SAND2019-4317PE

Exceptional service in the national interest

Sandia National Laboratories

Convergence of Operations Research with Safety and Security

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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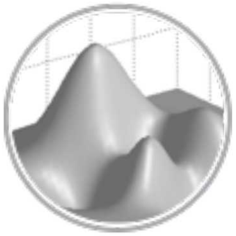
Research Group Skills

Modeling of Complex Systems

Rigorous systems modeling (steady-state and transient)

Large-scale, non-traditional, networked systems



Nonlinear and Discrete Mathematical Programming

Large-scale algorithms and problem formulation

Parallel algorithms for structured problems (e.g., uncertainty)

Software and Scientific Computing

Open-source domain-specific tools (WST, WNTR, EGRET)

General modeling and optimization tools (Pyomo, Schur-IPOPT)

Mathematical Programming

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

Mathematical programming (i.e. Optimization)

Problem types classified according to:

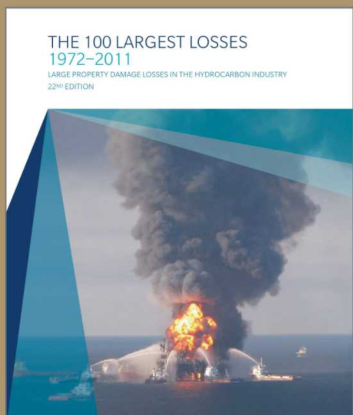
- Linearity/Nonlinearity of objective and constraints
- Continuous/Discrete/Mixed variables

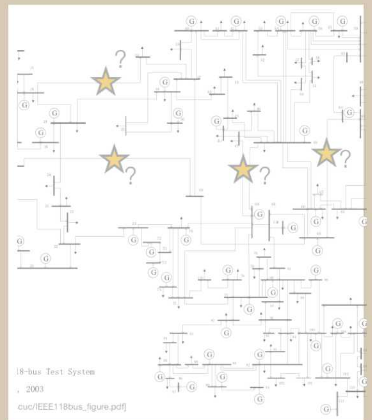
LP, QP, NLP, MILP, MINLP

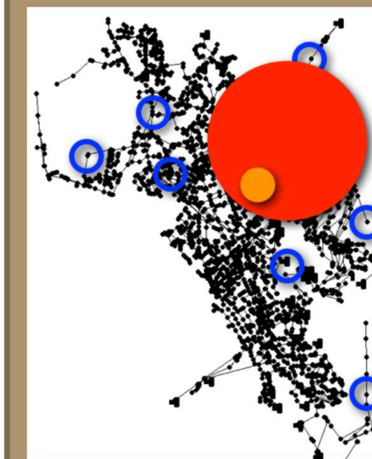
Useful for much more than… “optimization”

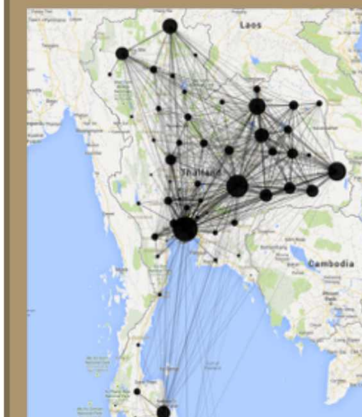
Convergence of Operations Research and …

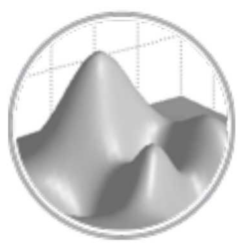
P2SAC, MKOPSC	FERC, Sandia	EPA, Sandia	U. Florida, Hopkins
Safety Systems Design	Powergrid Optimization	Water Security	Infectious Disease Spread

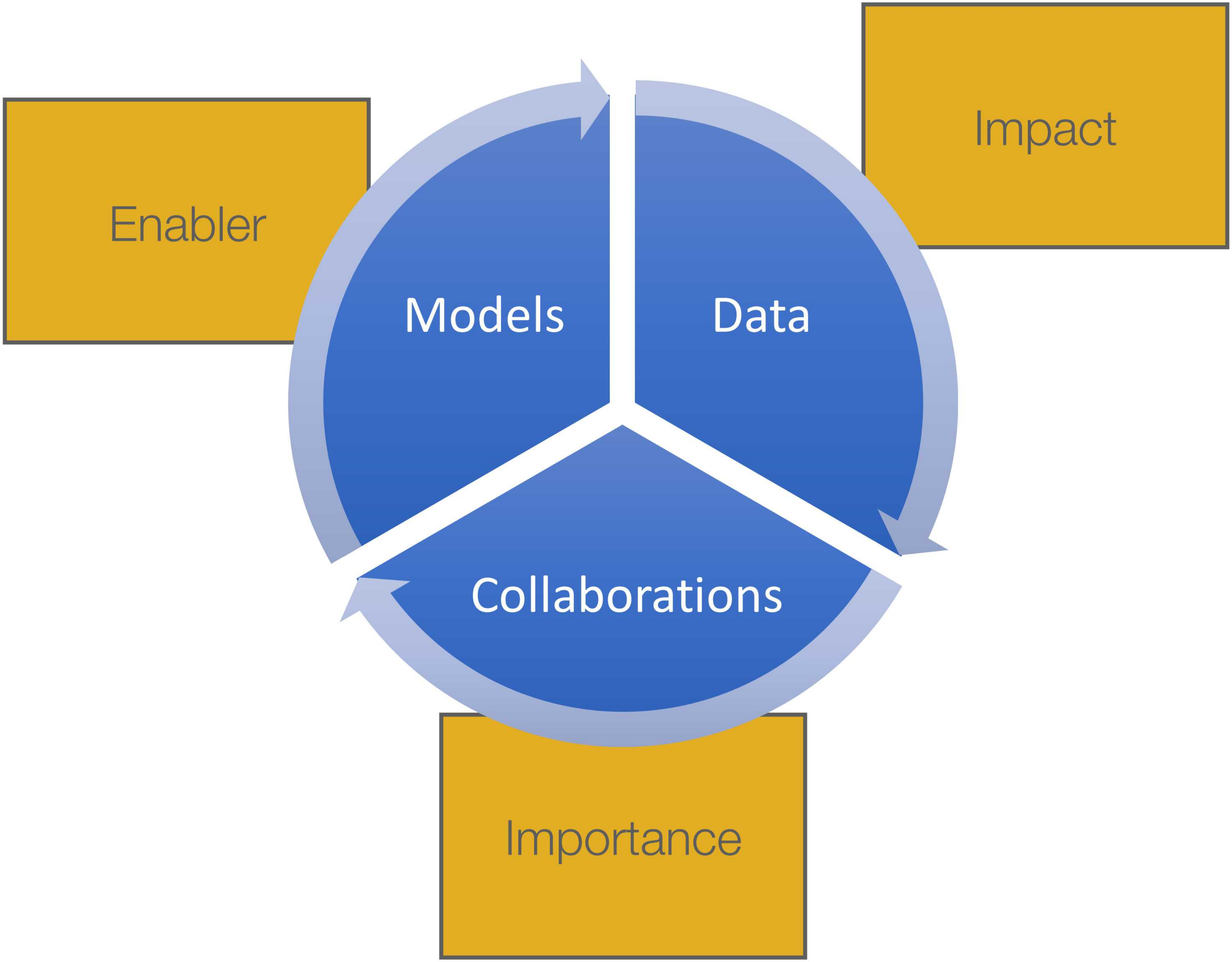




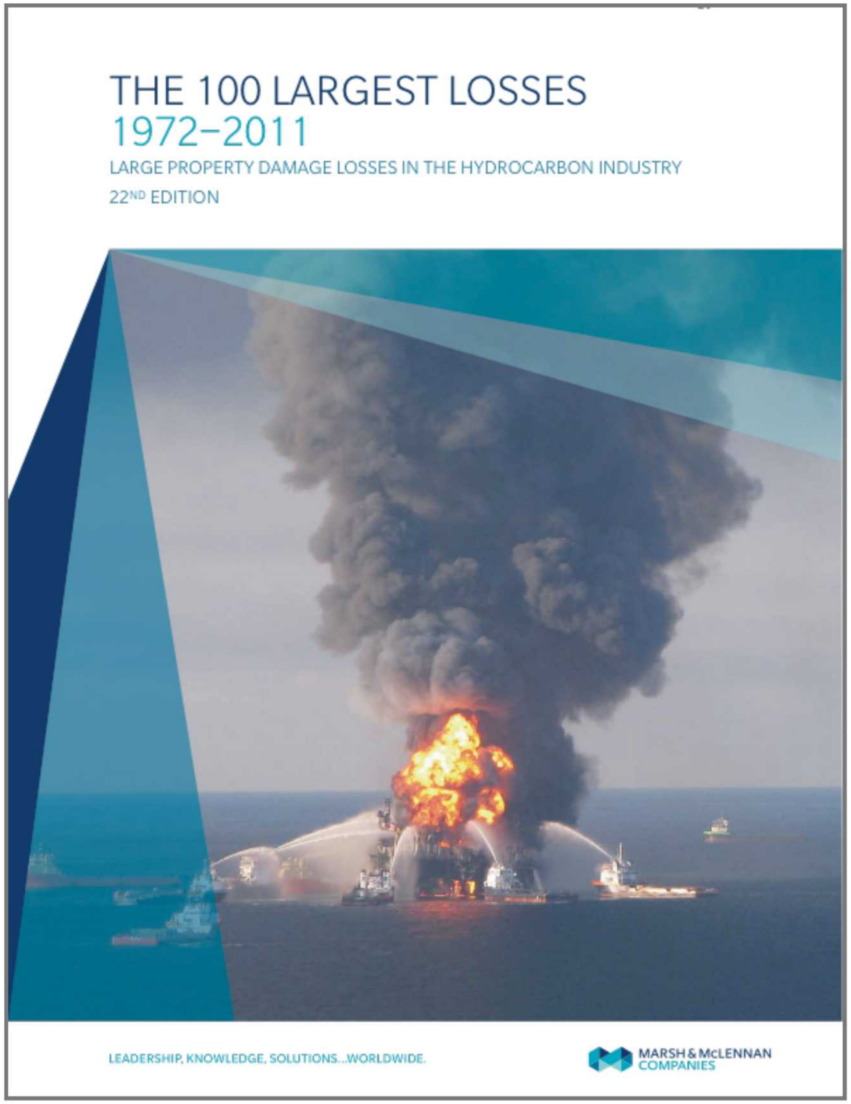







Enabler
Impact
Models
Data
Collaborations
Importance

The need for improved gas detector placement



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

70% attributed to fires and explosions

BSEE (2012), HSE (2007) and PSA (2012) data do not indicate a decreasing trend.

Less than 50% of all known releases are detected by gas detectors (HSE, 1997 & 2003)

-

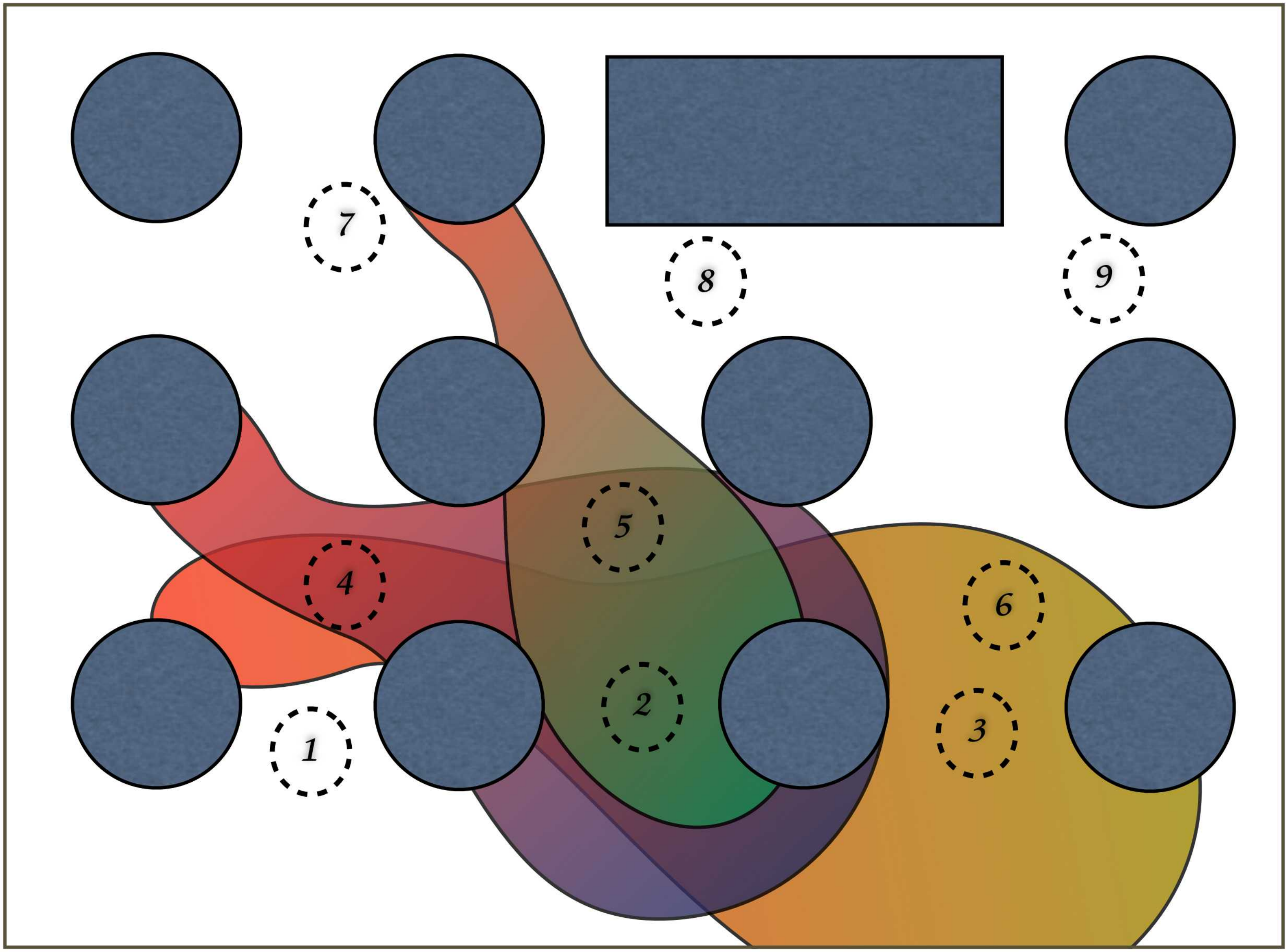
Significant uncertainty (leak location, weather, process conditions, etc.)

Highly complex geometries (difficult to model)

Design of gas detector systems currently done with rule-of-thumb, semi-quantitative methods.

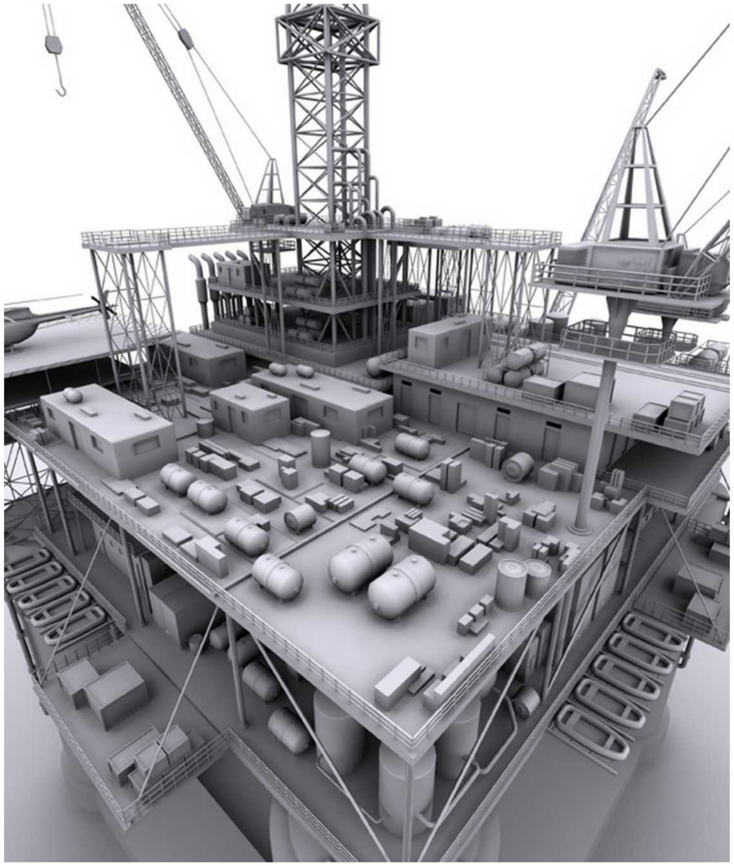
PURDUE CHEMICAL ENGINEERING

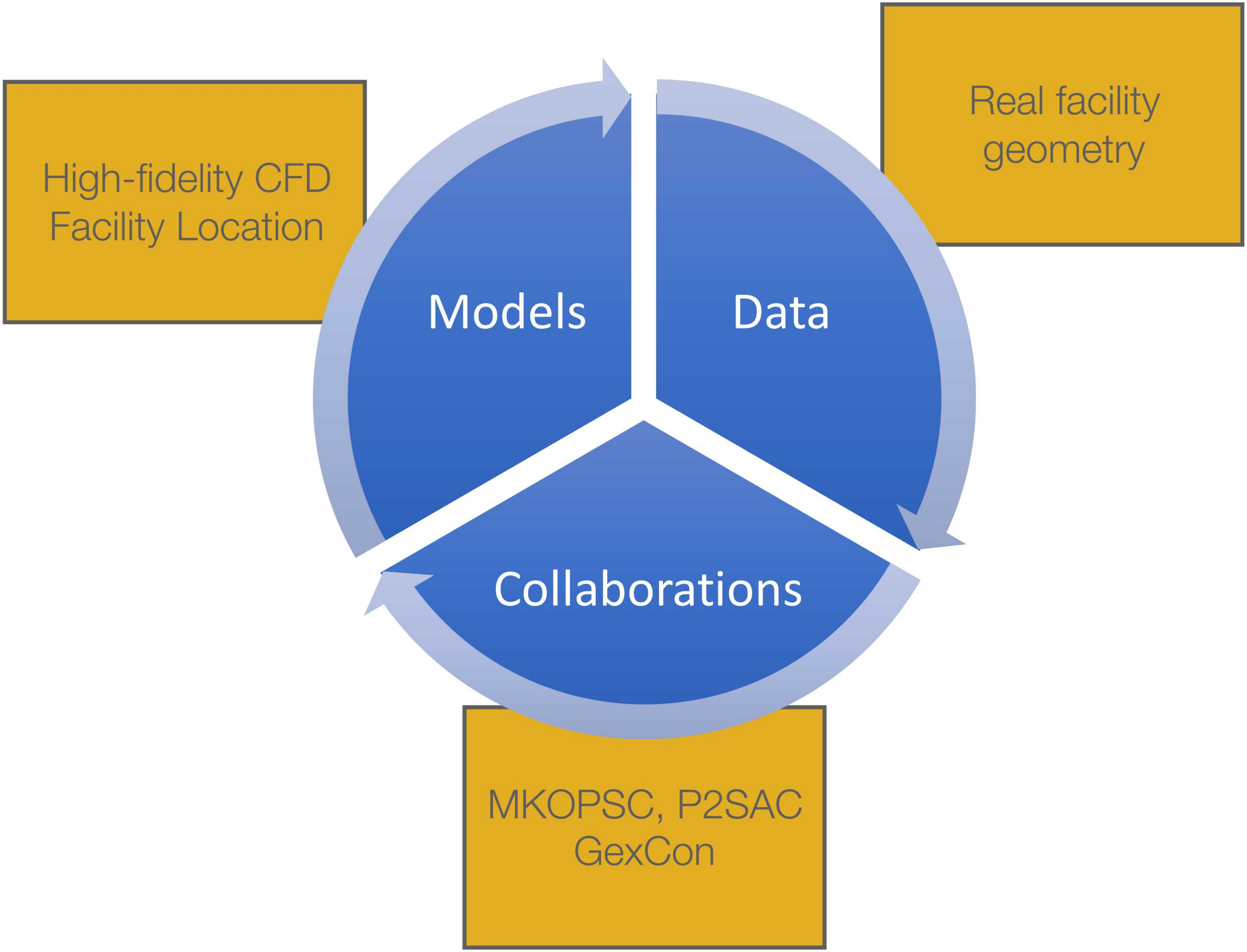
Optimal Placement of Detectors



Optimal Placement of Gas Detectors

- Significant uncertainty in:
  - Leak location
  - Weather conditions
  - Process conditions
- Problem scope:
  - Hundreds or thousands of scenarios
  - Hundreds or thousands of potential locations
  - Several different technologies
- Other challenges:
  - Most effective objective metric
  - Leak dispersion in complex geometries
  - Combinatorial explosion of decisions




High-fidelity CFD
Facility Location
Real facility
geometry
Models
Data
Collaborations
MKOPSC, P2SAC
GexCon

Optimization-based Approach

$$\min \quad \sum_{a \in \mathcal{A}} \alpha_a \sum_{i \in \mathcal{L}_a} d_{a,i} x_{a,i}$$

- Minimizes the expected detection time across all events

$$\text{s.t.} \quad \sum_{i \in \mathcal{L}_a} x_{a,i} = 1 \qquad \forall\, a \in \mathcal{A}$$

- Summation of probabilities of detection of scenario **a**

$$x_{a,i} \leq s_i \qquad \forall\, a \in \mathcal{A}, i \in \mathcal{L}_a$$

- A sensor location can only claim detection if a sensor exists in that location

$$\sum_{i \in \mathcal{L} \backslash \{D\}} s_i \leq p$$

- Constraint limiting the number of sensors allowed

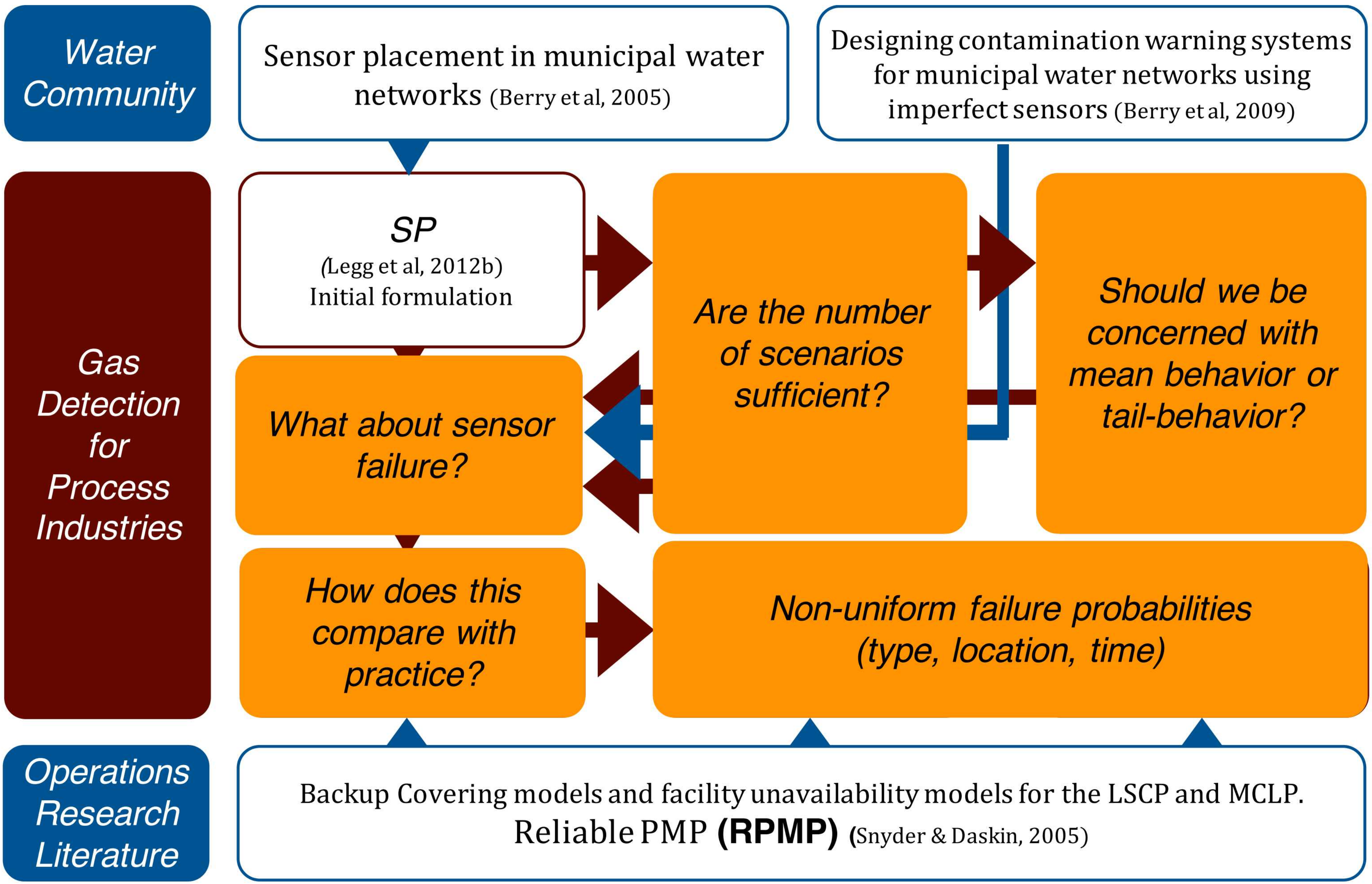
$$s_i \in \{0, 1\} \qquad \forall\, i \in \mathcal{L}$$

- Binary variable reflecting existence of a gas detector

$$0 \leq x_{a,i} \leq 1 \qquad \forall\, a \in \mathcal{A}, i \in \mathcal{L}_a$$

- Probability of 'first to detect' within the range of [0,1]

Gas Detector Placement Research



Gas Detector Placement Research

Water Community

Sensor placement in municipal water networks (Berry et al, 2005)

Designing contamination warning systems for municipal water networks using imperfect sensors (Berry et al, 2009)

Gas Detection for Process Industries

SP
(Legg et al, 2012b)
Initial formulation

SP-C
(Legg et al, 2012a)
Coverage constraints and the resilience of the formulation to unforeseen scenarios

SP-CVaR
(Legg et al., 2012c)
Improves the tail-behavior of the distributions of detection times

SP-U & SP-UV
(Benavides et al, 2014a)
Imperfect detector considerations: Unavailability and Voting

SP-UV Validation
(Benavides et al, 2014b)
SP-UV vs. Current detector placement practices in the industry

(Benavides et al, 2016)
Non-uniform unavailability
(1 backup level only)

(*J. Liu* et al, MKOPSC Symposium)
Non-uniform unavailability
(no limitation)

Operations Research Literature

Backup Covering models and facility unavailability models for the LSCP and MCLP.
Reliable PMP **(RPMP)** (Snyder & Daskin, 2005)

Optimal Gas Detector Placement

Mathematical optimization is computationally tractable (and useful) - Several formulations exist with realistic assumptions

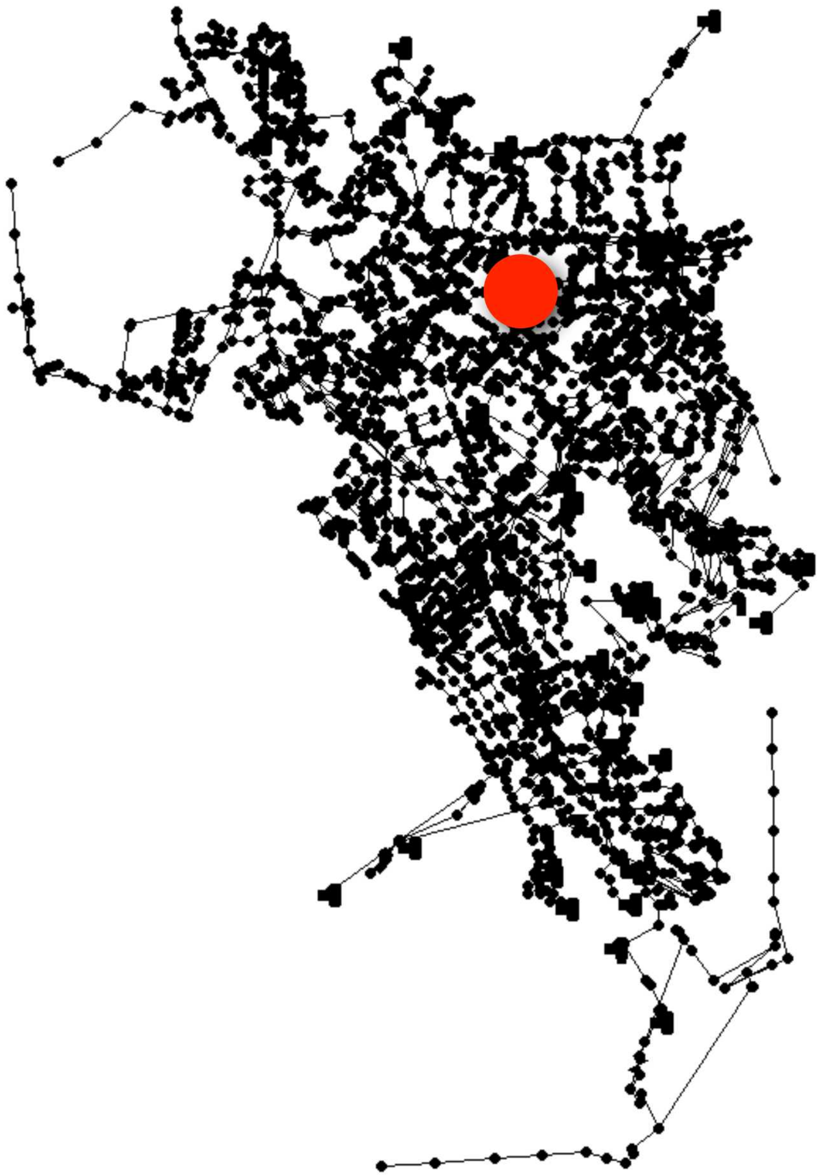
Optimization methods based on dispersion studies outperform common methods for gas detector placement

- Methods that use dispersion information outperform those that do not
- Methods that use optimization outperform those that do not

The volumetric approach (one of the most common) behaves the poorly (worse than random) with the data studied

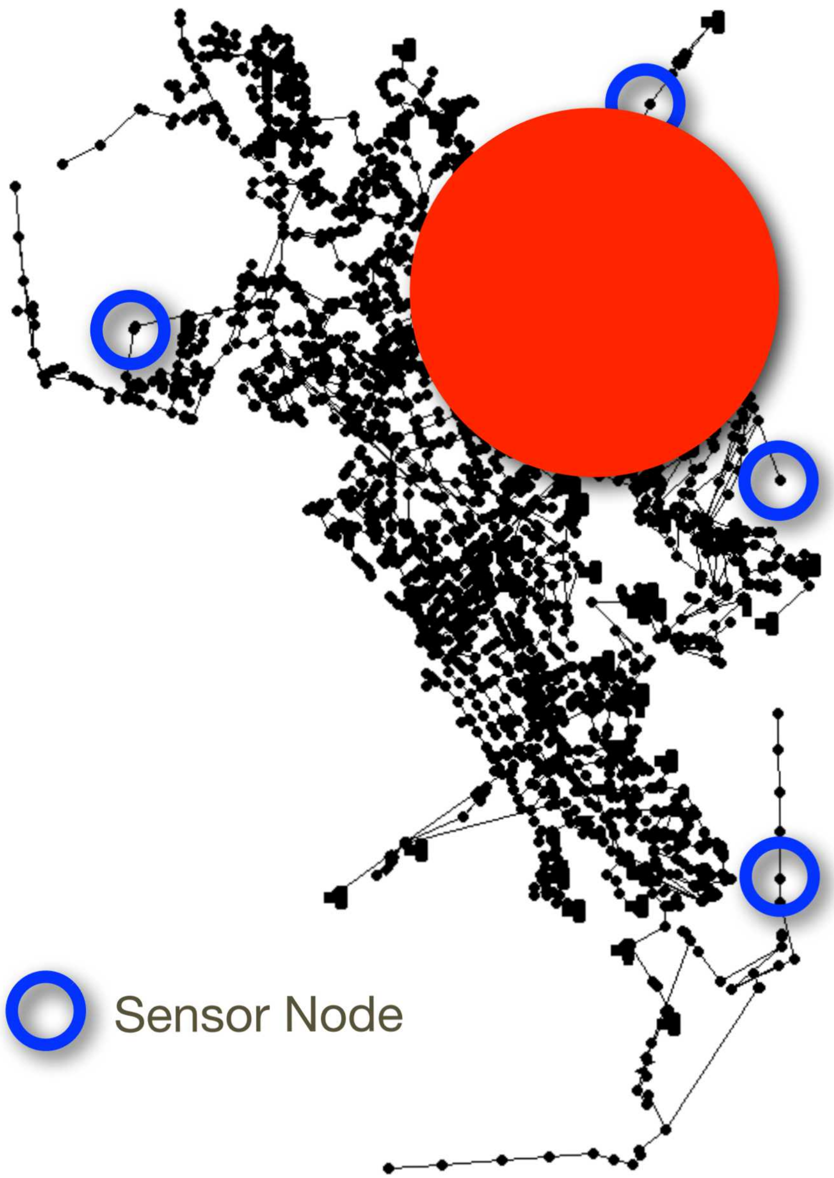
Similar results for all 4 data sets

Similar results when incomplete data used for placement (75% / 25%)

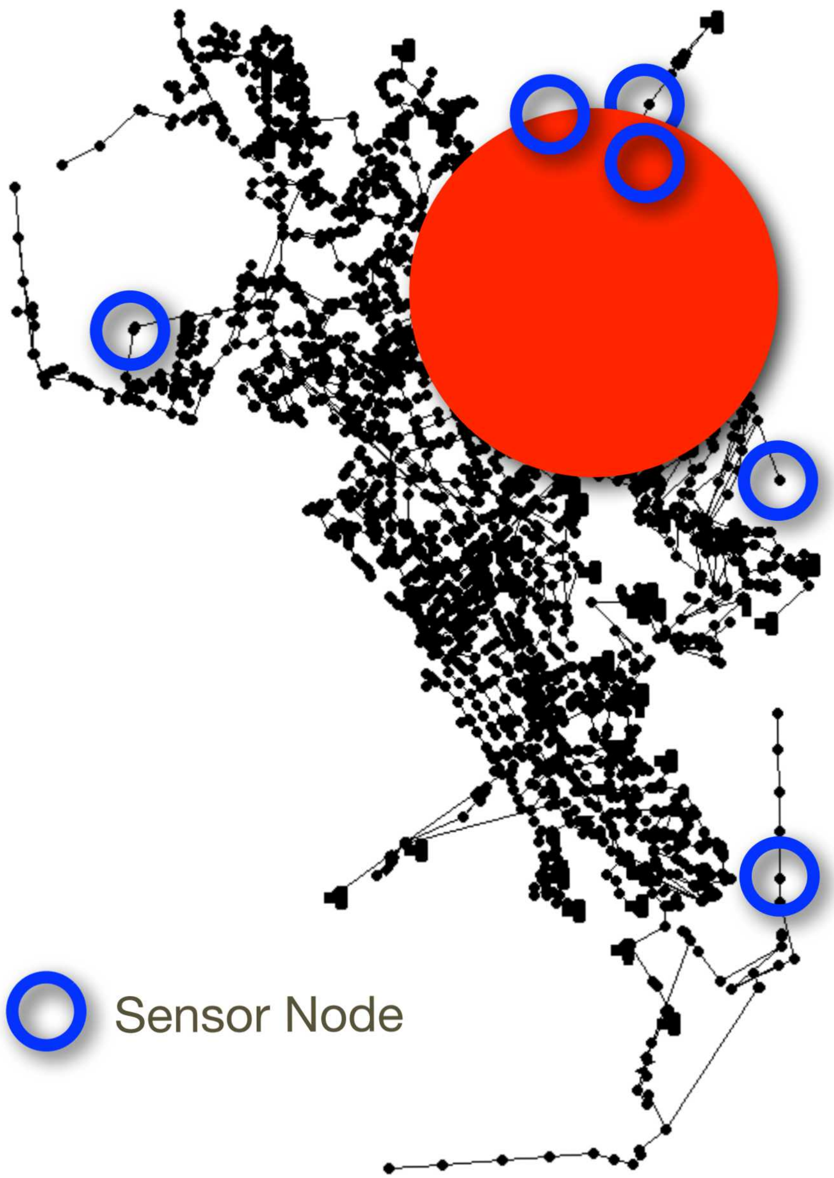


How do I best protect the public and the infrastructure?

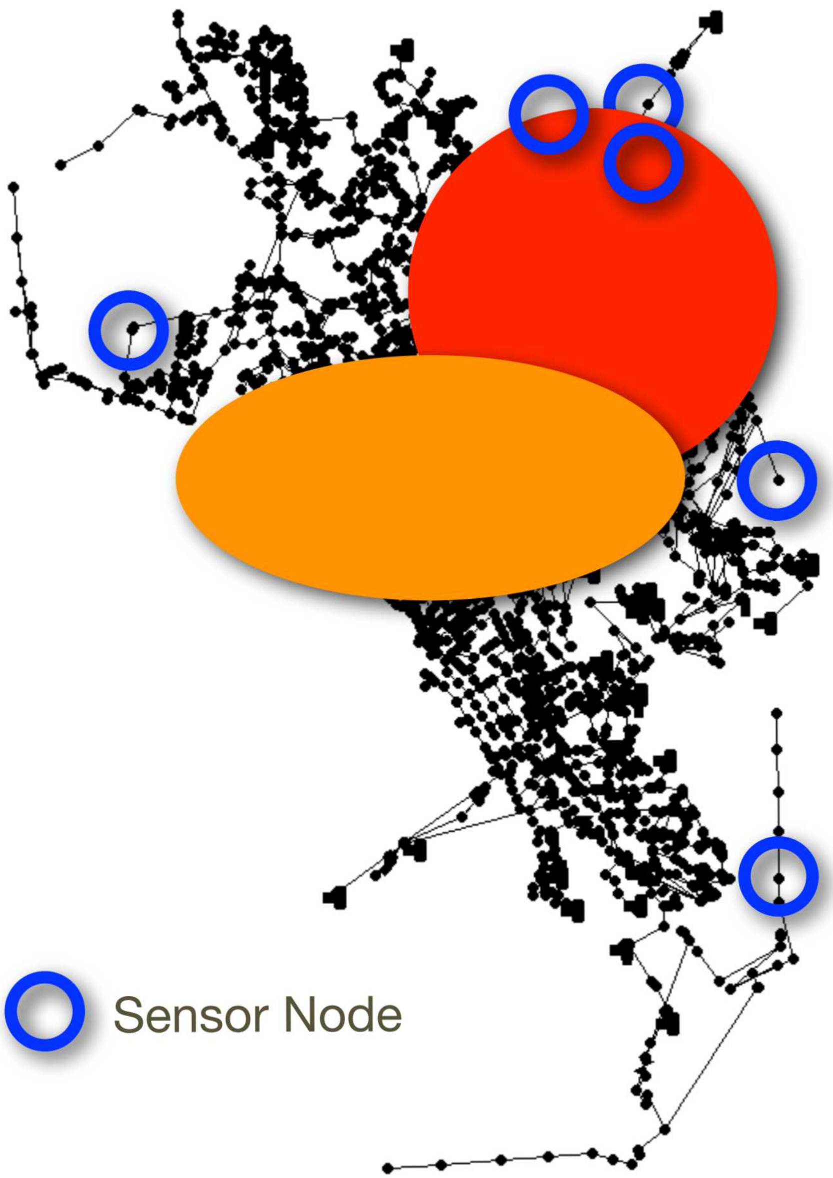
Early Warning and Response System



Early Warning and Response System

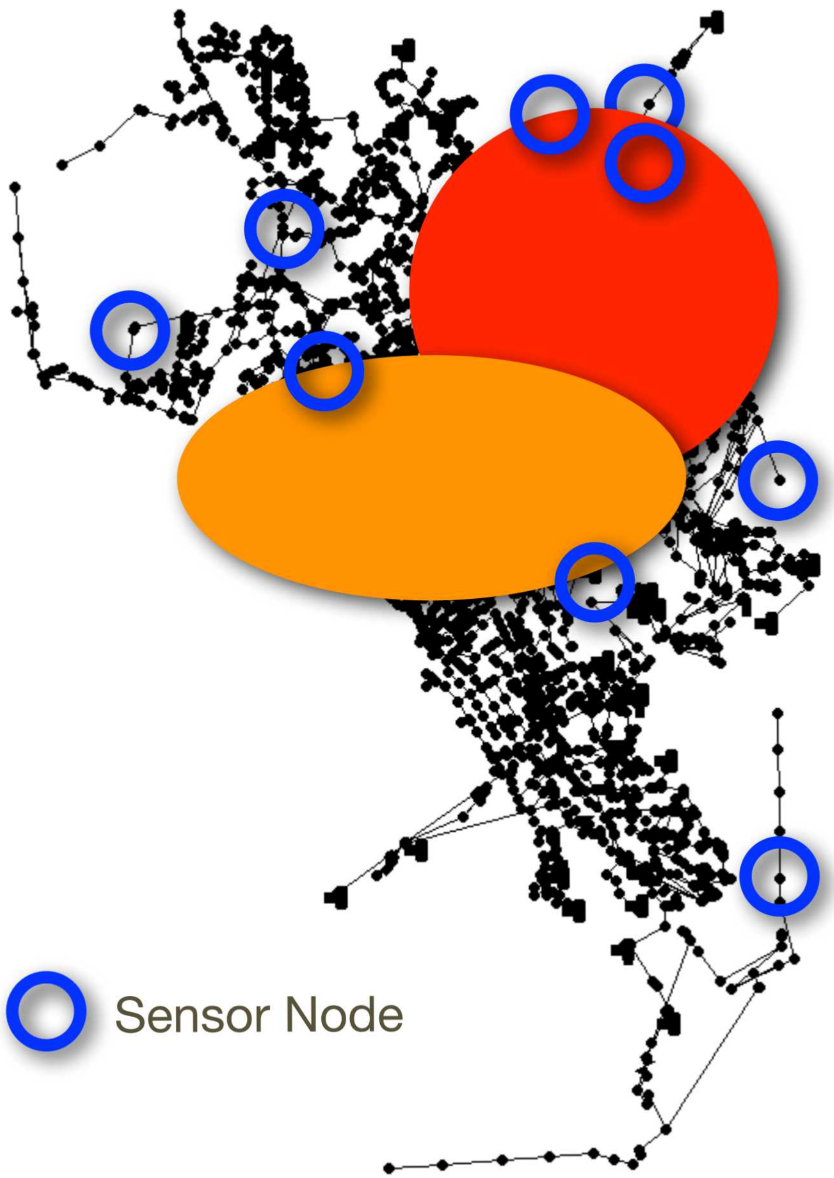


Early Warning and Response System

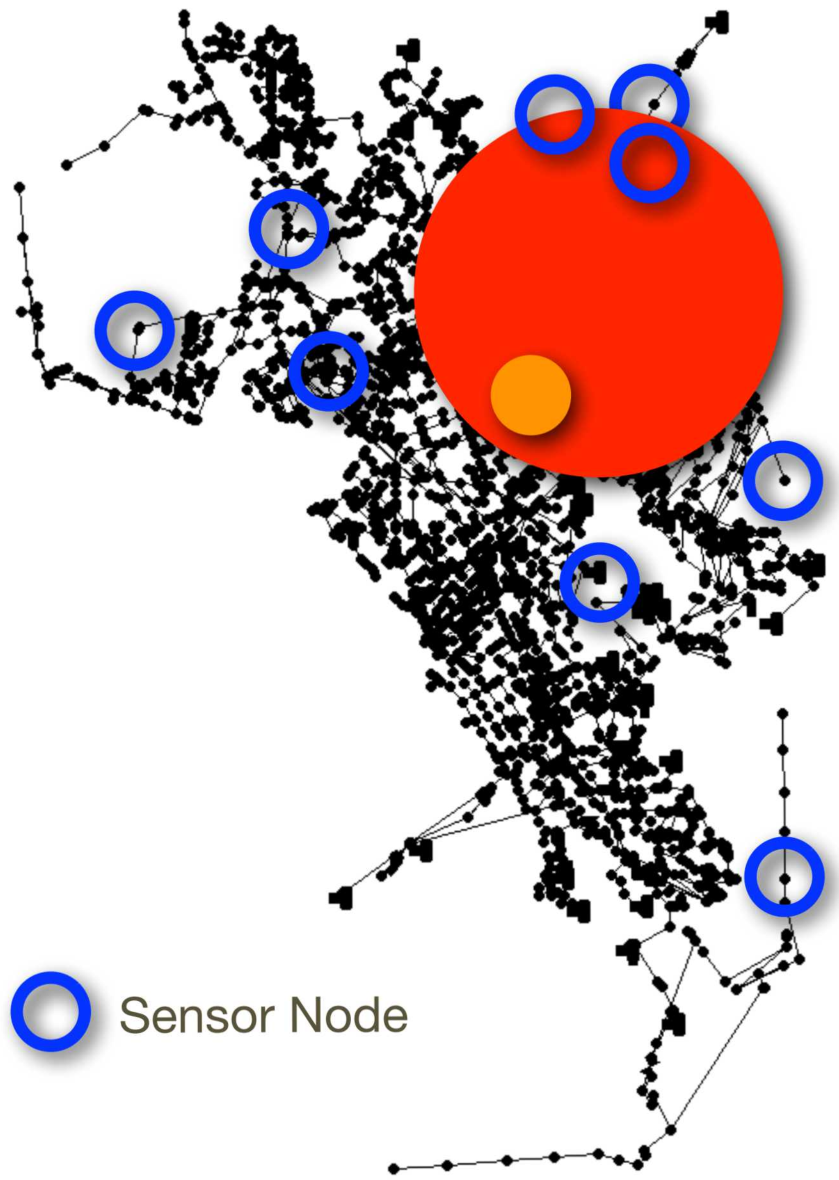


Sensor Node

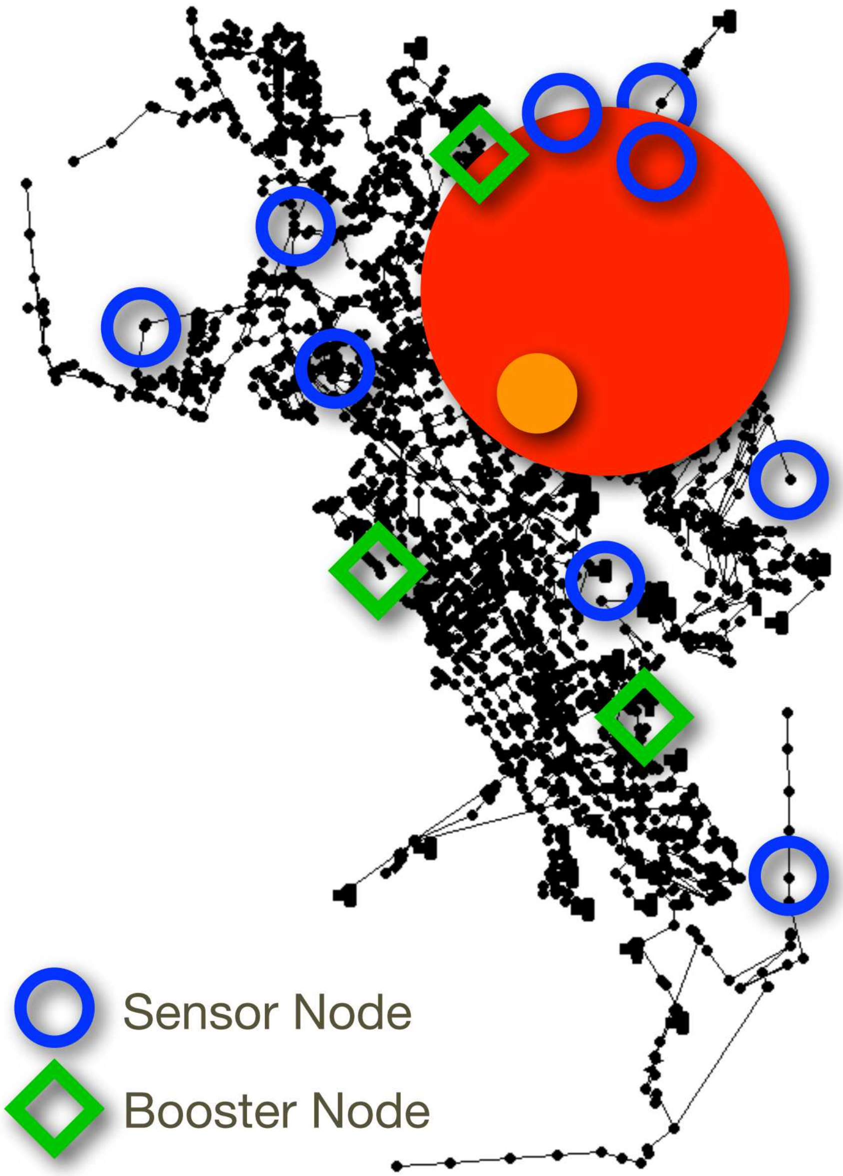
Early Warning and Response System



Early Warning and Response System



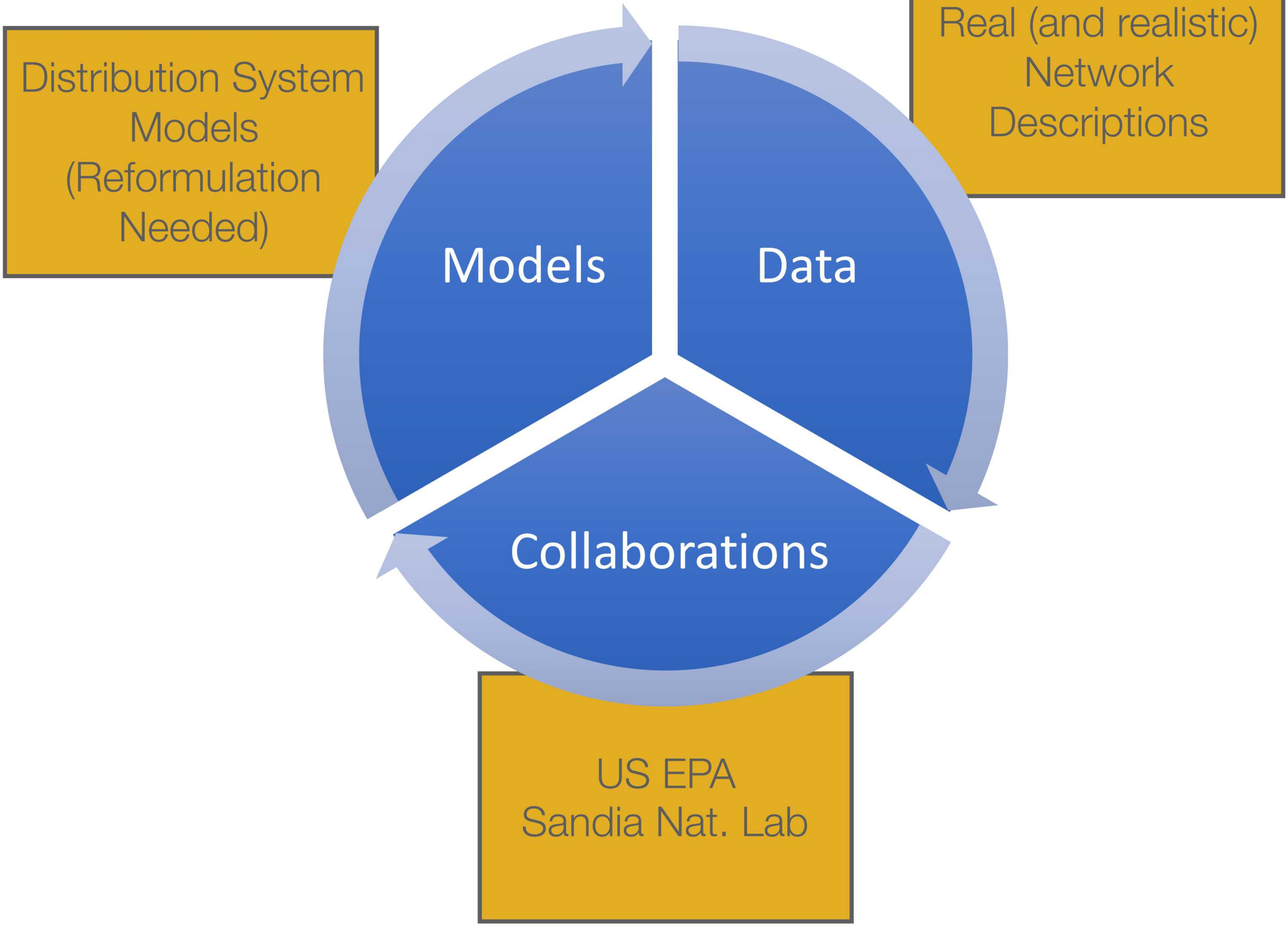
Early Warning and Response System



Sensor Technology

Monitoring & Mitigation System Design

Source/Plume Identification & Real-time Response


Distribution System Models (Reformulation Needed)
Real (and realistic) Network Descriptions
Models
Data
Collaborations
US EPA
Sandia Nat. Lab

Publications 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”, in progress

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.

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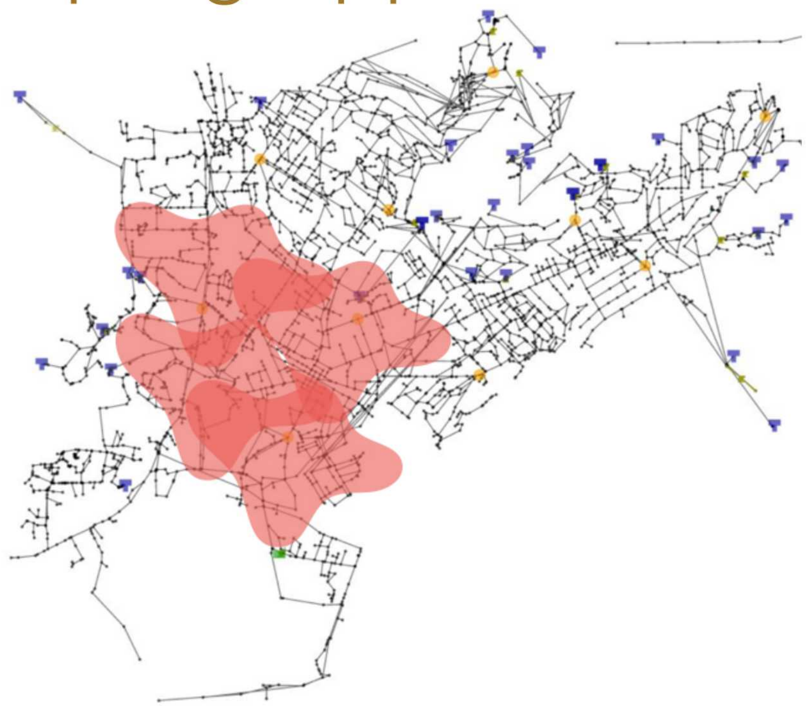
Optimal Real-time Sampling Approach

Given a contamination event:

What is the uncertainty in the plume?

Where can we take additional measurements to reduce uncertainty?



Account for uncertainty in:

Contamination location, time, profile

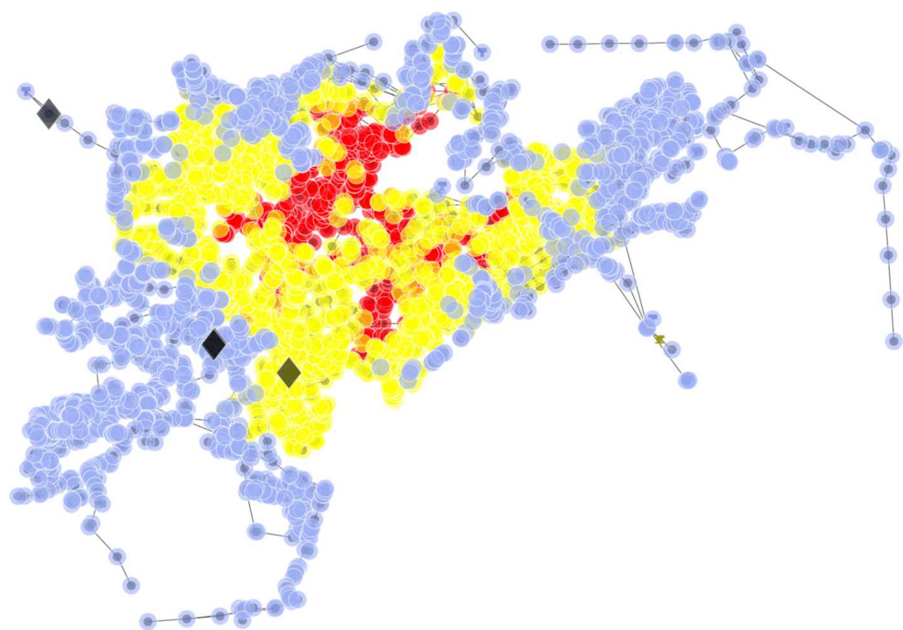
Hydraulics, reaction dynamics

Computational approach:

Pre-compute scenarios (M's)

Bayesian statistics:

- update scenario probabilities
- propagate probability of scenarios to probability of contamination
- use optimization to find best sampling locations to update the scenario probabilities

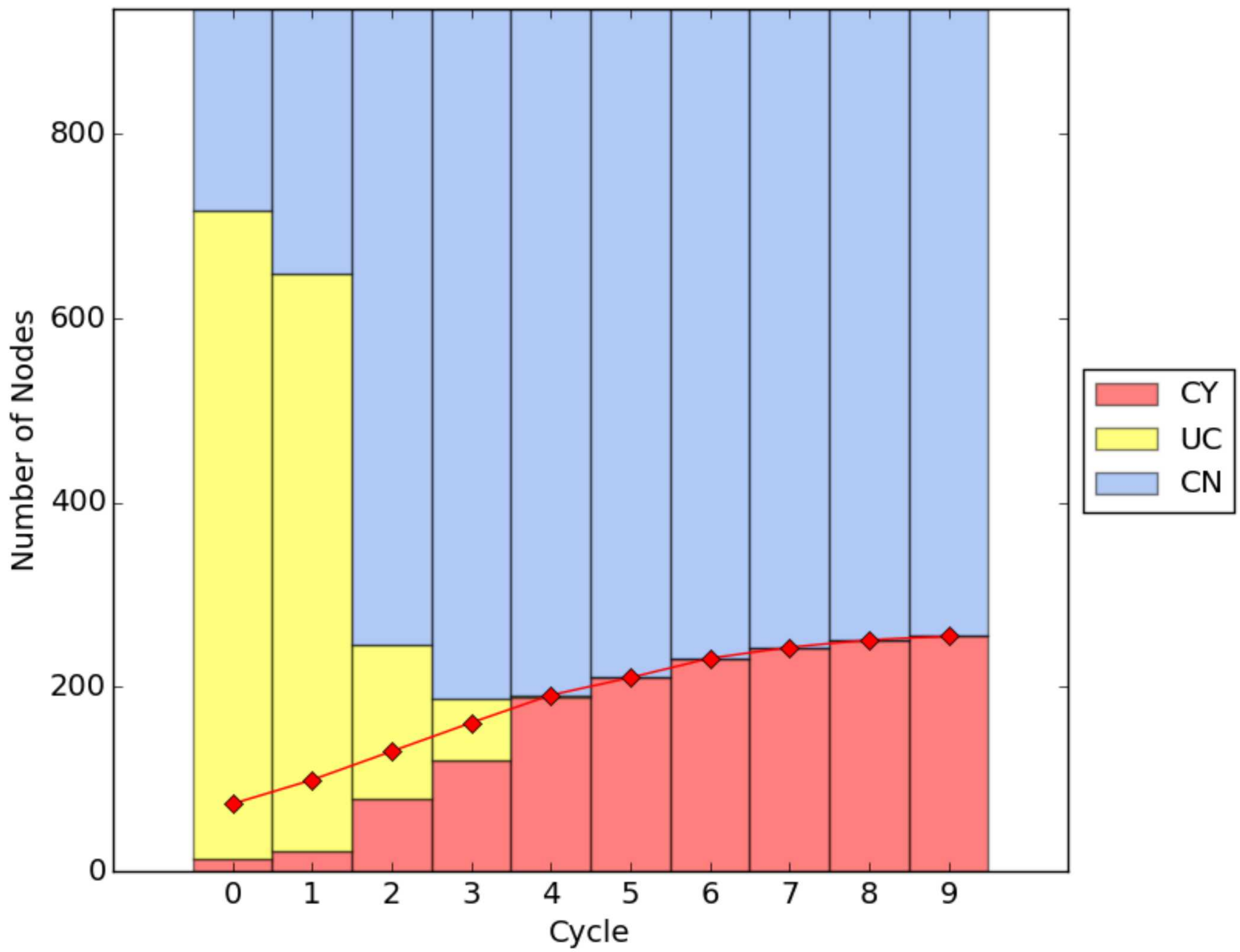


PURDUE CHEMICAL ENGINEERING

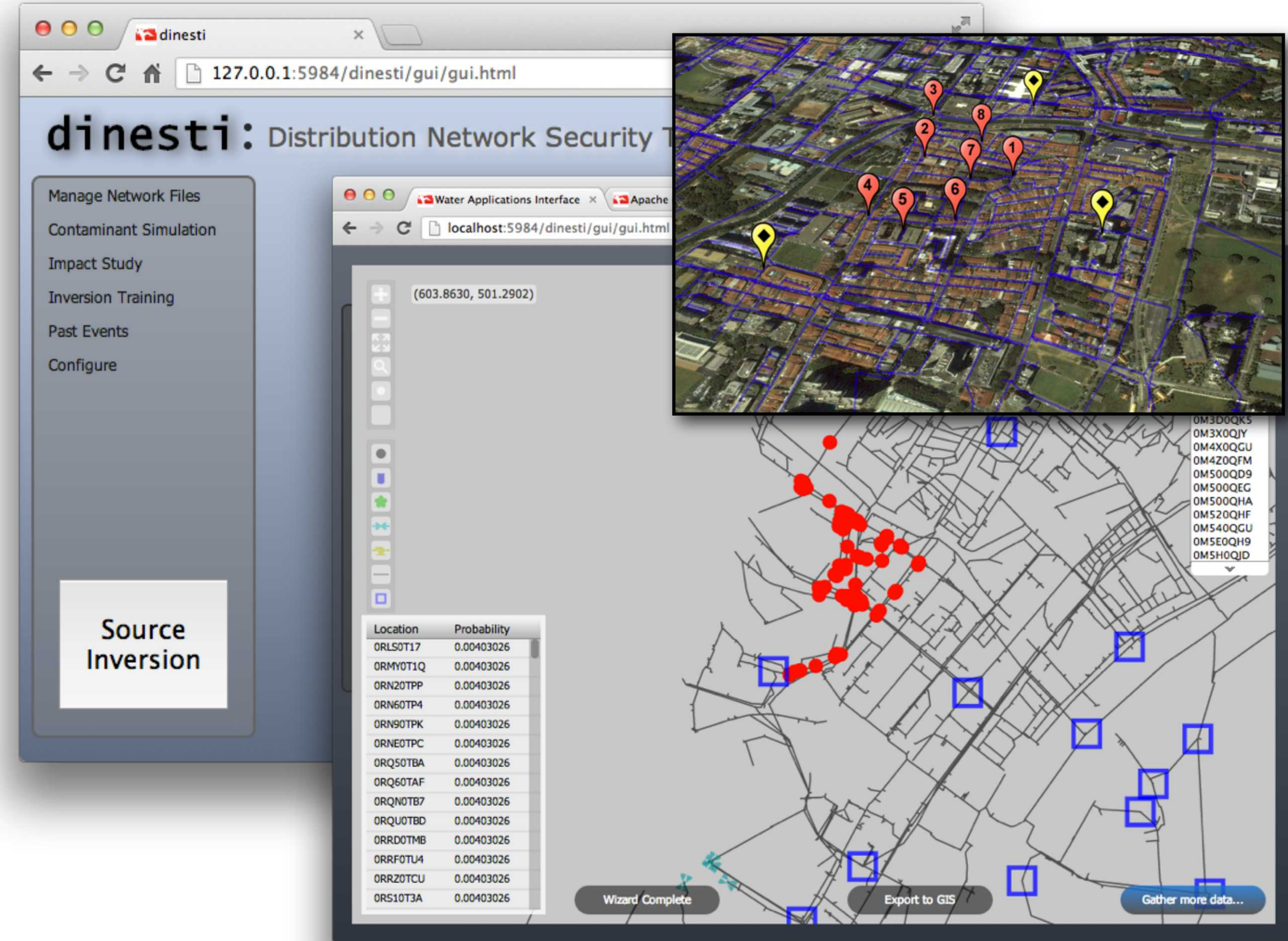
Maximization of number of expected scenarios that mismatch

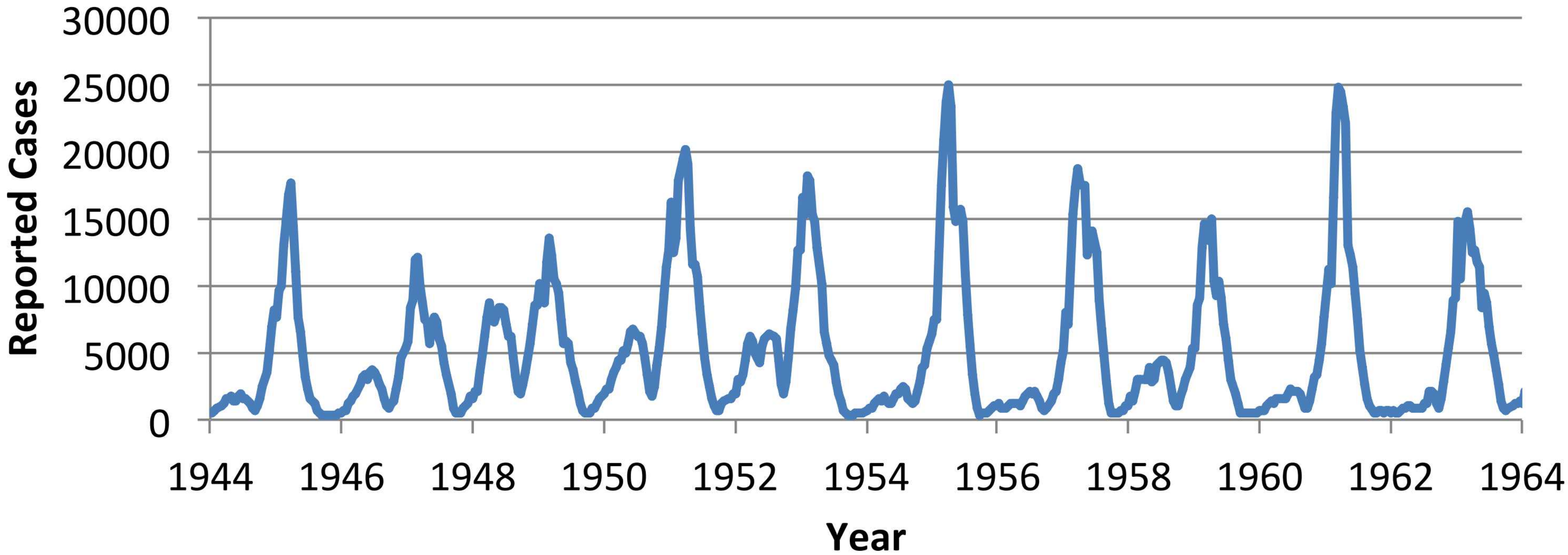
$$
\begin{aligned}
\max_{x} \quad & \sum_{s \in S} P_s^{\text{miss}} \\
\text{s.t.} \quad & P_s^{\text{miss}} = 1 - P_s^{\text{match}} && \forall s \in S \\
& P_s^{\text{match}} \geq \exp(\tilde{P}_s) && \forall s \in S \\
& \tilde{P}_s = \sum_{n \in N} x_n \ln(\alpha_{s,n}) && \forall s \in S \\
& \sum_{n \in N} x_n \leq S_{max} \\
& x_n \in 0, 1 \forall n \in N
\end{aligned}
$$

Uncertainty Reduction



Source Inversion Response System

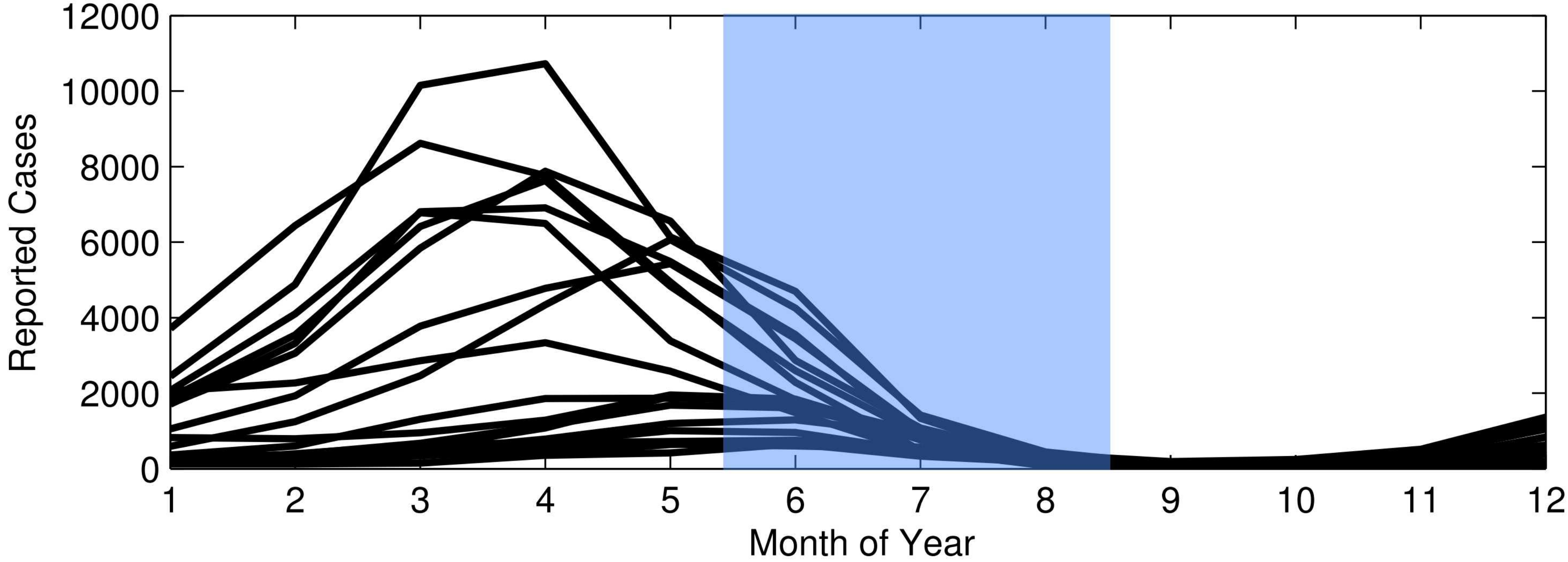




How do we use this data to better understand the spread of infectious disease?

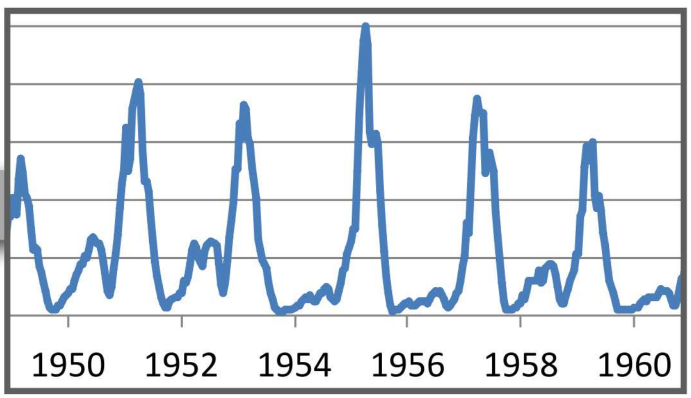
How would you use this data for improved intervention in an emerging childhood respiratory pandemic?

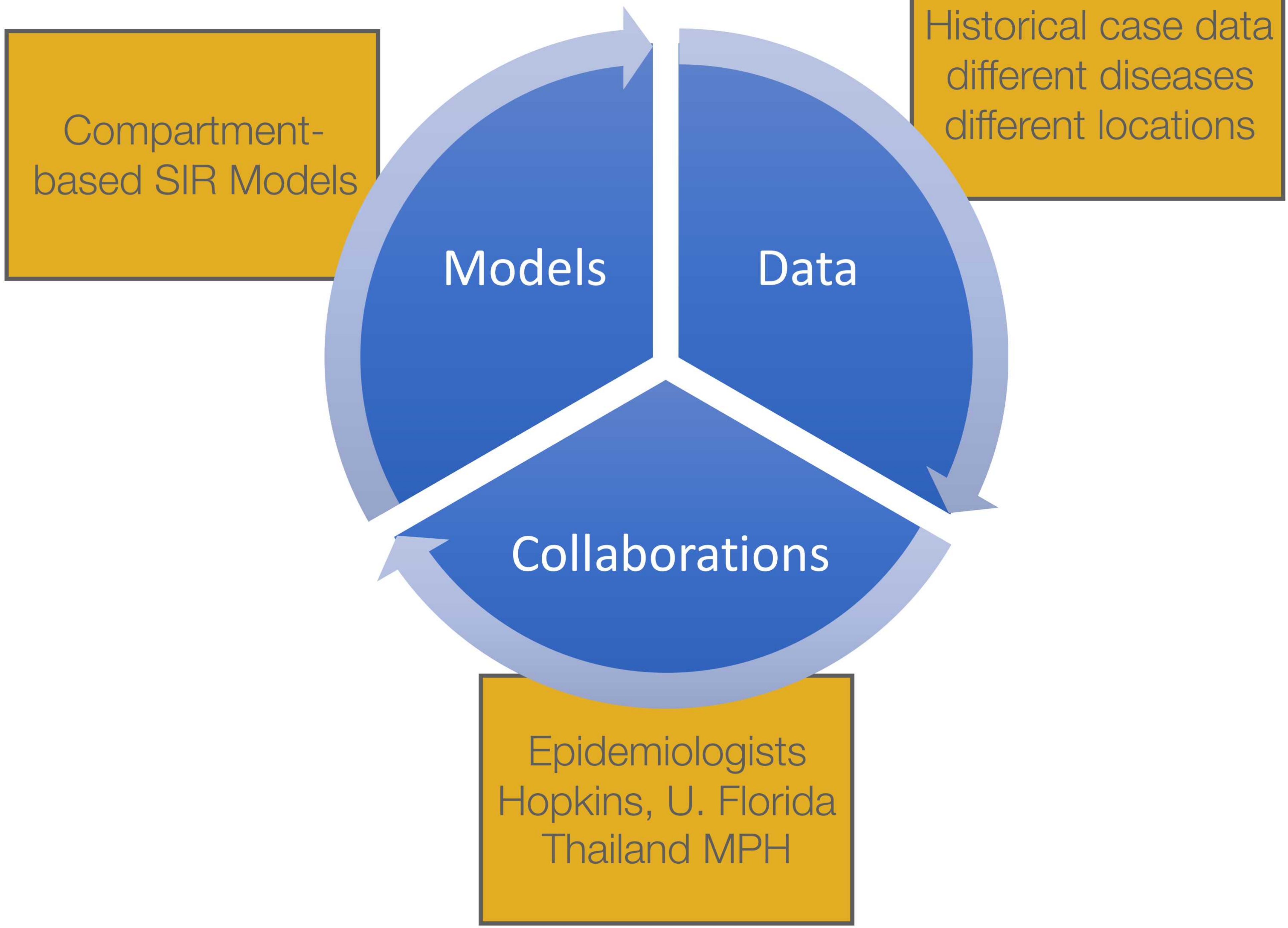
Seasonality in Input Drivers



Input Drivers

Nonlinear Disease Spread Dynamics

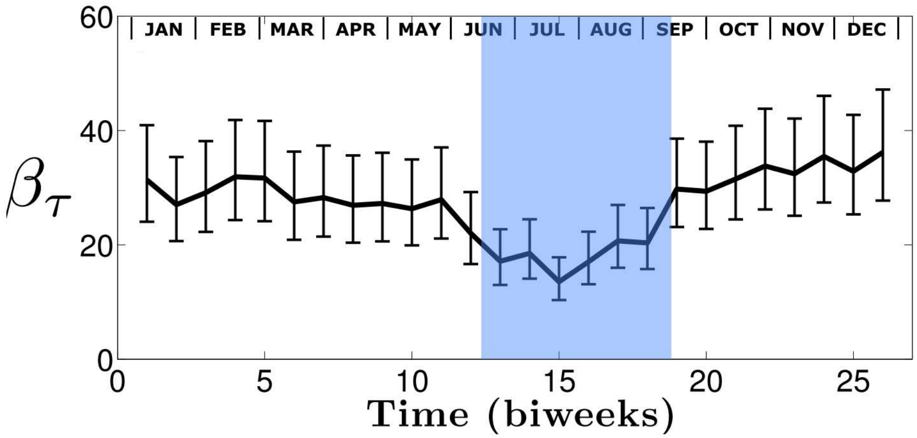



Compartment-based SIR Models
Historical case data
different diseases
different locations
Models
Data
Collaborations
Epidemiologists
Hopkins, U. Florida
Thailand MPH

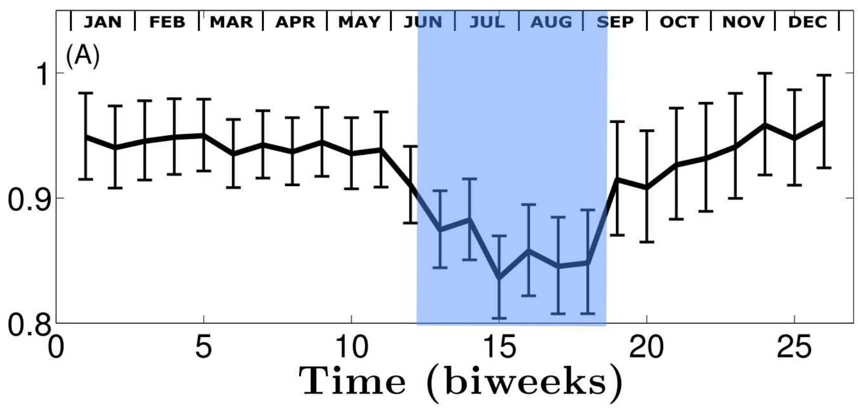
Estimating Seasonal Drivers in Childhood Infectious Diseases

- 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 & Easily Identified
- Estimation Challenges
  - Long-time Horizons (20-30 years)
  - Data aggregated monthly or biweekly
  - No Susceptible Information
  - Severe Under-reporting of Cases (1/2 for UK, 1/100 for Thailand)
  - Missing (1974, 1979), Substantial Noise, Time-Varying Reporting
- Available Data:
  - England & Wales: 60 (900) Cities 1944-1963
  - US: New York City, Baltimore, TYCO Data
  - Thailand: 76 Provinces 1972-1998
  - Library of Congress

Estimating Seasonal Drivers of Infectious Disease



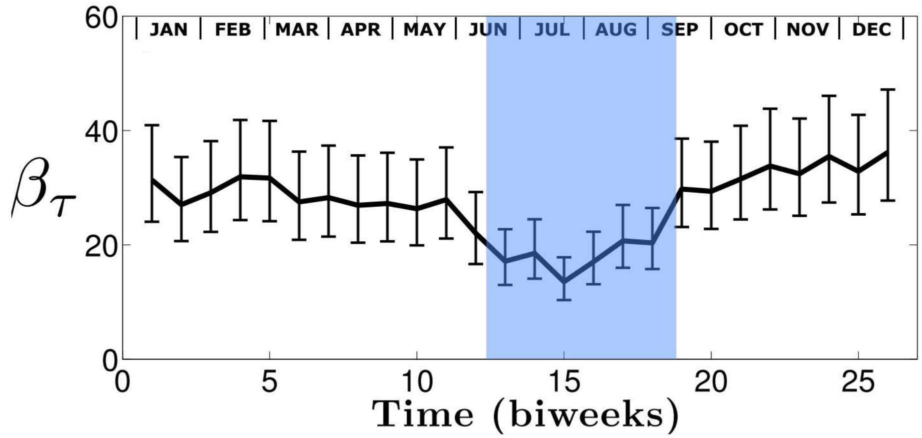
Estimating seasonality in transmission parameter (contacts)



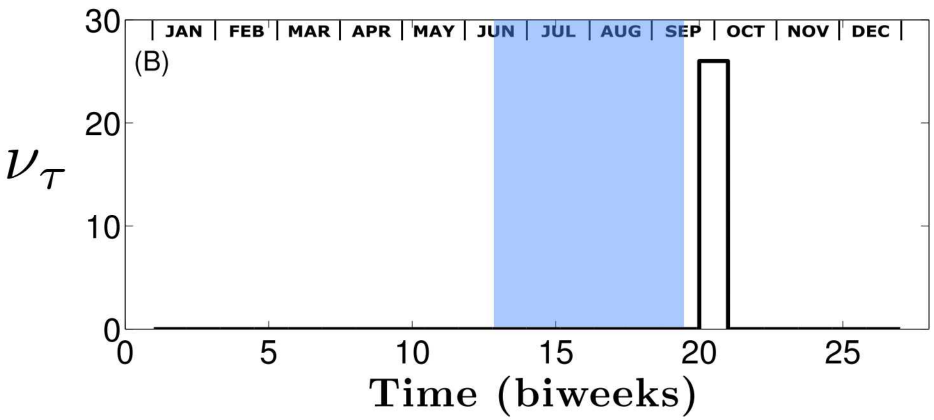
Estimating seasonality in exponential factor (mixing)

Estimated patterns correlate with school holidays and we can quantify impact of school closure

Estimating Seasonal Drivers of Infectious Disease



Estimating seasonality in transmission parameter (contacts)



Estimating seasonality in birth rate

Estimated patterns correlate with school holidays and we can quantify impact of school closure

Publications

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 and Conclusions

Mathematical programming provides rigorous, computationally tractable, solutions to many problems in safety and security

- Protection of critical infrastructure
- Improved system understanding
- Design of mitigation systems
- Real-time response

Rapid, dramatic improvements in optimization capabilities (modeling tools, algorithms)

Increased data and desire for rigorous analysis from many application areas

Successful convergence in research requires:

- Collaboration: Importance, community
- Data: Impact
- Models: Enabling technology

Acknowledgements

- Current Students/Researchers
  - Daniel Laky
  - Richard Shu
  - **Santiago Rodriguez**
  - **Jianfeng Liu**
  - Michael Bynum
  - Todd Zhen
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  - Arpan Seth
  - Yankai Cao
  - **Alberto Benavides-Serrano**
  - Yu Zhu
  - Ahmed Rabie
  - George Abbott III
  - Chen Wang
  - **Sean Legg**
  - **Daniel Word**
  - **Angelica Wong**
  - Xiaorui Yu
  - Gabriel Hackebeil
  - Shawn McGee
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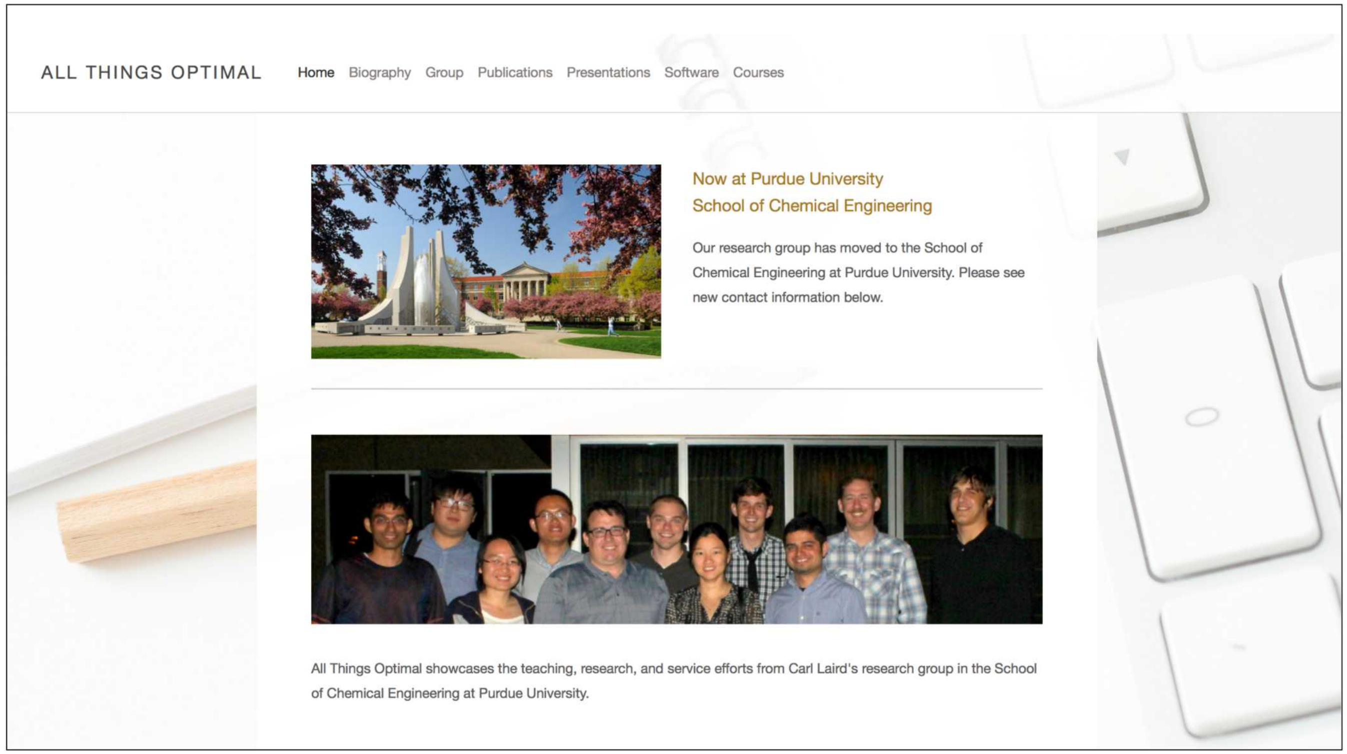
  - D. Cummings - JHSPH
  - S. Iamsirithaworn - MPHT
  - W. Hart, S. McKenna, J.P. Watson, K. Klise, John Siirola - Sandia
  - T. Haxton, R. Murray - EPA
  - Johan Akesson, Lund University
  - Sam Mannan, TAMU



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- National Science Foundation Cyber-Enabled Discovery and Innovation (CDI)-Type II
- National Science Foundation (CAREER Grant CBET# 0955205).
- Sandia National Laboratories, EPA, PUB Singapore
- MKOPSC, P2SAC