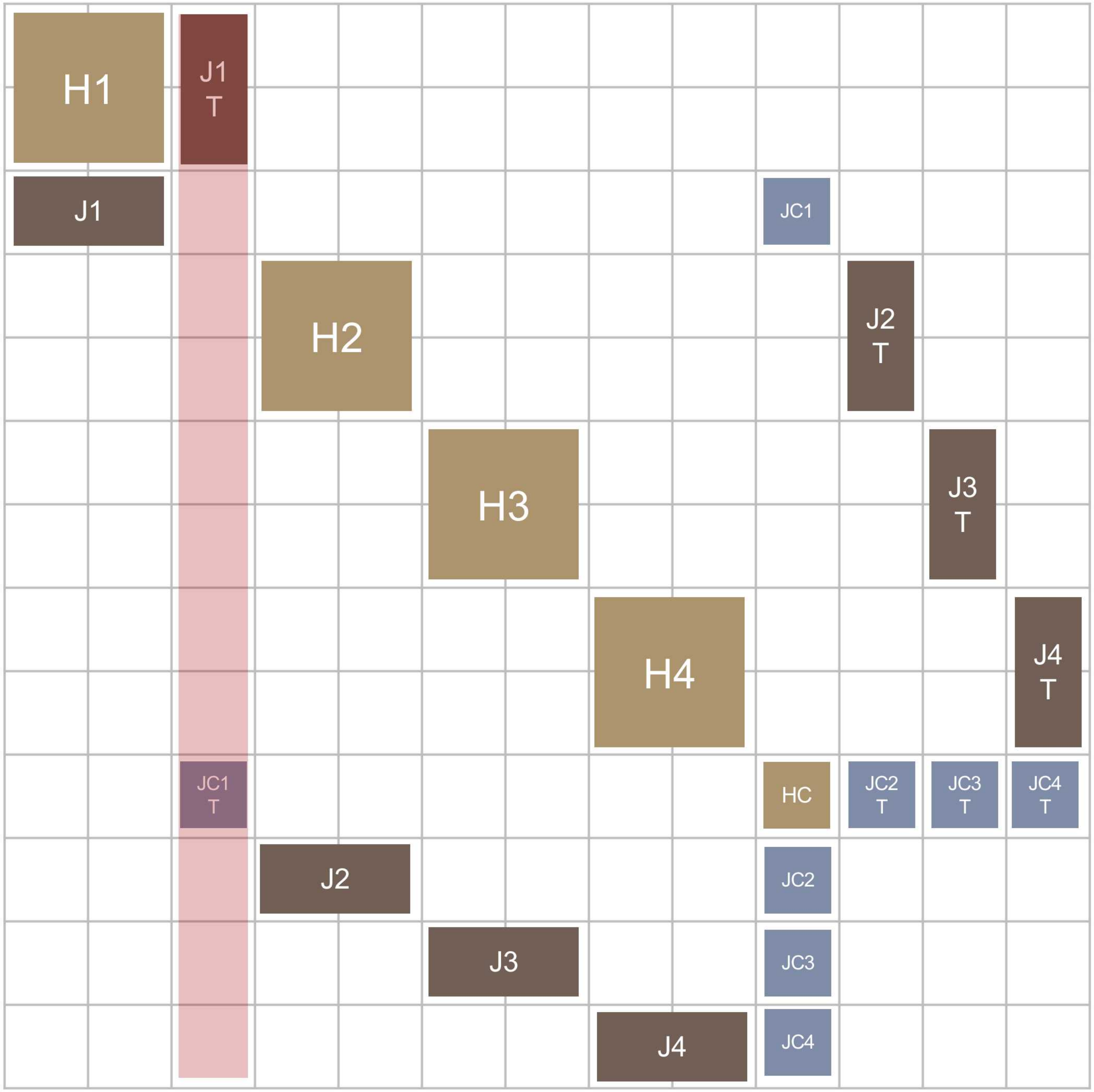
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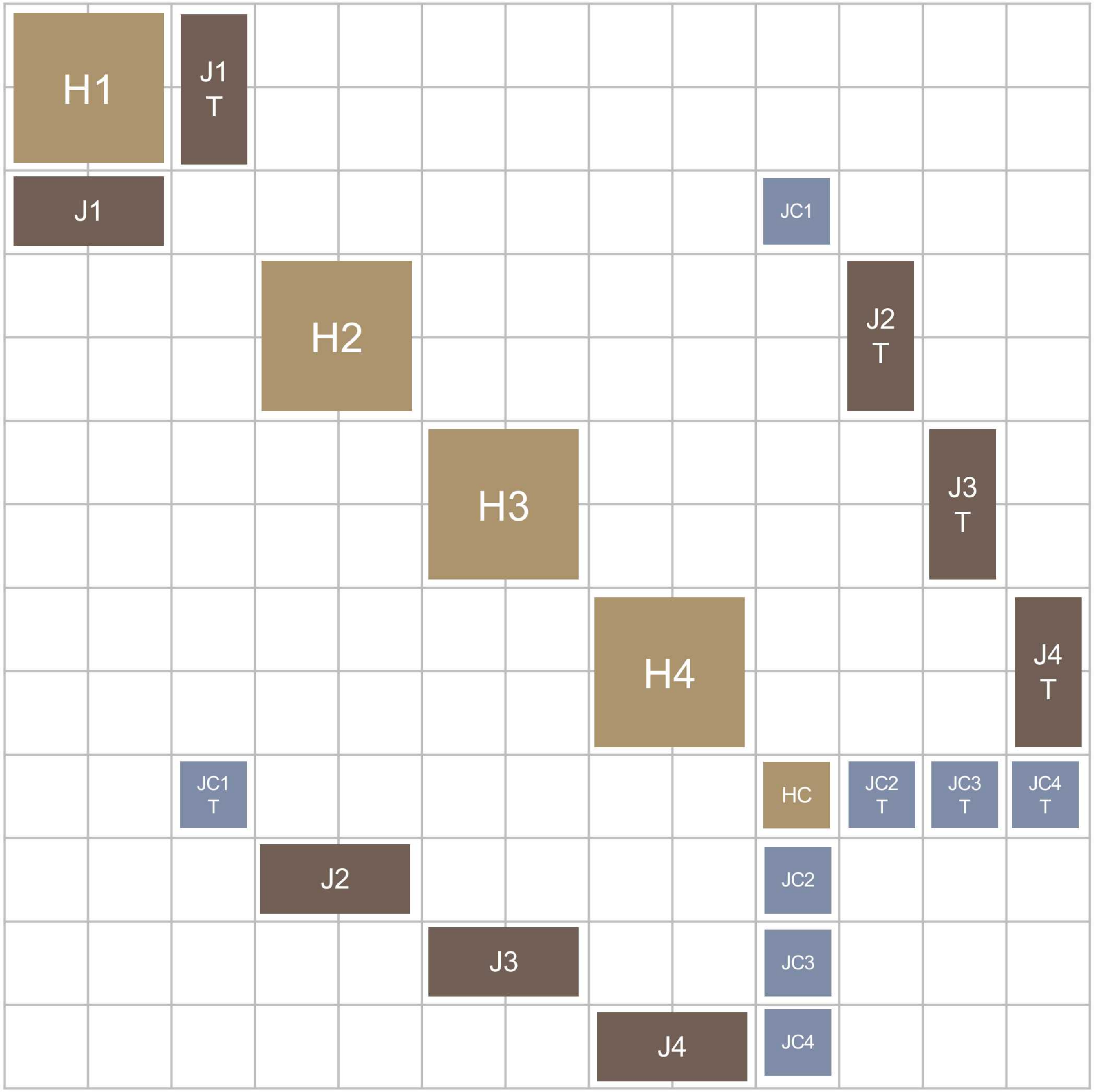
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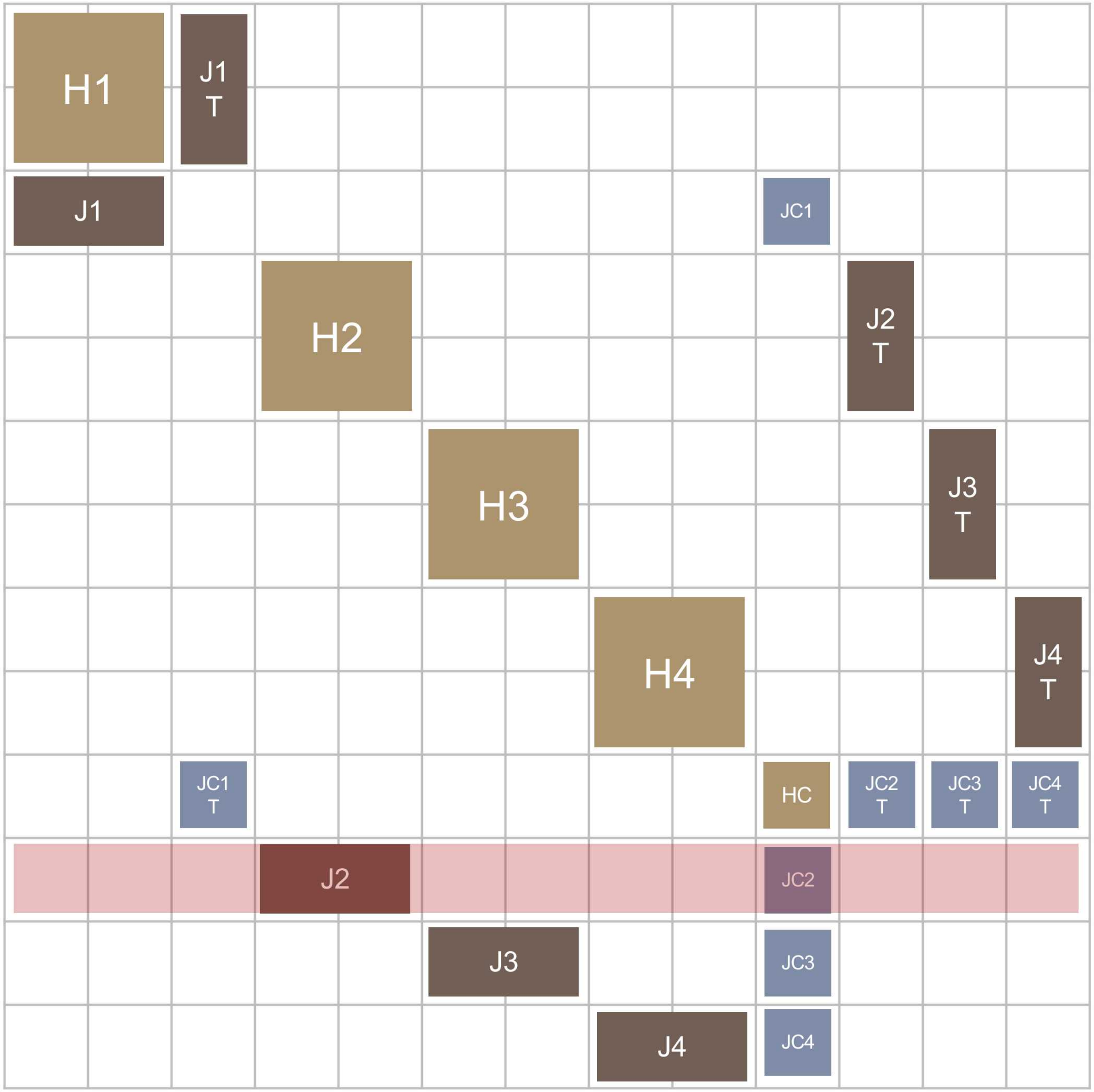
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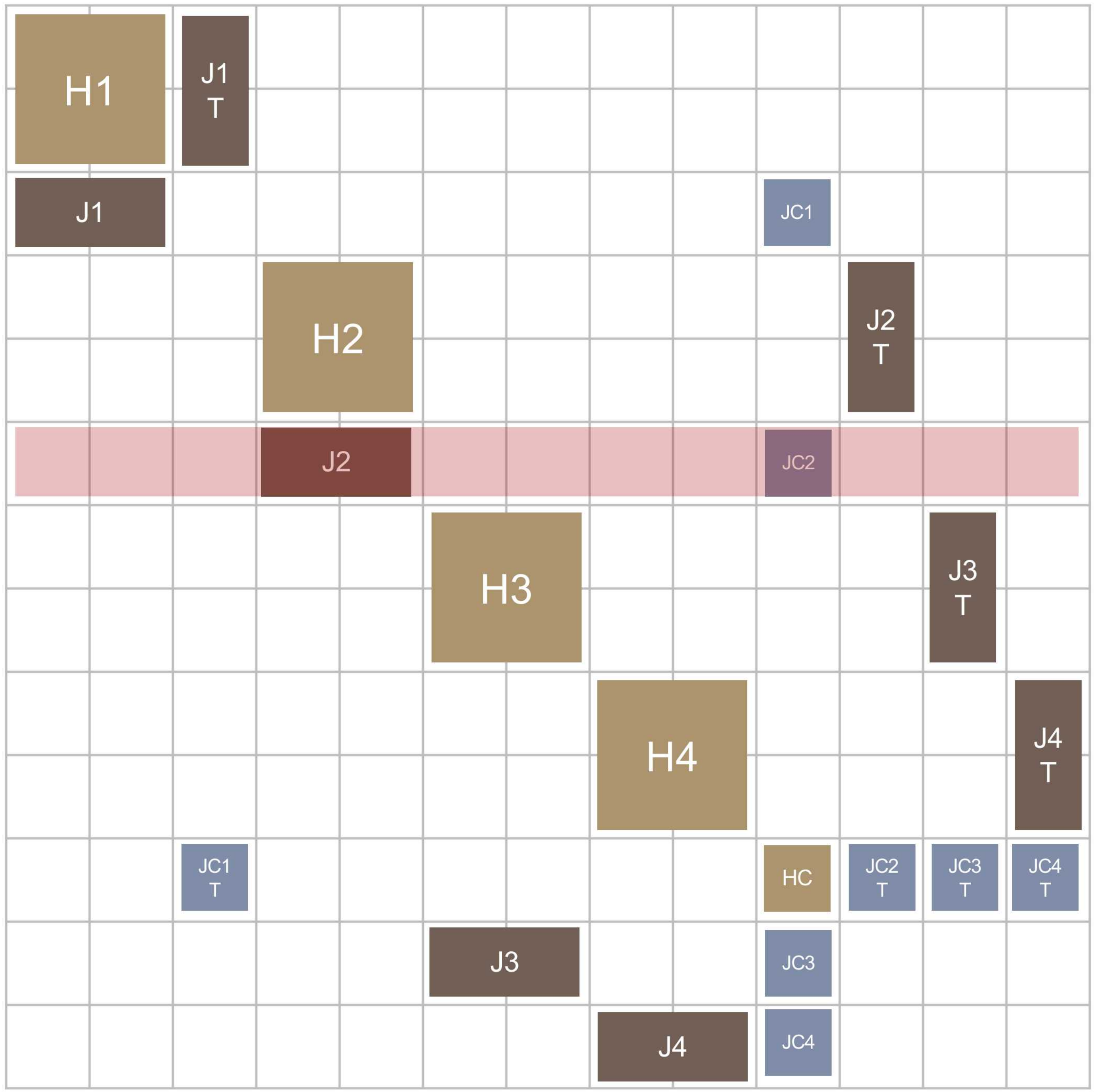
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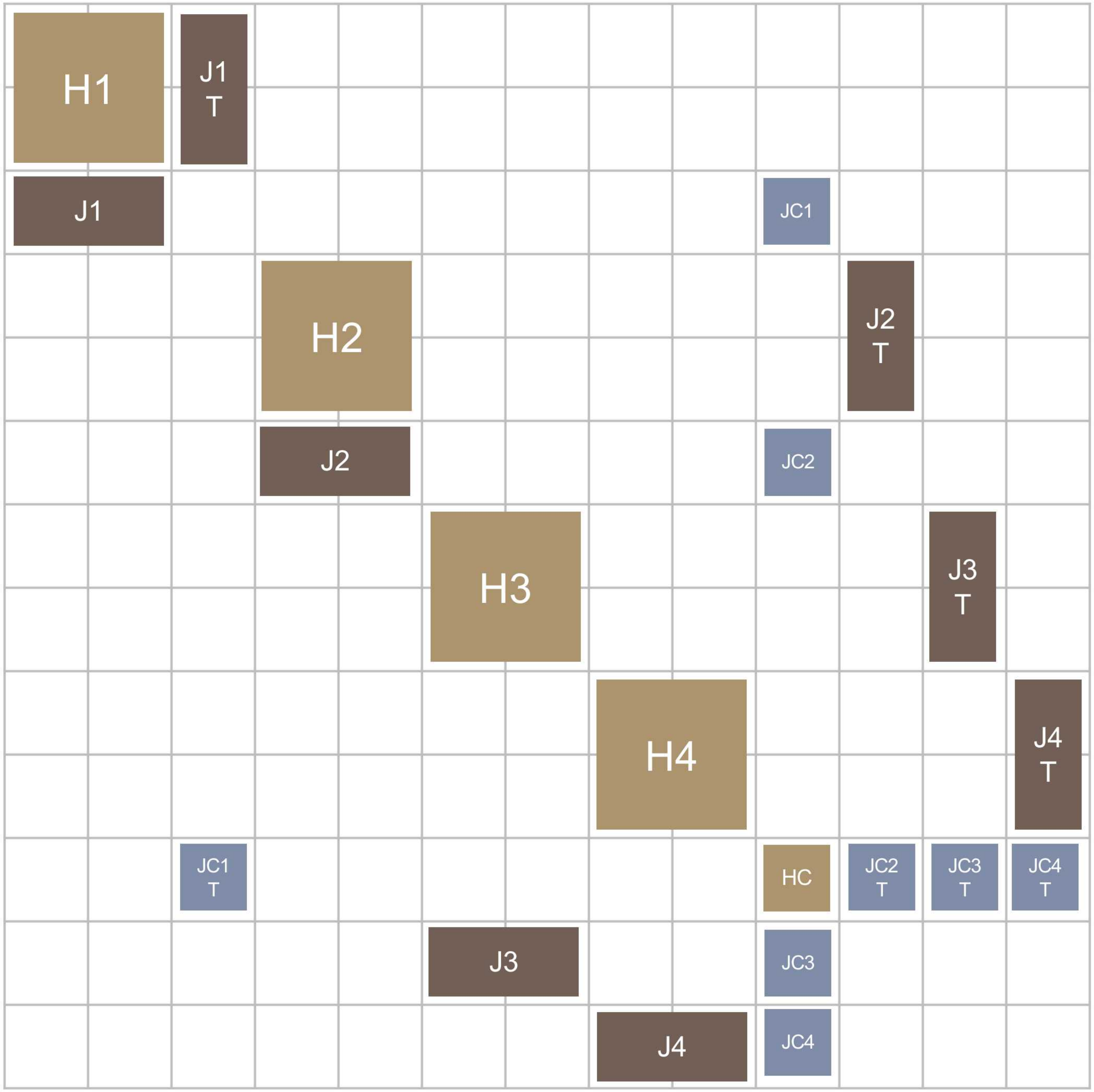
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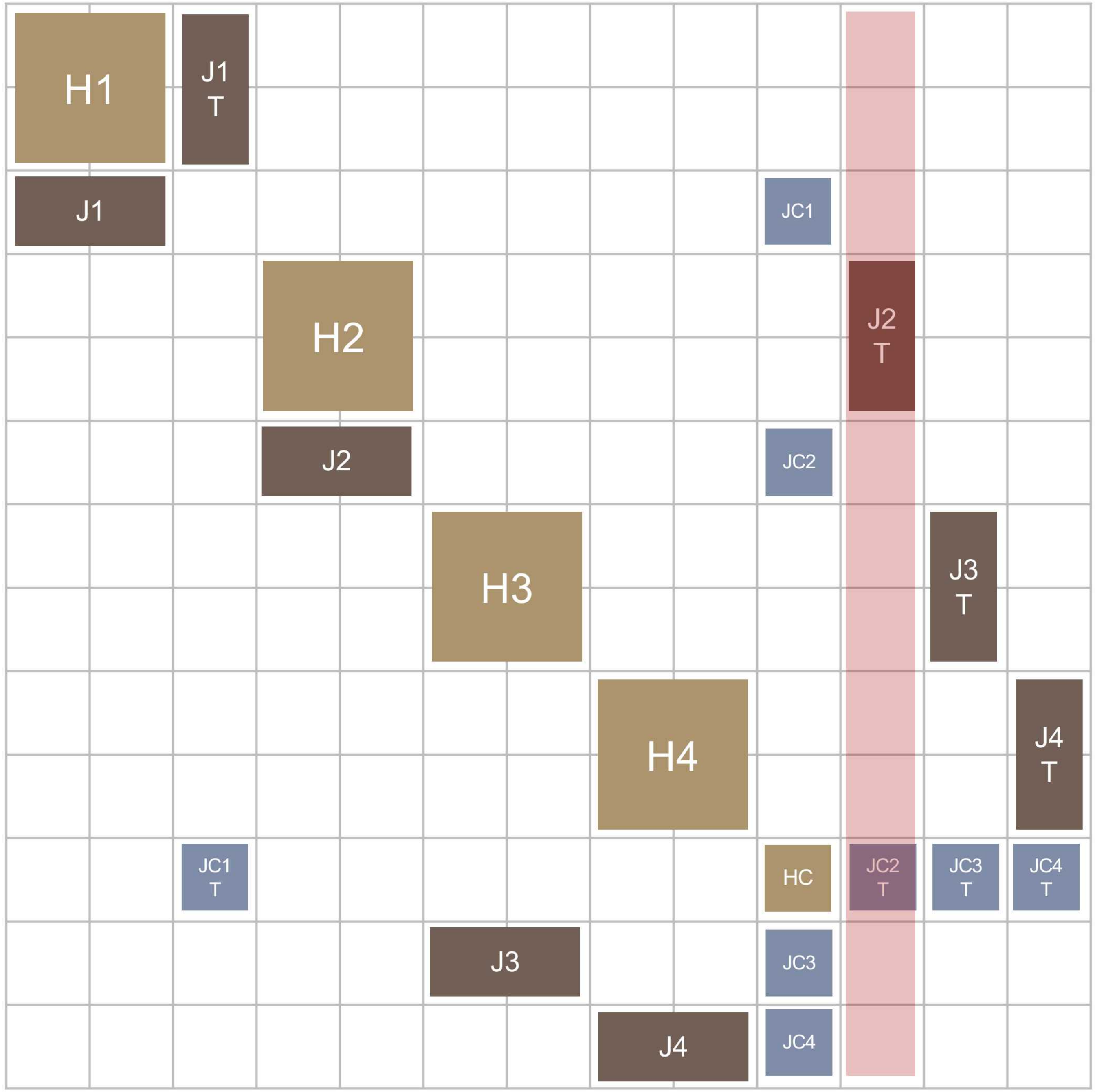
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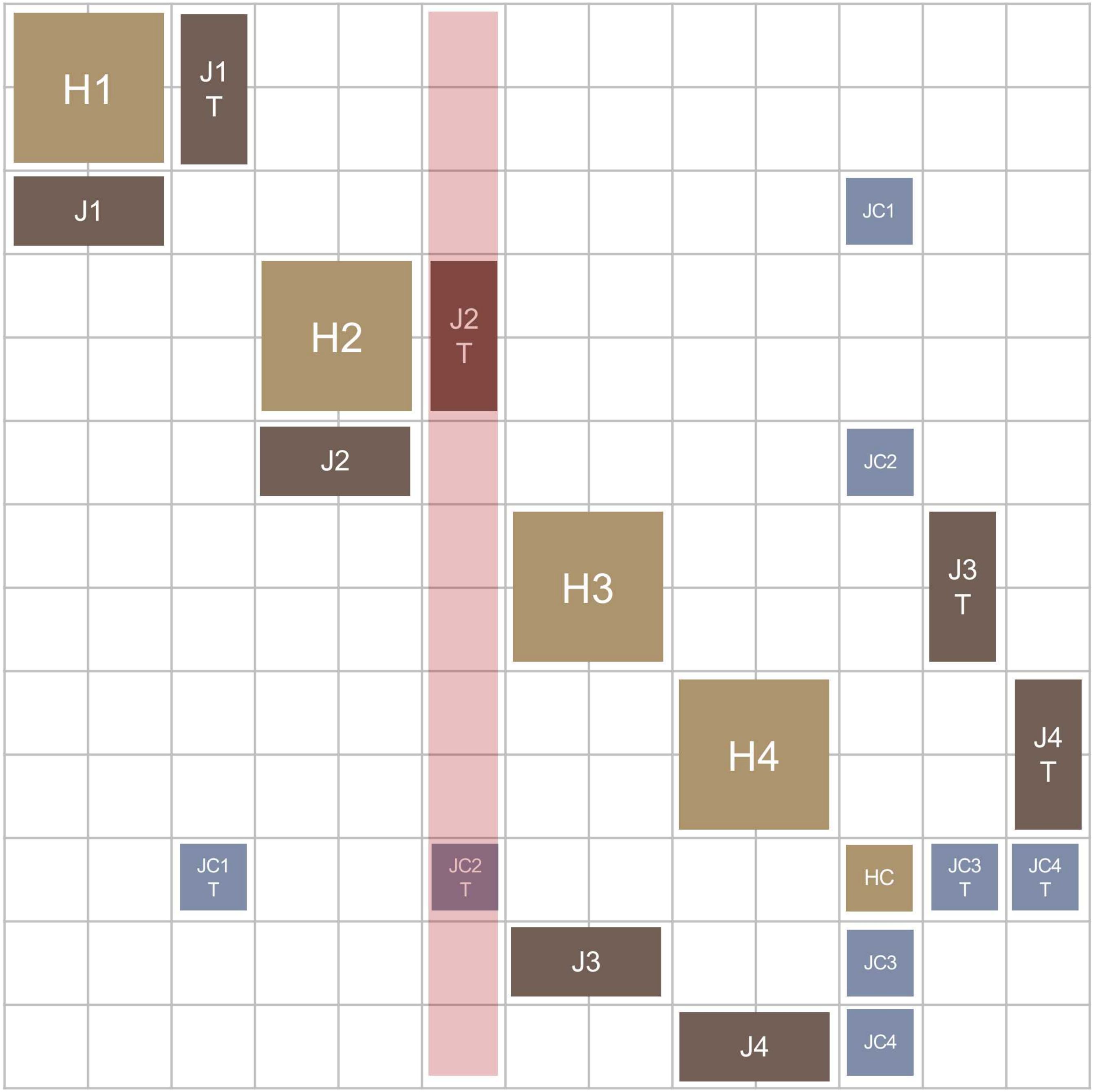
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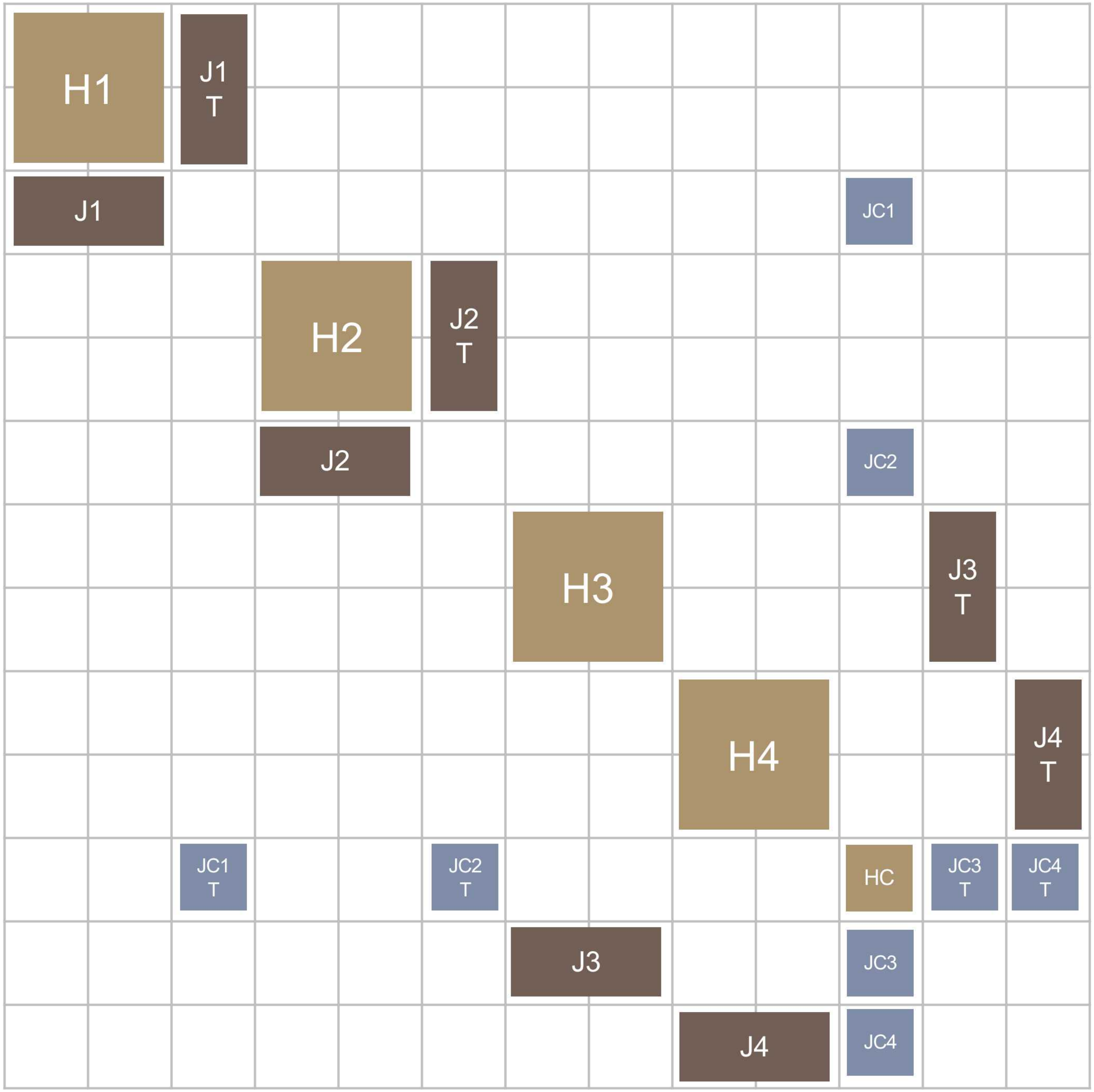
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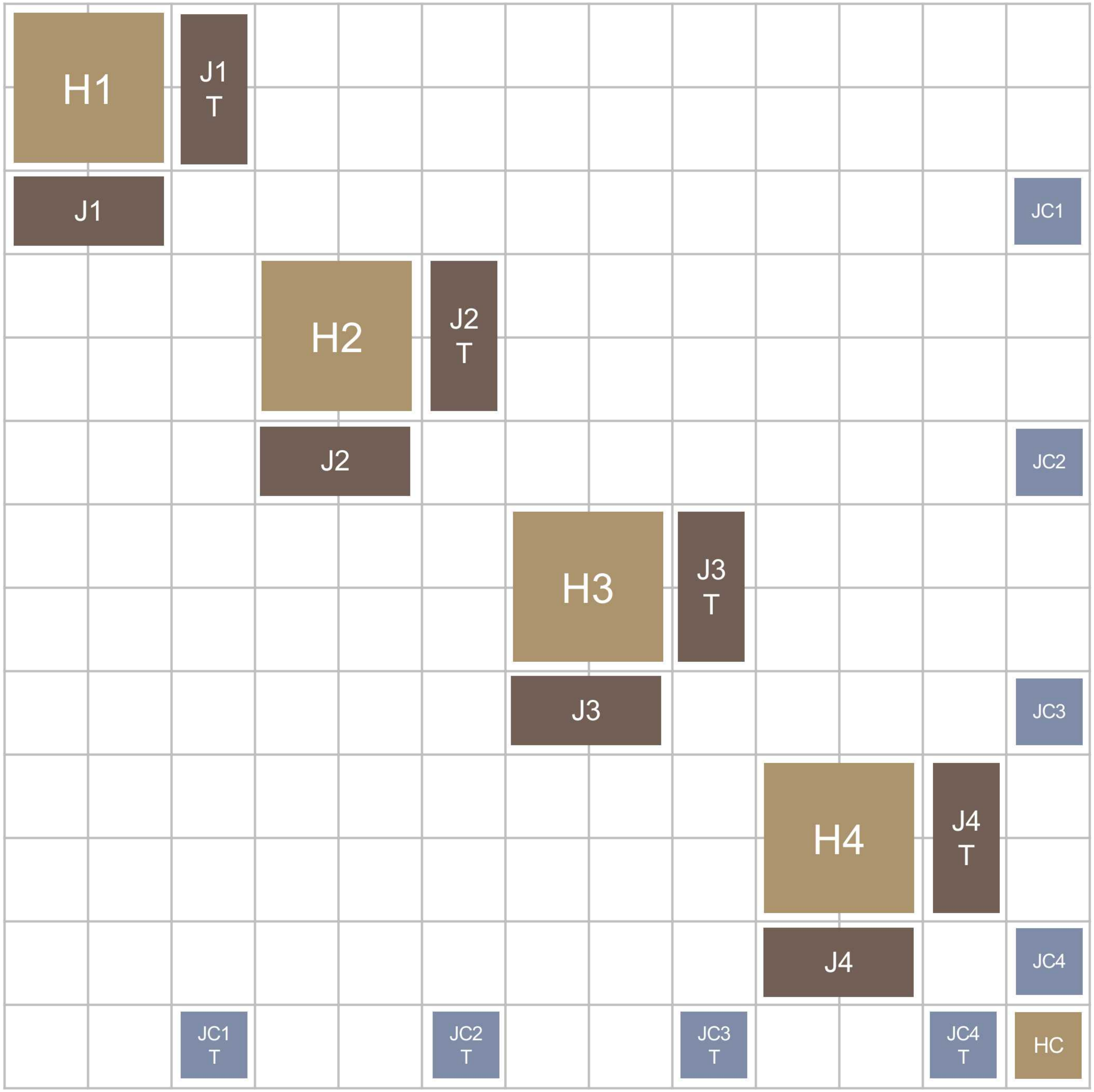
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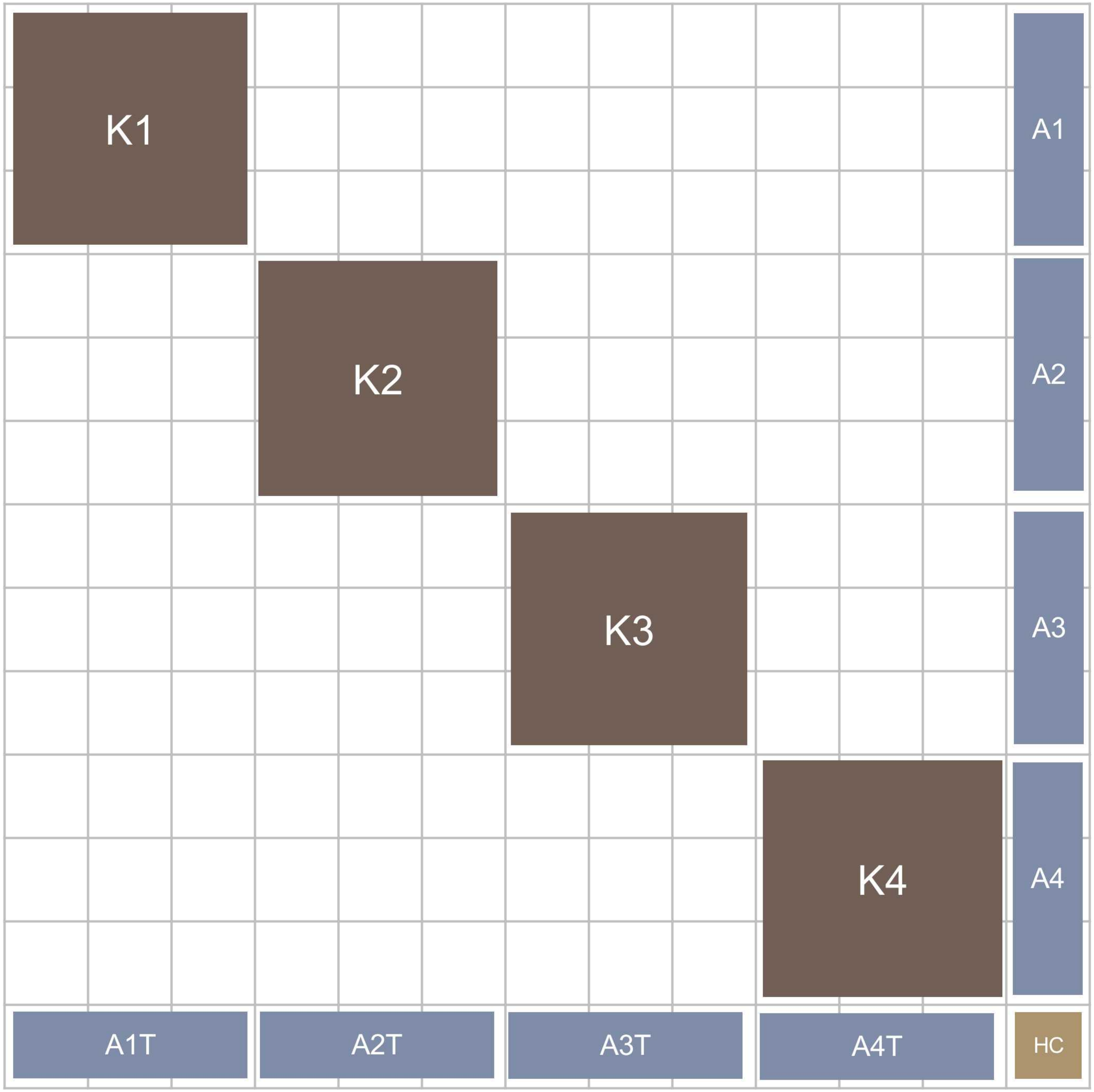
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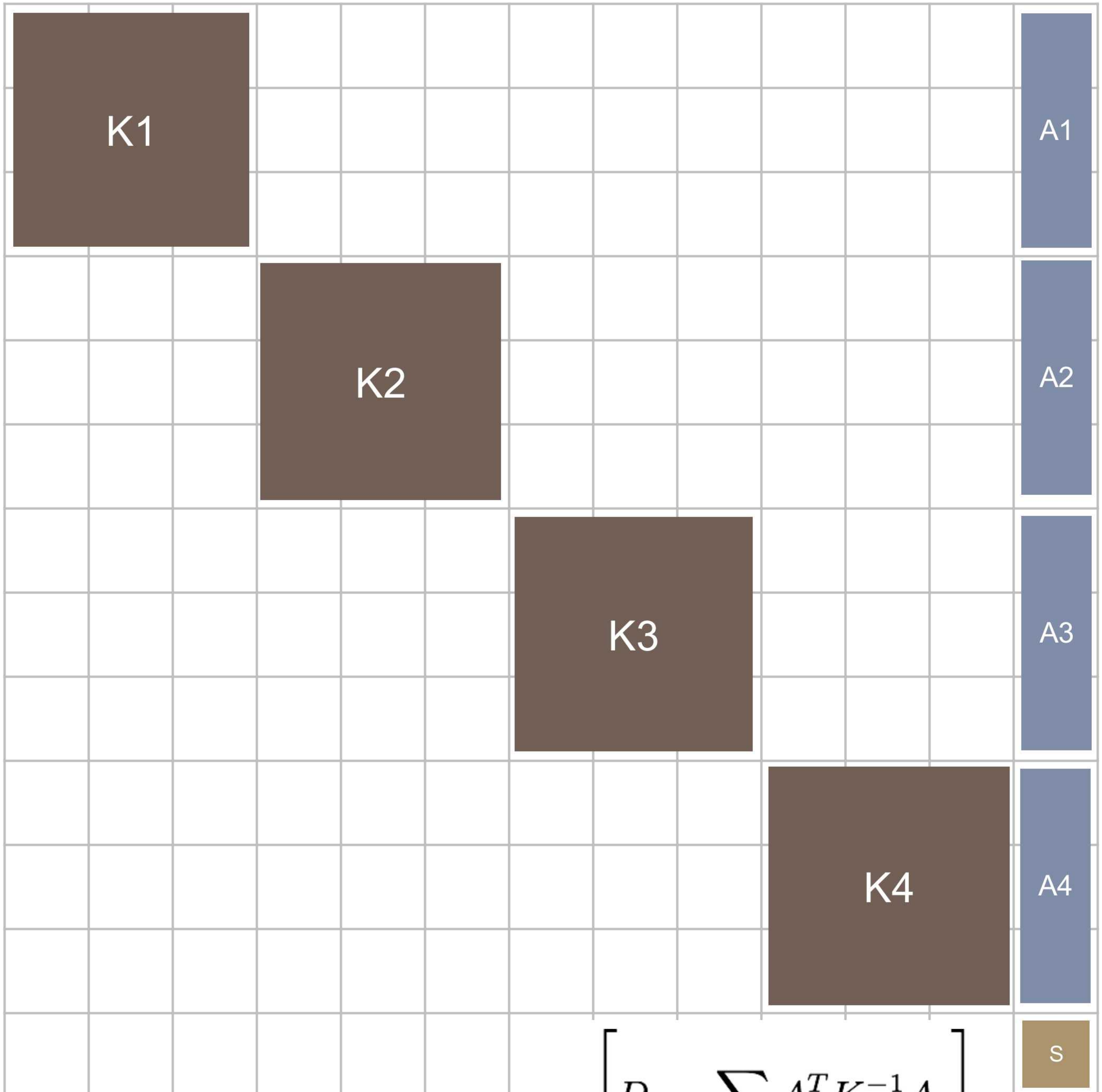

$$\left[D_y - \sum_{q \in Q} A_q^T K_q^{-1} A_q \right]$$

$$\left[D_y - \sum_{q \in Q} A_q^T K_q^{-1} A_q\right] \Delta y = r_y - \sum_{q \in Q} A_q^T K_q^{-1} r_q$$

1: for each i in $1, ..., n_e$

  1.1: factor K_i

Factor K Blocks

2: let $S = [-\delta_c I]$

3: let $r_{sc} = r_s$

4: for each i in $1, ..., n_e$

  4.1: for each column j in A_i^T

    4.1.1: solve the system $K_i q_i^{<j>} = [A_i^T]^{<j>}$

    4.1.2: let $S^{<j>} = S^{<j>} + A_i q_i^{<j>}$

  4.2: solve the system $K_i p_i = r_i$

  4.3: let $r_{sc} = r_{sc} - A_i p_i$

Form Schur-Complement

5: solve $S \Delta\nu_s = r_{sc}$ for $\Delta\nu_s$

Solve Schur-Complement

6: for each i in $1, ..., n_e$

  6.1: solve $K_i \Delta\nu_i = r_i - A_i^T \Delta\nu_s$ for $\Delta\nu_i$

Solve Remaining Vars

$$\left[D_y - \sum_{q\in Q} A_q^T K_q^{-1} A_q\right] \Delta y = r_y - \sum_{q\in Q} A_q^T K_q^{-1} r_q$$

1: ~~for each i in $1, \ldots, n_e$~~

1.1: factor K_i

Factor K Blocks

2: let $S = [-\delta_c I]$

3: let $r_{sc} = r_s$

4: ~~for each i in $1, \ldots, n_e$~~

4.1: for each column j in A_i^T

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Solve Remaining Vars

Explicit Schur-Complement Decomposition

LDPE Process

- Parameter estimation problem [Zavala et al. 2008]

Water network optimization

- Spatial decomposition of network [Zhu, 2011]

Operation of air separation plants

- Dynamic load change under uncertainty
- Optimal operation with uncertain demand and energy pricing [Zhu, Legg, Laird, 2011a,b]

N-1 Contingency constrained ACOPF (current work)

Explicit SC does not scale well to large coupling variables

- Excellent when number of coupling variables is small (~100 variables)
- Time to form and factor the Schur-complement becomes bottleneck

Implicit-PCG-SC for problems with significant coupling

Implicit PCG Approach for Strongly Coupled Systems

Solve Schur-complement implicitly, iteratively using PCG
- Never Explicitly Form Schur-complement
- Requires Only 1 Backsolve of K-block per PCG Iteration

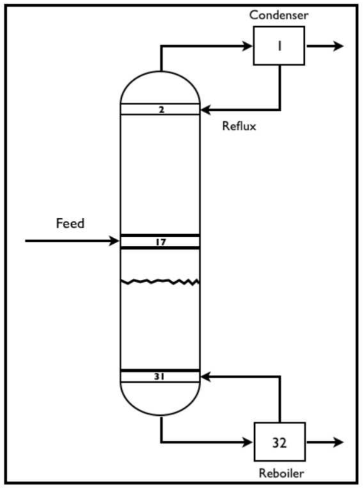
$$\left[D_y - \sum_{q \in Q} A_q^T K_q^{-1} A_q \right] \Delta y$$

Preconditioner for the Schur-complement system
- Automatic preconditioning [J.L. Morales, and J. Nocedal, 2000]
- L-BFGS update using CG steps from the previous IP iteration
- In practice, significantly fewer than n PCG iterations

Schur-complement must be positive semi-definite
- closely tied to the inertia condition

Parallel Performance: Optimization Under Uncertainty

Sandia National Laboratories



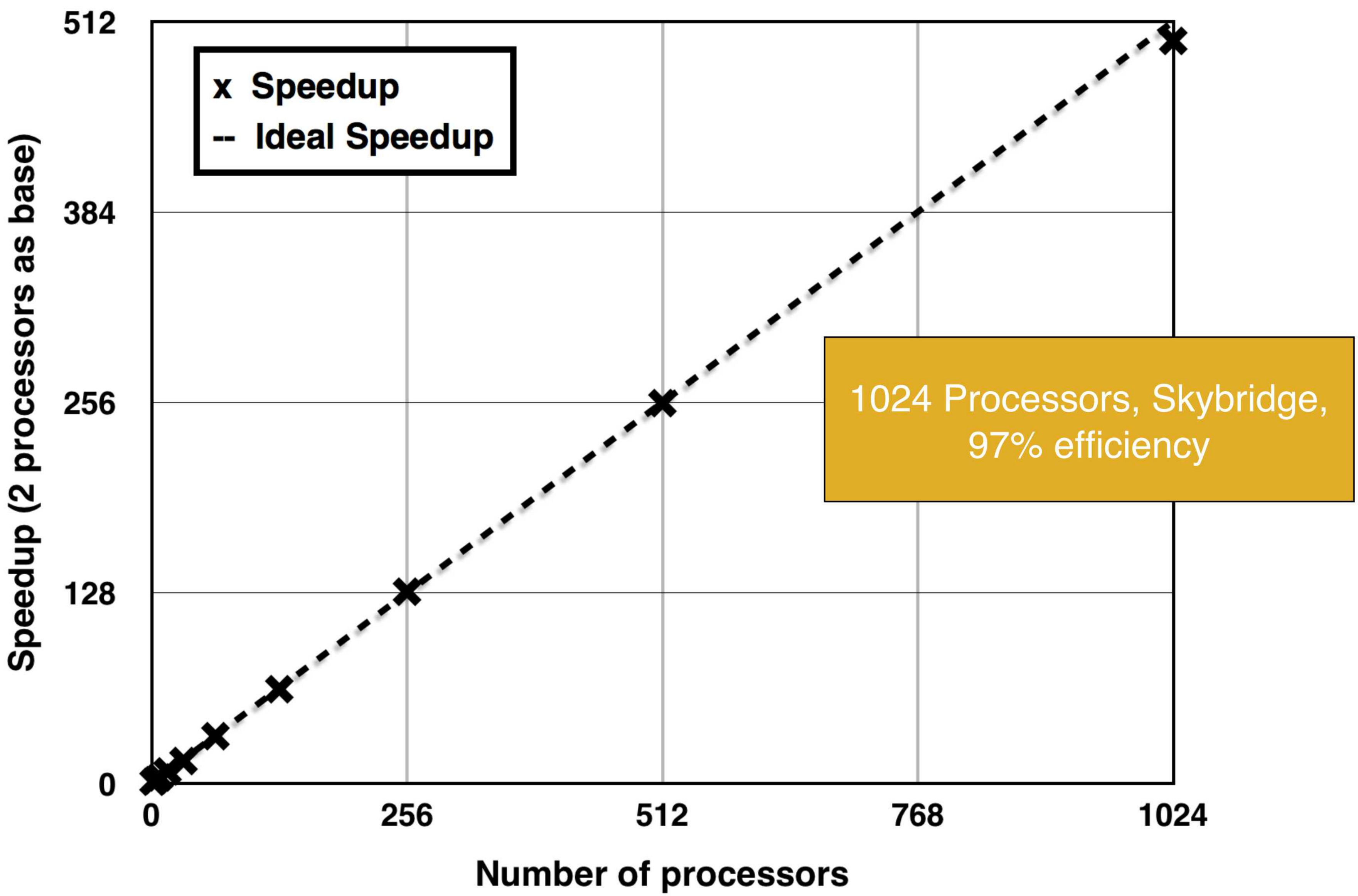
- 32 state variables, 35 algebraic variables
- Discretize model (OCFE)
- Uncertainty in mole fraction of the feed stream
- 96 scenarios, 32 processors

[Benallou, Seborg, and Mellichamp (1986)]

Case	# Vars.	# Coupling Vars.	FS-S time(s)	ESC-S time(s)	ESC-P time(s)	PCGSC-S time(s)	PCGSC-P time(s)
1	1430550	150	10.3	79.1	2.6	17.9	0.6
2	2861100	300	-	-	10.8	-	1.1
3	4291650	450	-	-	32.1	-	2.4
4	5722200	600	-	-	70.3	-	3.2
5	7152750	750	-	-	90.5	-	4.3
6	8583300	900	-	-	160.5	-	5.3
7	10013850	1050	-	-	218.0	-	6.3
8	11444400	1200	-	-	286.6	-	8.1

Kang, J., Word, D.P., and Laird, C.D., "An Interior-point Method for Efficient Solution of Block-structured NLP Problems using an Implicit Schur-complement Decomposition", Computers and Chemical Engineering, vol 71, Dec. 2014, pp 563-573

Parallel Performance: Strong Scaling



Summary and Conclusions

Tremendous opportunities for rigorous mathematical programming approaches in science and engineering

Emerging science and engineering problems continue to push the capabilities of scientific computing tools

No more free lunch…

Summary and Conclusions

Applications, Architectures, Algorithms, Adoption

- Need to understand the applications, assumptions
  - Structure: Uncertainty, discretization, spatial/network, data
- Need to understand architectures
  - E.g. Big-Iron clusters, shared-memory multi-core, GPU
  - Not all parallel architectures created equal
- Need for new algorithms
  - Tailored decomposition based on interior-point methods
  - Problem level decomposition strategies
  - Strategies are problem and architecture dependent
- Need to make tools available for other researchers
  - Open-source parallel algorithms
  - Pyomo: Optimization Modeling in Python

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Ahmed Rabie
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Chen Wang
Sean Legg
Daniel Word
Angelica Wong
Xiaorui Yu
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