Meeting with STAC Members
June 13, 2023

CAST Optimization: Intermediate Status

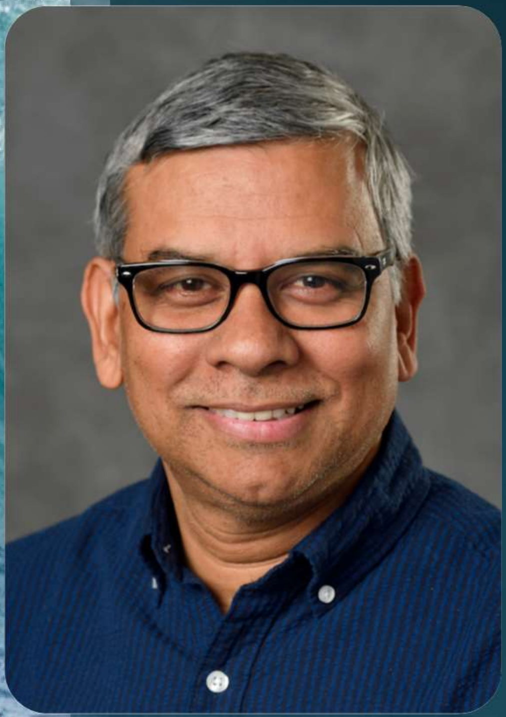
Kalyanmoy Deb, Pouyan Nejadhashemi, Gregorio Toscano, and Hoda Razavi

MICHIGAN STATE UNIVERSITY

Agenda

1. Introduction to Michigan State University (MSU) Team
2. STAC Workshop Report, 2016: Goals and Applications
3. Objectives and Main Tasks of the Project
4. Current Status of the Project
5. Short Demo (video)
6. Future Plan

Kalyanmoy Deb



- **Title:**
  - **University Distinguished Professor**
  - **Koenig Endowed Chair Professor**
    - **Dept of Electrical and Computer Engineering**
    - **Dept of Computer Science and Engineering**
    - **Dept of Mechanical Engineering**

- **Expertise and Achievements:**
  - **Optimization, Multi-objective optimization, Machine Learning, Modeling**
  - **36 years of experience in optimization and its applications**
  - **Author of popular evolutionary optimization methods: NSGA-II, NSGA-III**
  - **Author of two text-books on optimization, 610 research papers**
  - **185,000 Google Scholar citations, h-index: 133**
  - **Director, Computational Opt. and Innovation (COIN) Lab at MSU**

Pouyan Nejadhashemi

- **Title:**
  - **University Foundation Professor**
    - **Department of Biosystems and Agricultural Engineering**
    - **Department of Plant, Soil and Microbial Sciences**
  - **Elected board member**
    - **International Environmental Modelling & Software Society**
- **Expertise and Achievements:**
  - **Soft computing applications in water resources management**
  - **Computational Ecohydrology**
  - **Evaluation and development of watershed and water quality models**
  - **$41M in grant funding**
  - **130 peer-reviewed publications**
  - **180 scientific presentations**
  - **Director, Center for Intelligent Water Resources Engineering (CIWRE)**

Gregorio Toscano

- **Title:**
  - **CBPO CAST optimization researcher**
  - **Associate Professor - Center for Research and Advanced Studies, Mexico**
  - **PhD in Evol. Multi-Criterion Optimization, 2005**

- **Expertise and Achievements:**
  - **Multi-objective optimization, Computational Intelligence, and Machine Learning**
  - **Multi-objective Micro-GA, Multi-objective PSO**
  - **Full Stack**
  - **Programming Languages**
  - **7,692 Google Scholar citations**

Hoda Razavi

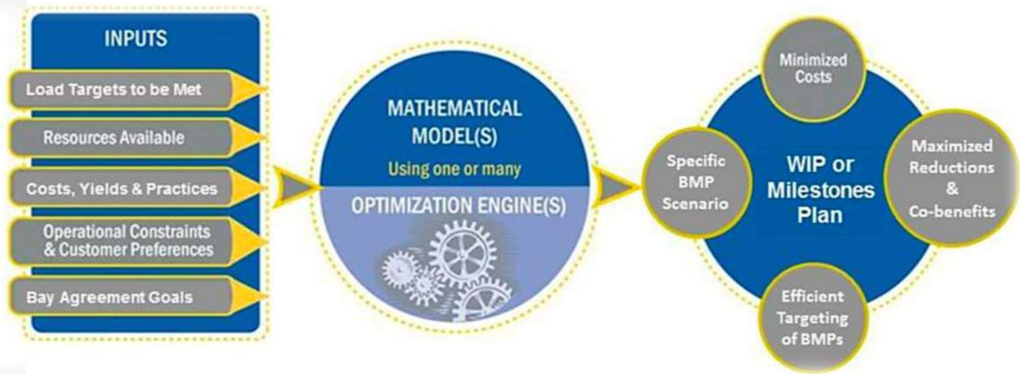
- **Title:**
  - **PhD Student, Biosystems and Agricultural Engineering, Michigan State University**
  - **MS Water and Hydraulic Structures, Civil Engineering, Khajeh Nasir Toosi University of Technology**
  - **BS Civil Engineering University of Tehran**

- **Expertise:**
  - **Watershed/water quality modeling**
  - **Environmental flow**
  - **Multi-objective optimization**
  - **Uncertainty quantification**
  - **Water resources management**
  - **Data-driven models**
  - **Climate change impacts**

"Cracking the WIP" - Designing an Optimization Engine to Guide Efficient Bay Implementation STAC Workshop Report, 2016

Goals:

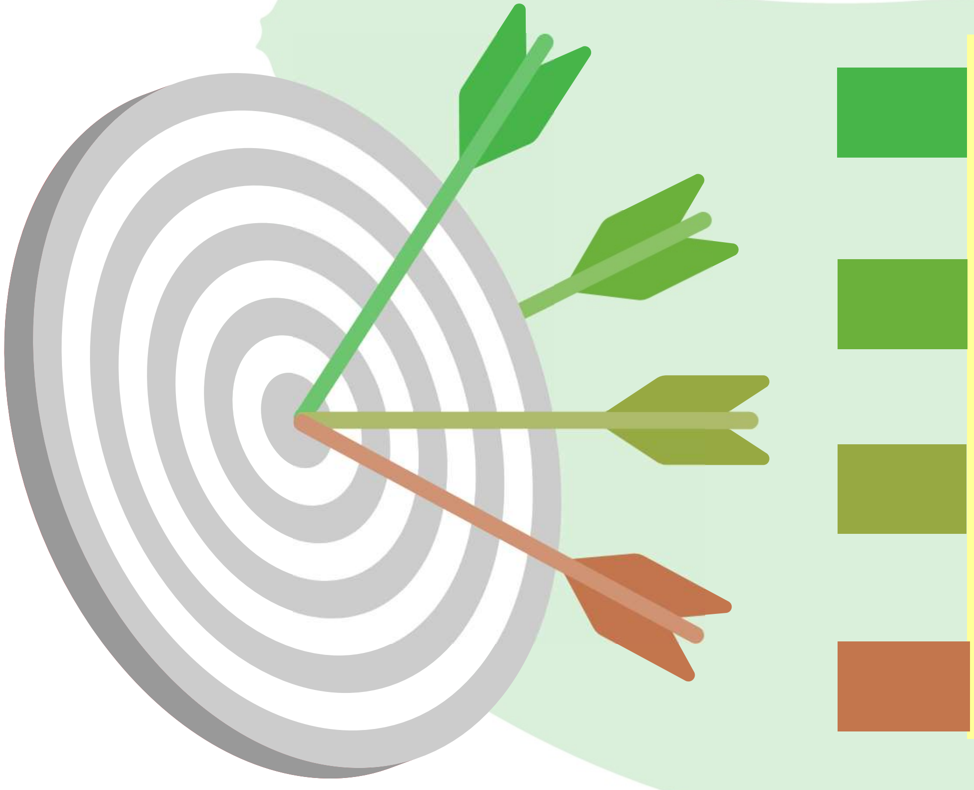
1. **Cost minimization** was a key goal for the partners
2. **Maximizing co-benefits**, particularly those supporting Chesapeake Bay Watershed Agreement goals
3. **Maximizing load reduction** reliability
4. Equitable distribution of effort among jurisdictions
5. Equitable distribution of effort among source sectors
6. Limits on retirement of agricultural land
7. Ability to use the tool at **various scales**



Applications: STAC Workshop Report, 2016

Under development	Future Application	
• Address optimization of multiple co-benefits • Minimize costs of BMP implementation • Optimal use of BMPs on land use by county • Make Bay TMDL load targets achievable • Make Phase III WIP scenario that achieves nitrogen, phosphorus, and sediment targets for the lowest cost with the ability to tweak to see the different scenario costs	• Rethink the allocation of responsibilities by sector, by geography, by funding • Recognize the value/influence of ecosystem services in local decision making • Assist with the development of grant applications • Help local governments document co-benefits of WIP implementation • Identify cost savings within a source sector	• Provide a basic resource for planners to understand advantages and disadvantages of implementation options • Assist progress towards other management strategy objectives • Help in development of state implementation plans (Bay Milestones and WIPs) • Help in development of local implementation plans (local and Bay TMDLs) • Develop sector implementation plans cost effectively

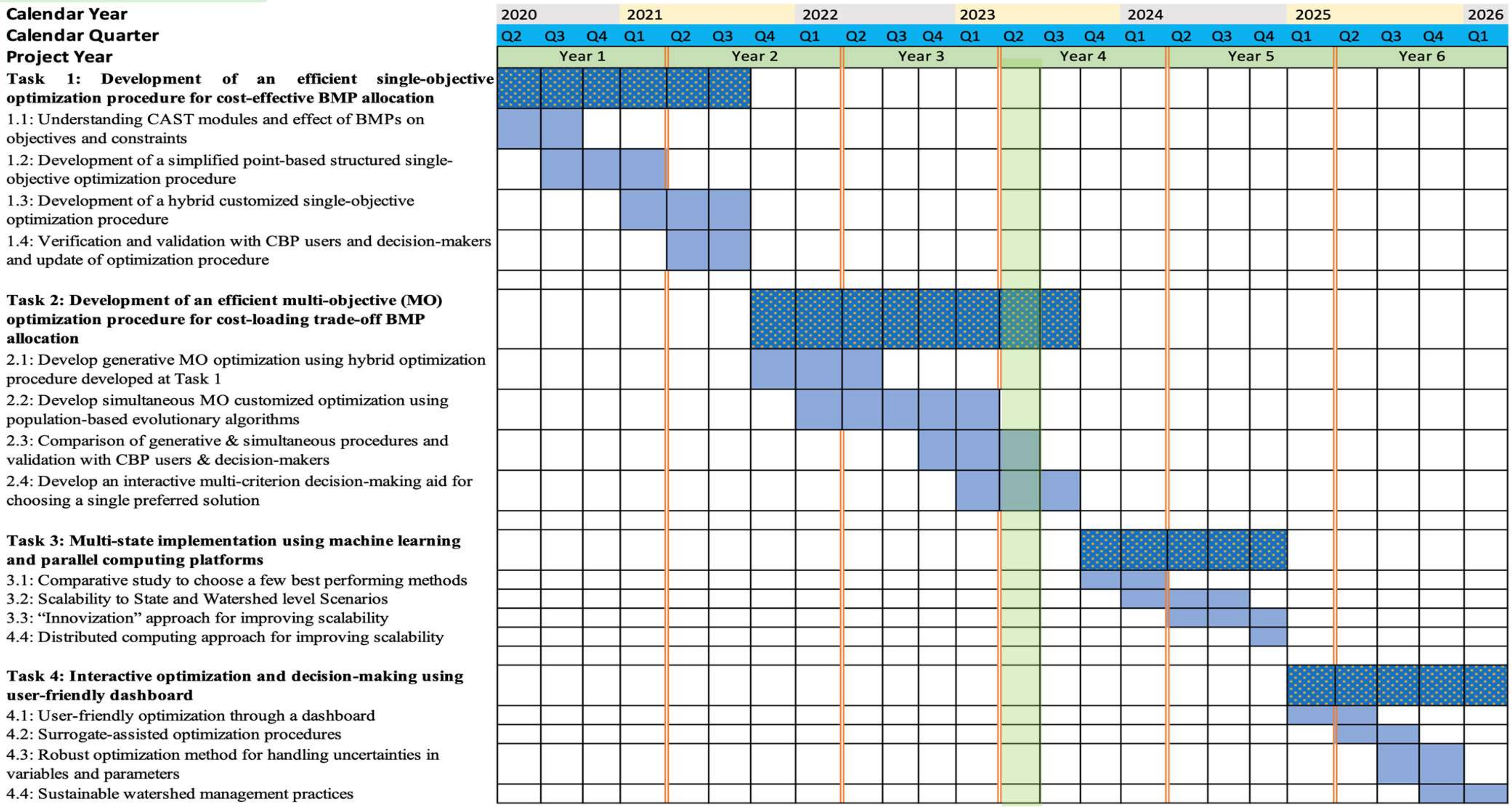
Objective of the MSU-Optimization Project



Investigate, develop, program, verify, and implement an optimization system built around the CBP's CAST Model to:

- Improve the water quality
- At the lowest cost

Timeline of the Project



We are here

Timeline of the Project

Calendar Year	2020	2021	2022	2023	2024	2025	2026

Q4 Q1

Year 6

Task 1: Development of an efficient single-objective optimization procedure for cost-effective BMP allocation

1.1: Understanding CAST modules and effect of BMPs on objectives and constraints

1.2: Development of a simplified point-based structured single-objective optimization procedure

1.3: Development of a hybrid customized single-objective optimization procedure

1.4: Verification and validation with CBP users and decision-makers and update of optimization procedure

4.2: Surrogate-assisted optimization procedures

4.3: Robust optimization method for handling uncertainties in variables and parameters

4.4: Sustainable watershed management practices

We are here

Timeline of the Project

Calendar Year	2020			2021				2022				2023				2024				2025				2026
Calendar Quarter	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1
Project Yea…																							…ear 6	

Task 1: … optimization…
1.1: Understa… objectives and…
1.2: Develop… objective opti…
1.3: Develop… optimization p…
1.4: Verificati… and update of…

Task 2: Dev… optimization… allocation
2.1: Develop… procedure dev…
2.2: Develop… population-ba…
2.3: Comparis… validation wit…
2.4: Develop… choosing a si…

Task 3: Mult… and parallel…
3.1: Compara…
3.2: Scalabilit…
3.3: "Innoviz…
4.4: Distribut…

Task 4: Inte… user-friendly…
4.1: User-friendly optimization through a dashboard
4.2: Surrogate-assisted optimization procedures
4.3: Robust optimization method for handling uncertainties in variables and parameters
4.4: Sustainable watershed management practices

Task 2: Development of an efficient multi-objective (MO) optimization procedure for cost-loading trade-off BMP allocation

2.1: Develop generative MO optimization using hybrid optimization procedure developed at Task 1

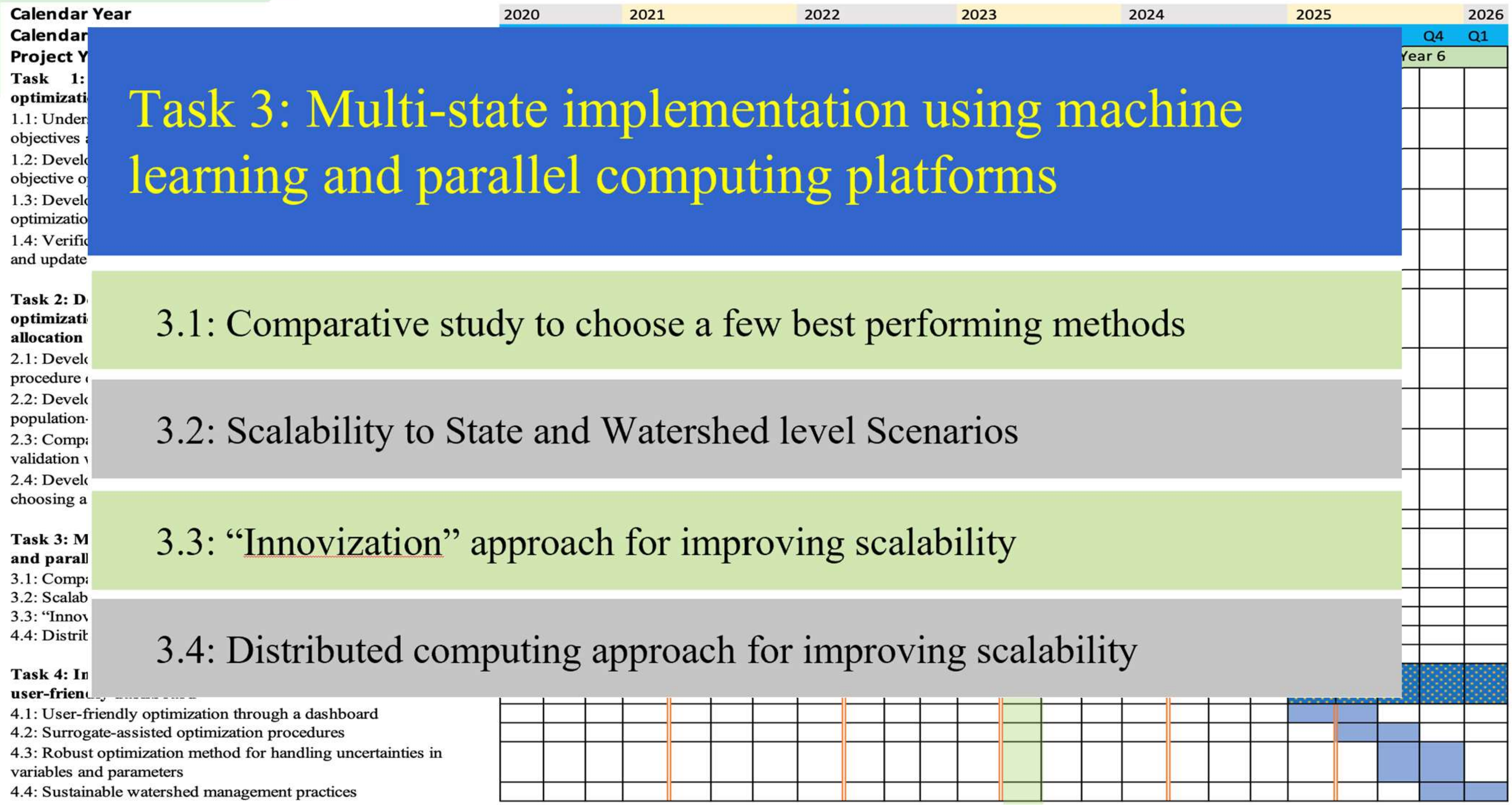
2.2: Develop simultaneous MO customized optimization using population-based evolutionary algorithms

2.3: Comparison of generative & simultaneous procedures and validation with CBP users & decision-makers

2.4: Develop an interactive multi-criterion decision-making aid for choosing a single preferred solution

We are here

Timeline of the Project



Task 3: Multi-state implementation using machine learning and parallel computing platforms

3.1: Comparative study to choose a few best performing methods

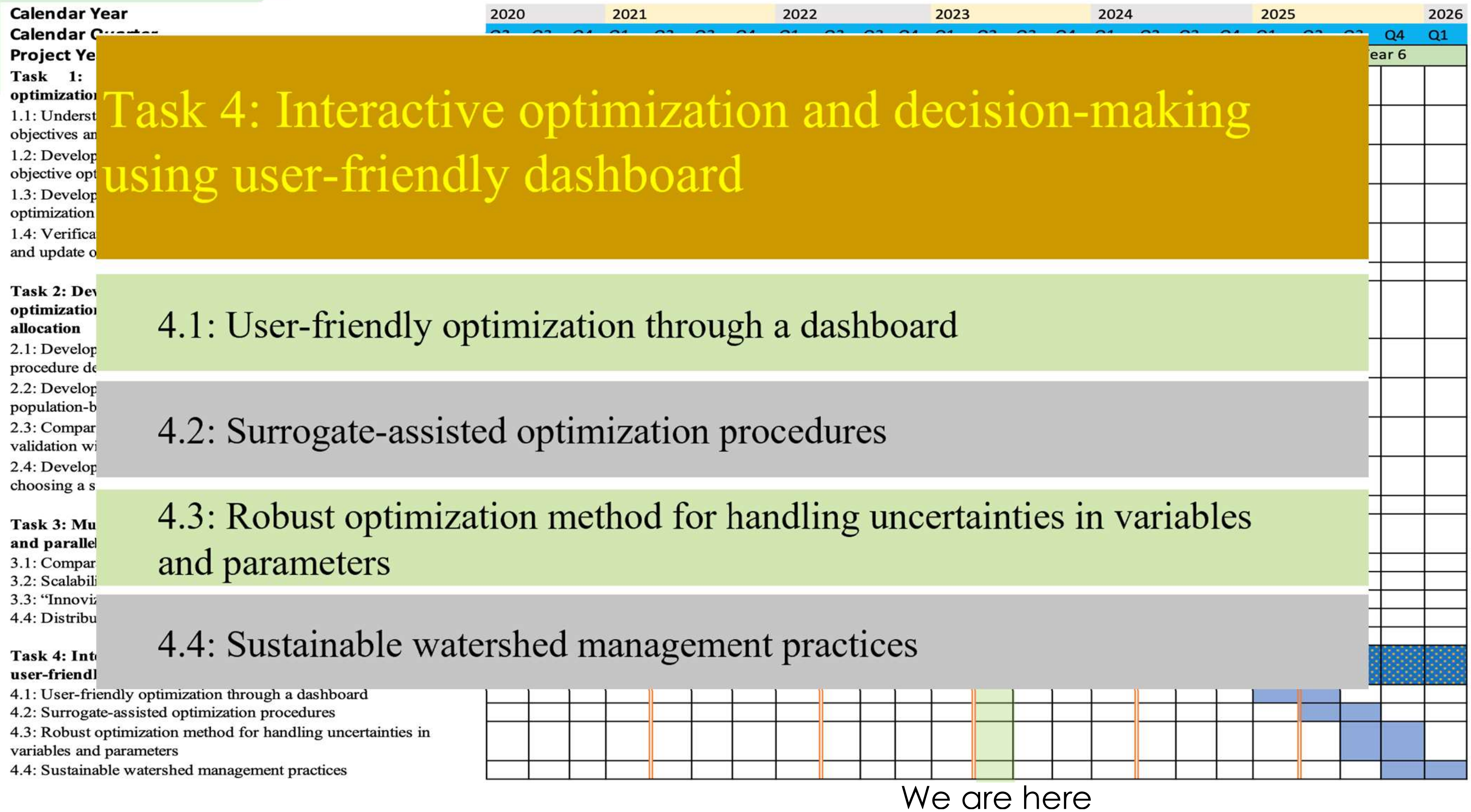
3.2: Scalability to State and Watershed level Scenarios

3.3: "Innovization" approach for improving scalability

3.4: Distributed computing approach for improving scalability

We are here

Timeline of the Project



Task 4: Interactive optimization and decision-making using user-friendly dashboard

4.1: User-friendly optimization through a dashboard

4.2: Surrogate-assisted optimization procedures

4.3: Robust optimization method for handling uncertainties in variables and parameters

4.4: Sustainable watershed management practices

Related Optimization Research at MSU

Point and population-based optimization and their combined use

A case study on a billion-variable resource allocation problem

Multi-objective optimization (MO) and decision-making

- **Evolutionary multi-objective optimization (EMO)** algorithms to find multiple Pareto solutions
- "**Innovization**": Knowledge extraction from learning from Pareto solutions
- **Multi-criterion decision-making (MCDM)** to choose a preferred Pareto solution

Point and Population Based Optimization Methods: Adv and Disadv

Point-Based

Best for simplistic problems, difficult to modify for different problem classes

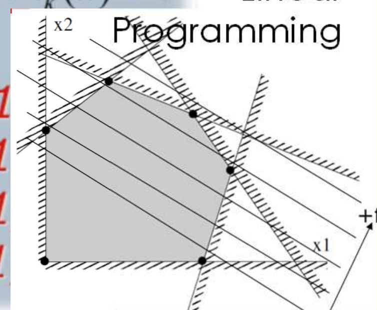
Ideal for local search

Nonlinear Programming

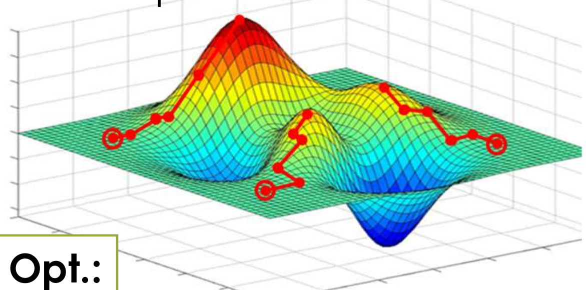
$$\nabla f(x) - \sum_{j=1}^{J} u_j \nabla g_j(x) - \sum_{k=1}^{K} v_k \nabla h_k(x) = 0$$

$$g_j(\mathbf{x}) \geq 0 \qquad j = 1$$
$$h_k(\mathbf{x}) = 0 \qquad k = 1$$
$$u_j g_j(\mathbf{x}) = 0 \qquad j = 1$$
$$u_j \geq 0 \qquad j = 1$$

Linear Programming



Math. optimization

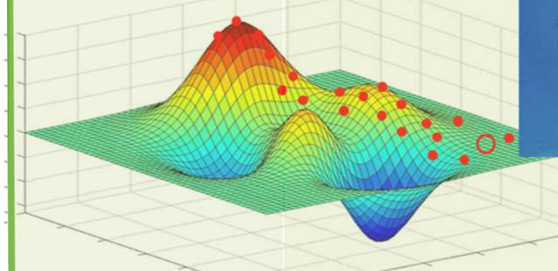


Single-obj Opt.:

Search for a point which minimizes an objective function satisfying constraints

Population-Based

Evolutionary optimization



Other Metaheuristics

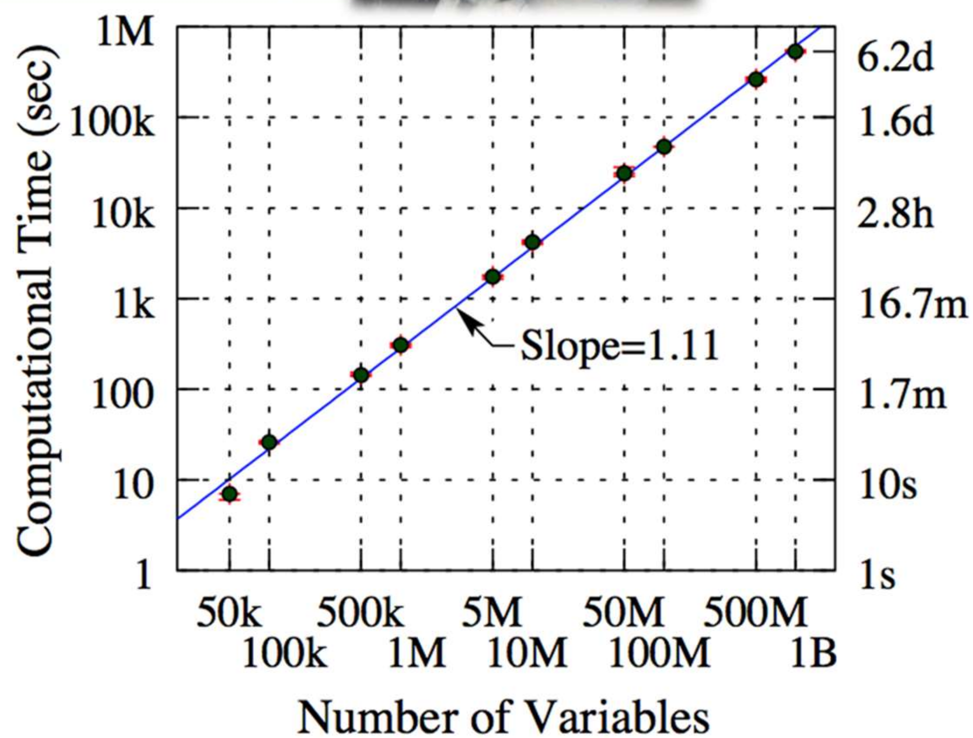
Best for complex problems, flexible to suit a problem class

Ideal for global search

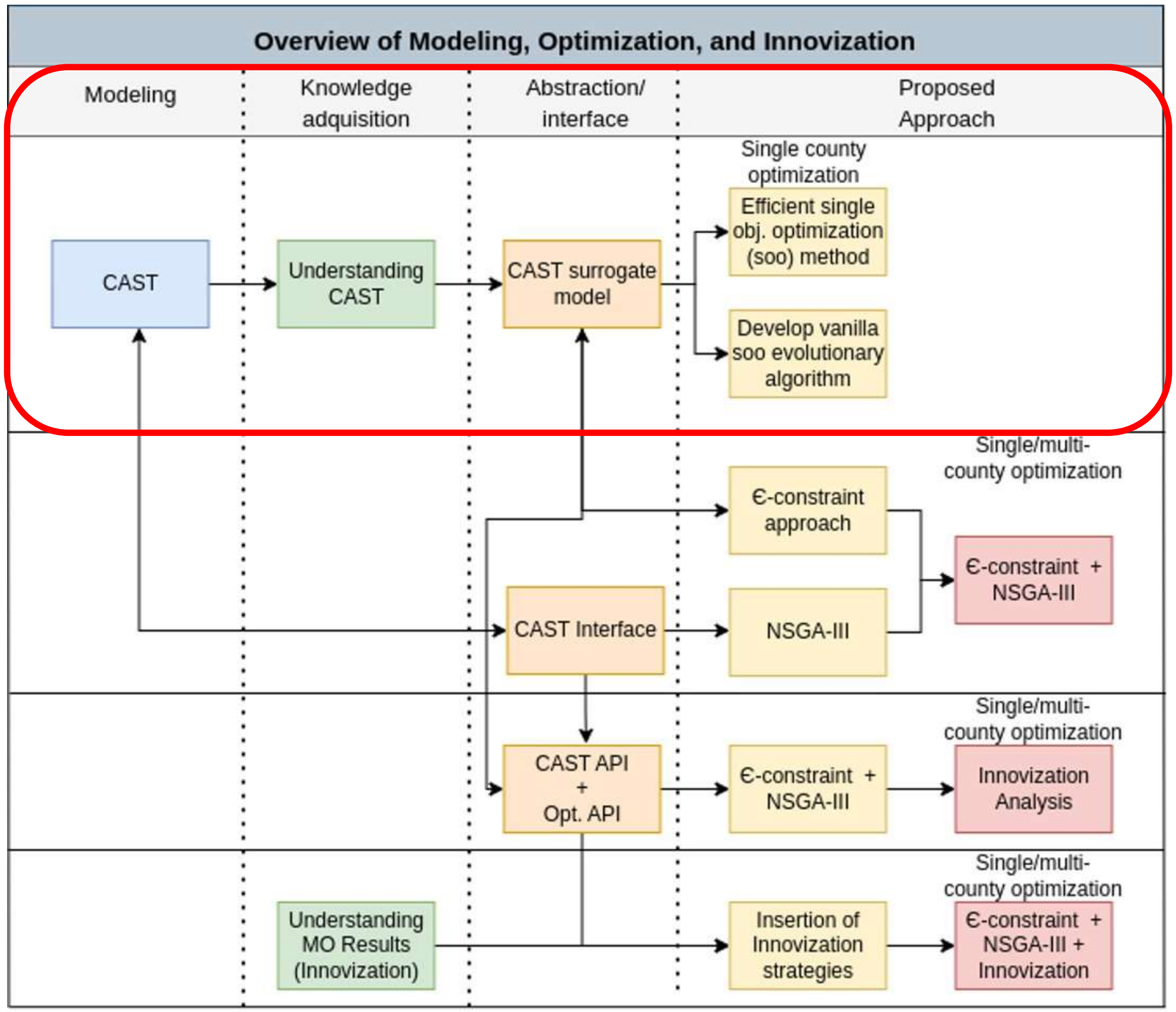
Population-based Optimization:

A Case Study on Resource Allocation Problem

- Casting scheduling problem requiring **50,000 variables**
- CPLEX software could not solve 2,000-variable version
- Customized Evol. Algorithm (population based) solves **Billion-variable** version
  - Polynomial time performance



Deb, K. and Myburgh, C. (2017). A Population-Based Fast Algorithm for a Billion-Dimensional Resource Allocation Problem with Integer Variables. *European Journal of Operational Research, 261*(2), 460–474.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Chesapeake Bay Watershed Optimization Problem

Allocate a specific BMP to

- Land River Segment (LRS)
- Agency
- Load source

Minimize {Cost, Loadings}

Large number of variables will require **large computational time**

Surrogate model:

s: LRS
h: Agency
u: Load source
b: BMP

West Virginia Counties

County	#Variables	#Constraints	Base N_2 (f_2^{base})
Berkeley	14,090	1,813	977,896
Grant	25,228	3,448	1,049,450
Hampshire	12,783	1,700	1,012,797
Hardy	18,607	2,491	1,344,295
Jefferson	12,303	1,606	1,018,012
Mineral	20,260	2,698	763,864
Monroe	3,102	399	48,655
Morgan	11,880	1,665	271,134
Pendleton	33,083	4,352	1,133,327
Preston	1,470	193	4,683
Tucker	1,012	144	1,702
Total	153,818	20,509	7,625,818

$$\text{Min. } f_1(\mathbf{x}) = \sum_{s\in S} \sum_{h\in H_s} \sum_{u\in U} \sum_{b\in B_u} \tau_b x_{s,h,u,b},$$

$$\text{Min. } f_2(\mathbf{x}) = \sum_{s\in S} \sum_{h\in H_s} \sum_{u\in U} \left[\alpha_{s,h,u} \phi_{s,h,u} \prod_{G^B\in\mathcal{G}^B} \left(1 - \sum_{b\in G^B} \eta^N_{s,h,b} \frac{x_{s,h,u,b}}{\alpha_{s,h,u}} \right) \right],$$

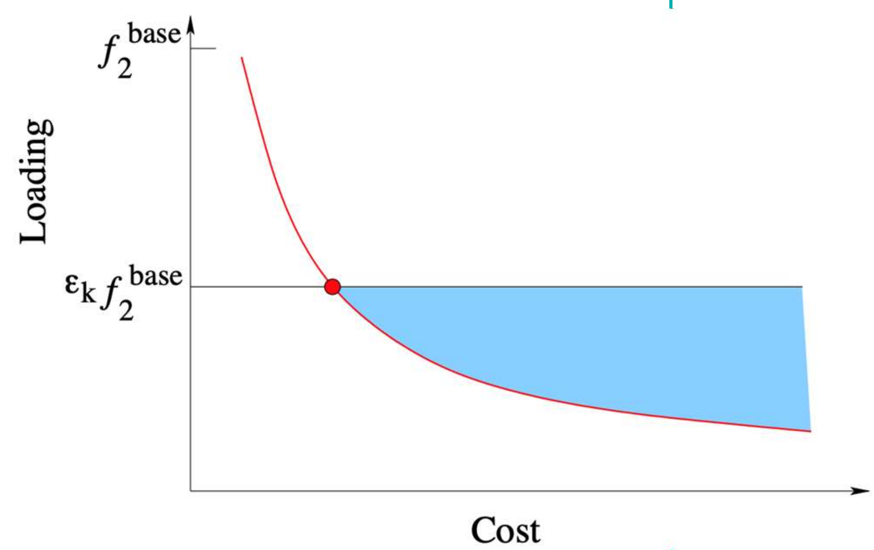
$$s.t. \quad \sum_{b\in G^B} x_{s,h,u,b} = \alpha_{s,h,u}, \quad \forall s\in S,\ h\in H_s,\ u\in U_s,\ G^B\in\mathcal{G}^B,$$

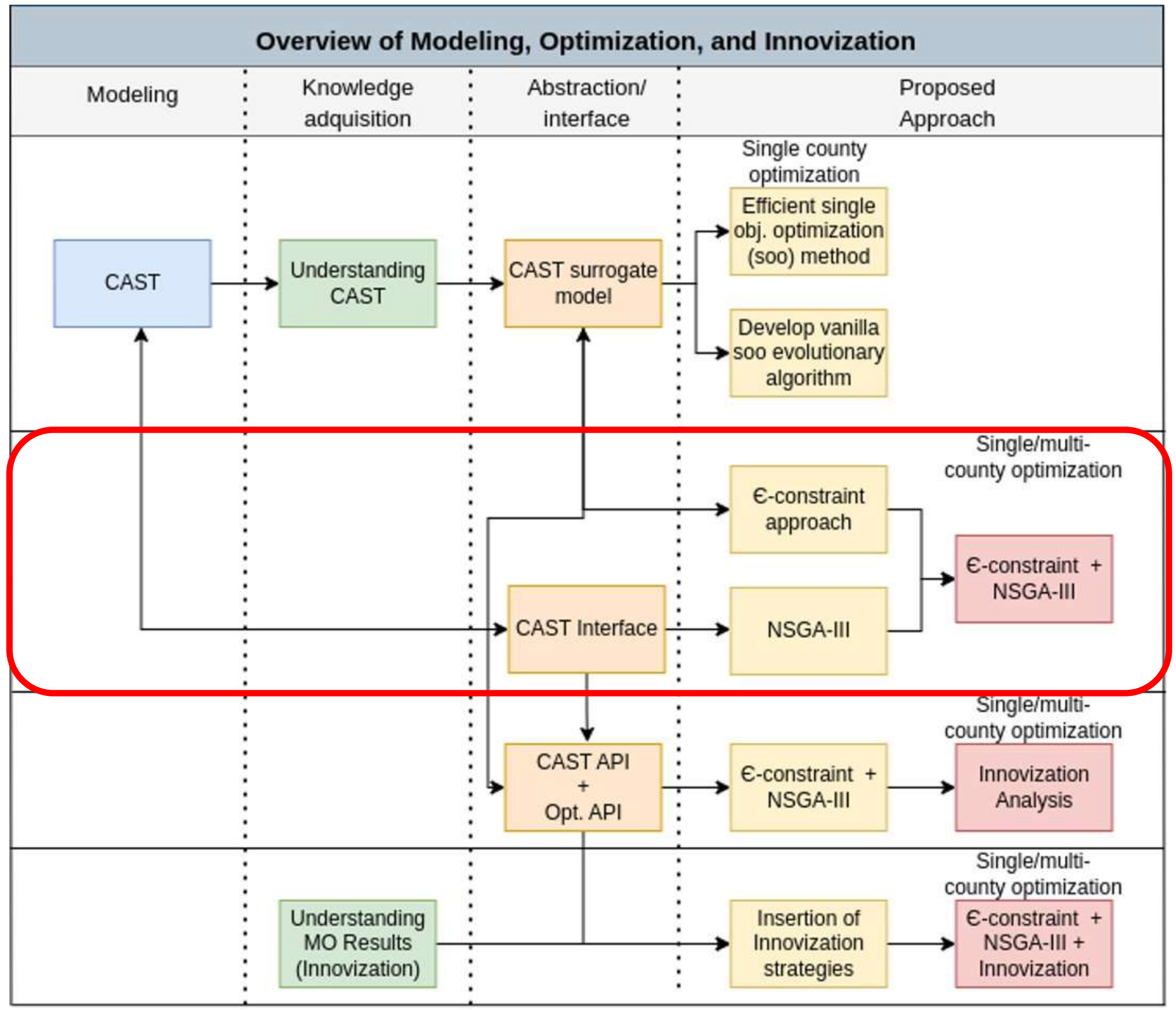
$$x_{s,h,u,b} \geq 0, \quad \forall s\in S,\ h\in H_s,\ u\in U_s,\ b\in B_u.$$

Converting Multiple Objectives Into One

- Convert second objective into a constraint
- **Epsilon-Constraint method**
  - Vary ϵ_k to generate a set of trade-off solutions

$$
\begin{aligned}
&\text{Minimize} && f_1(\mathbf{x}), && \text{(Cost)}\\
&\text{Subject to} && f_2(\mathbf{x}) \leq \epsilon_k f_2^{\text{base}}, && \text{(N2)}\\
& && \mathbf{x} \in \mathbf{X},
\end{aligned}
$$





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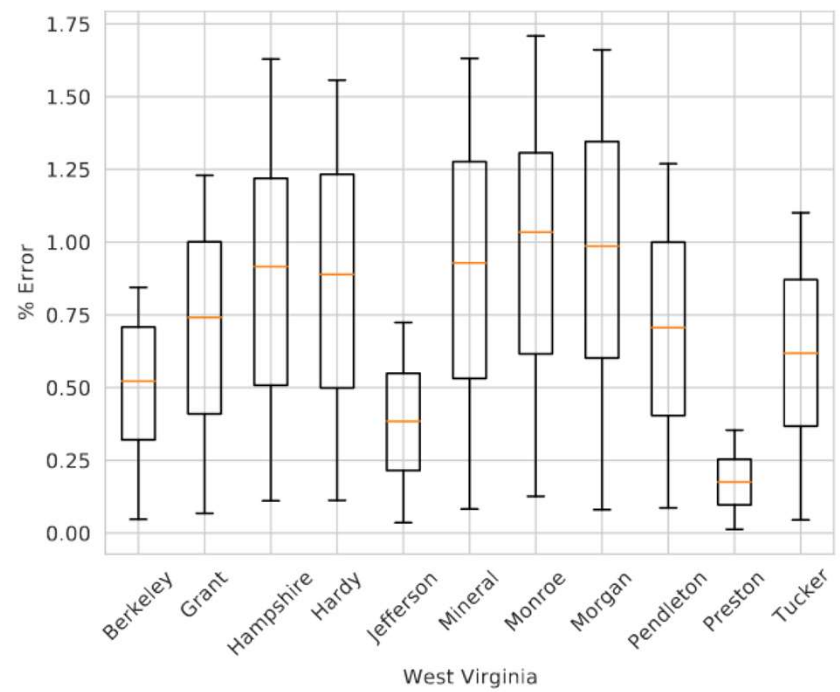
Surrogate Model Error

- **10,000 BMP scenarios** are evaluated using **surrogate model and CAST** on West Virginia counties

- Observed **small error** in Nitrogen loading value

- **Supports the use of surrogate model based optimization, if needed**

Surrogate Model Percent Error Compared To CAST

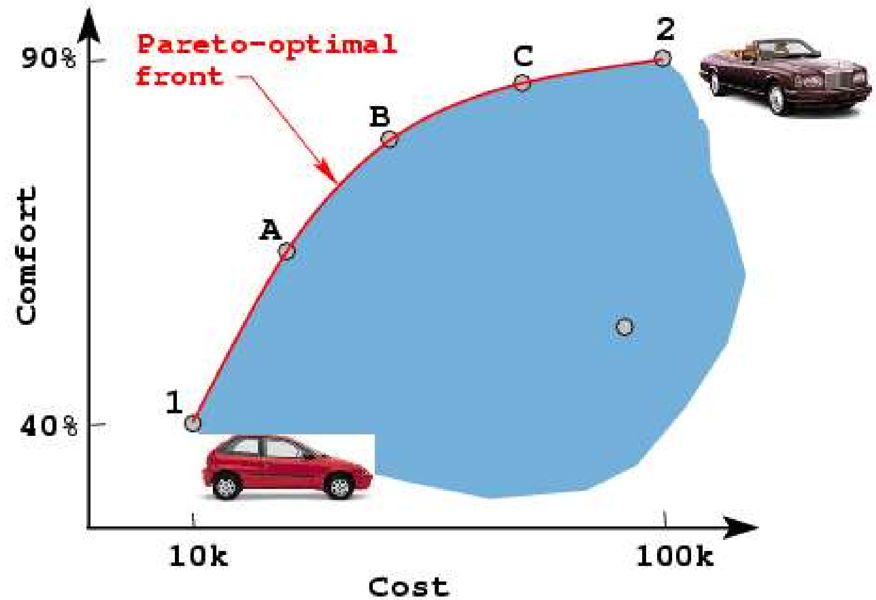


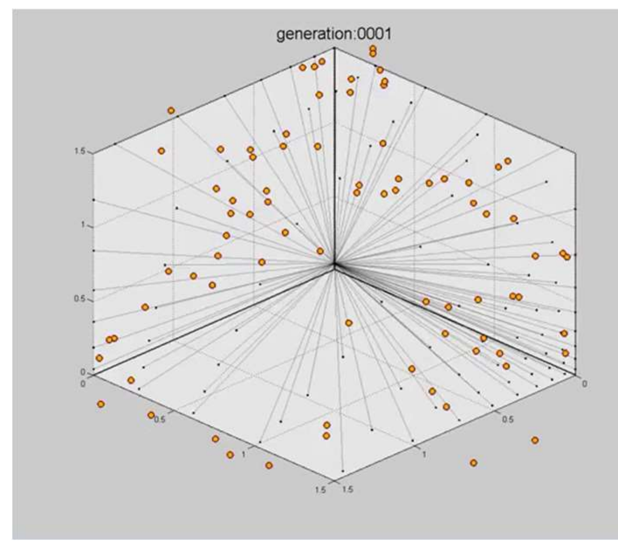
Multi-Objective Optimization

Results in a set of Pareto-optimal solutions

- **Step 1:** Find multiple trade-off solutions
- **Step 2:** Choose a preferred solution

- **Evol. Multi-objective optimization (EMO)**
- NSGA-III can handle 2-15 objectives with constraints



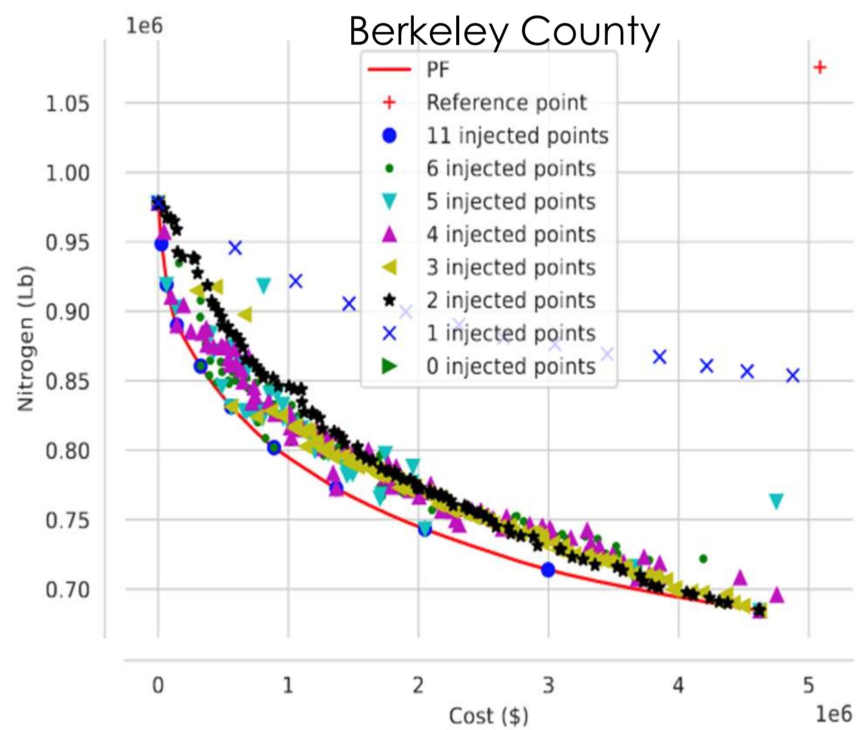


Customized NSGA-III for CBW Problem

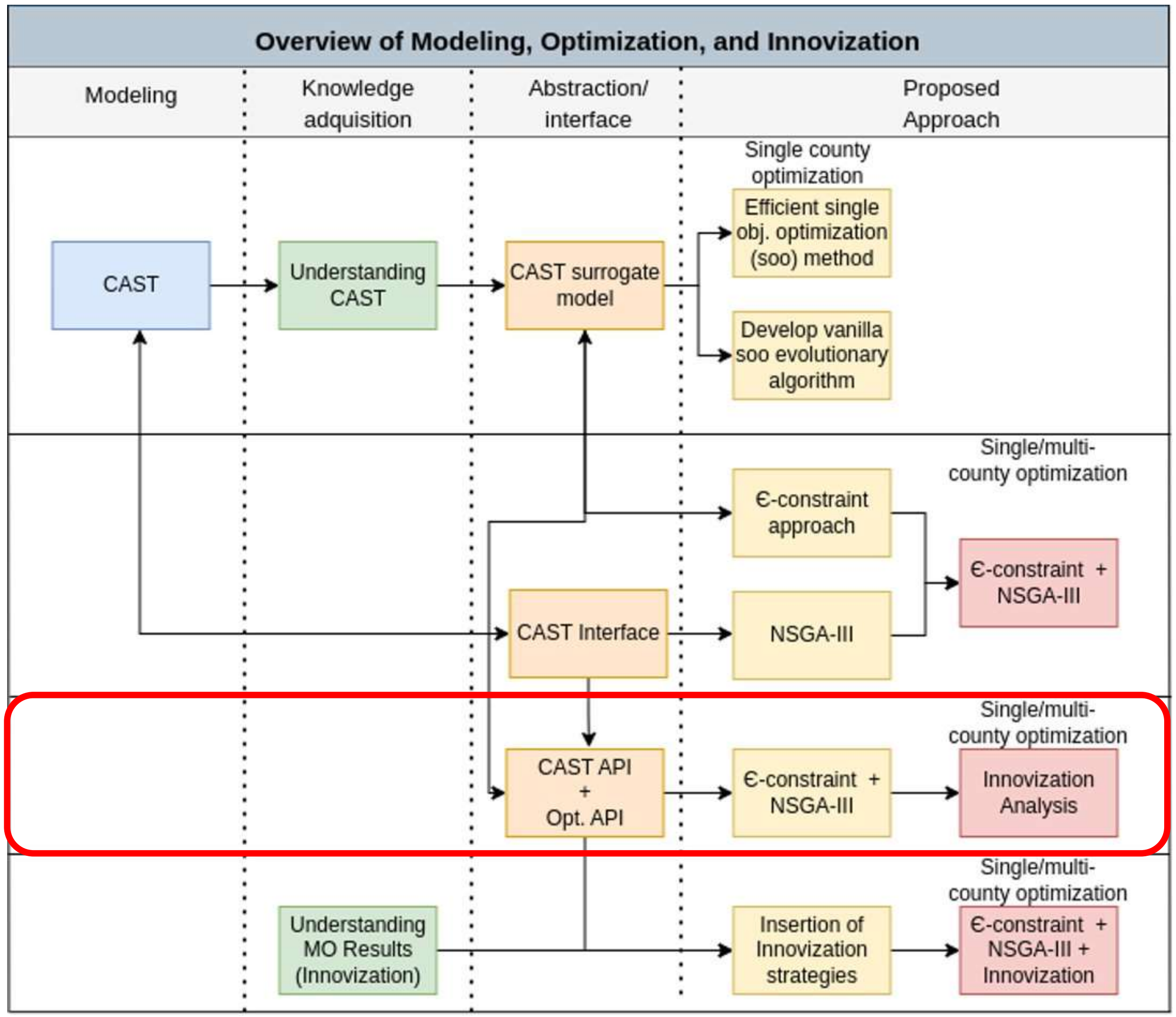
- NSGA-III initialized with **Eps-Constraint solutions**
- Repair operator to fix constraint violation
- Optimize surrogate model

Major finding:

At least 3 injected solutions make NSGA-III efficient



Toscano, G., Hernandez-Suarez, J. S., Blank, J., Nejadhashemi, P., Deb, K. and Linker, L. (2022). Large-scale Multi-objective Optimization for Water Quality in Chesapeake Bay Watershed. Proceedings of 2022 Congress on Evolutionary Computation (CEC-2022), IEEE Press. (pp. 1–8). BEST PAPER AWARD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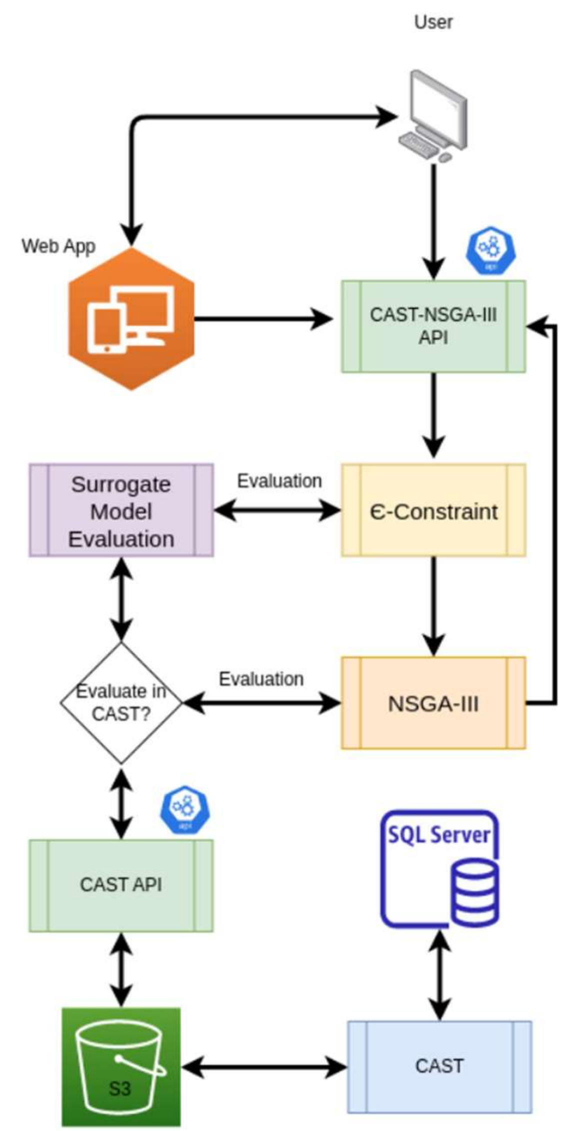
API-based Linking of CAST with NSGA-III

Automatic Programming Interface (API)

- Allows multiple users with different programming environments to interact
- Makes application modular



NSGA-III Linked with CAST

NSGA-III calls CAST to evaluate using Restful APIs

Mixed Heterogeneity:

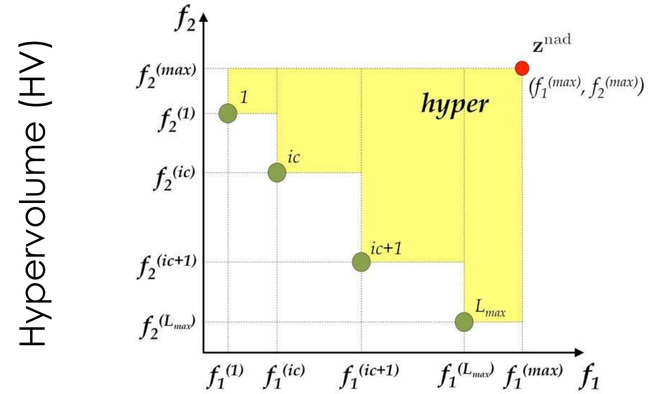
- **50/50:** 50% surrogate, 50% CAST
- **95/5:** 95% surrogate, 5% CAST
- **1:** All surrogates, evaluate final solutions by CAST

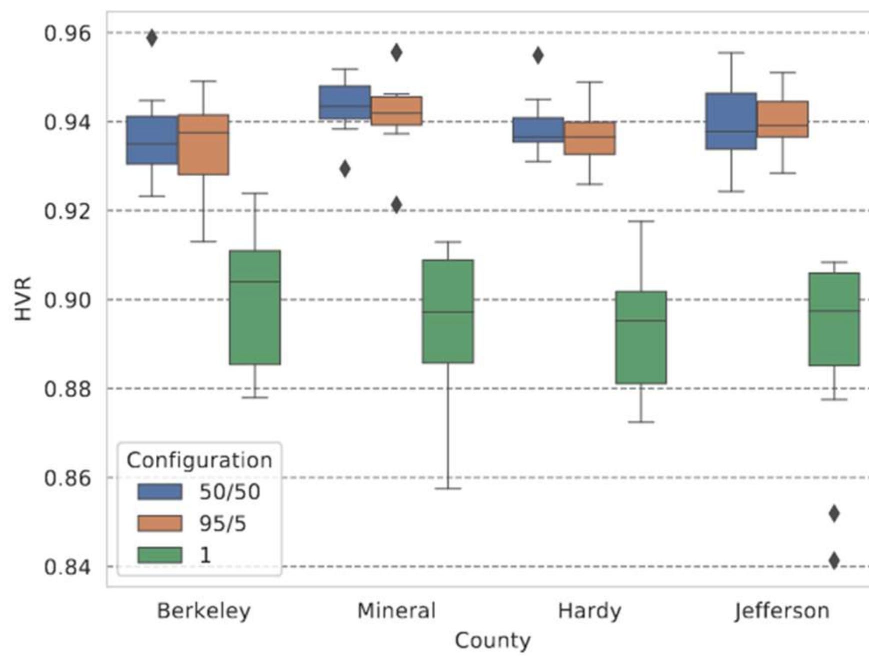
Time (min)

	50/50	95/5	1
Best	138.90	17.53	2.70
Worst	152.96	20.55	3.80
AVG	143.79	18.20	3.18
STD	2.61	0.69	0.33

Major finding:

95/5 is almost as good but requires less time

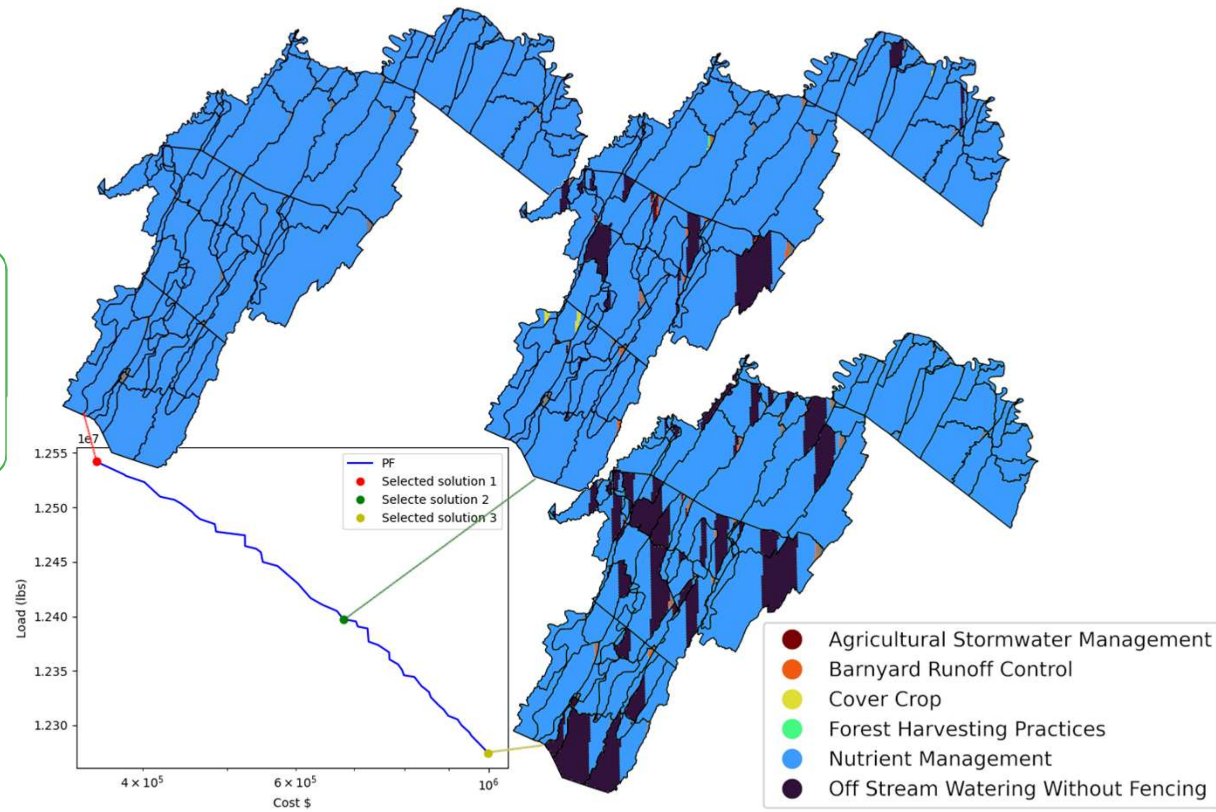




Alternate Solutions Using Multi-objective Optimization

Evaluate alternate solutions before picking a single preferred solution

Analyze solutions for extracting knowledge for future use



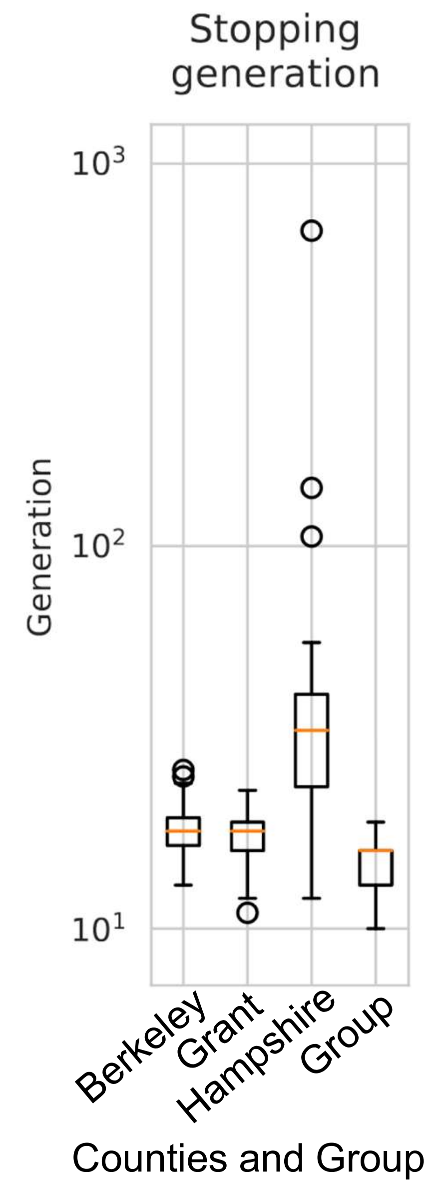
Multi-County Optimization

Observation:

- Some combinations of counties make the problem easier to solve compared to individual counties
  - Ex: Group gets optimized faster than Hampshire county

Major finding:

This provides promise for extending the proposed optimization method to multi-state and to watershed level



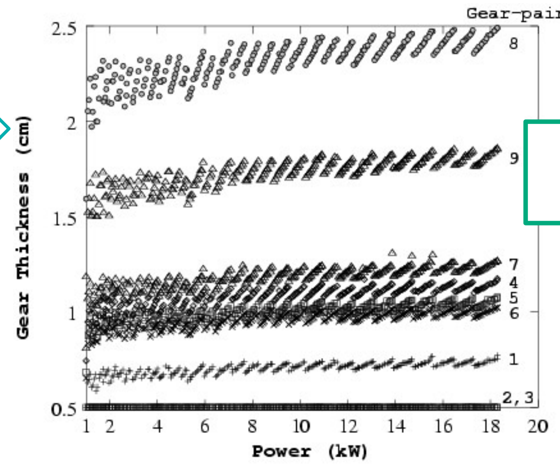
"Innovization"

Innovation through Optimization

Finding **patterns** in Pareto-optimal solutions for knowledge discovery using AI/ML methods

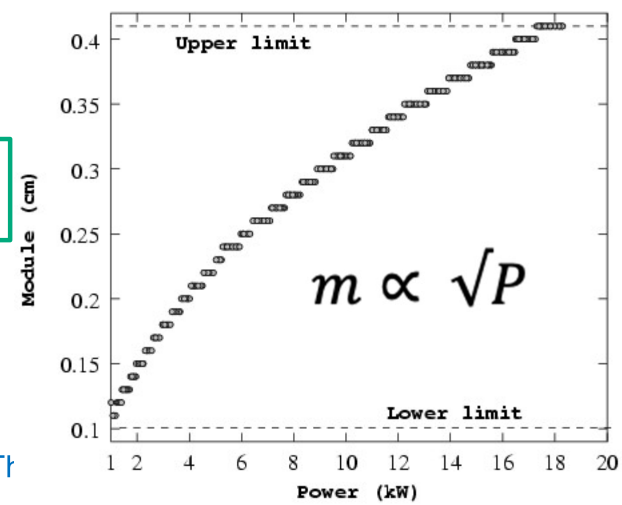
- Optimality conditions must manifest as common patterns
- Extract patterns and re-optimize

A Gear-box design with 28 variables

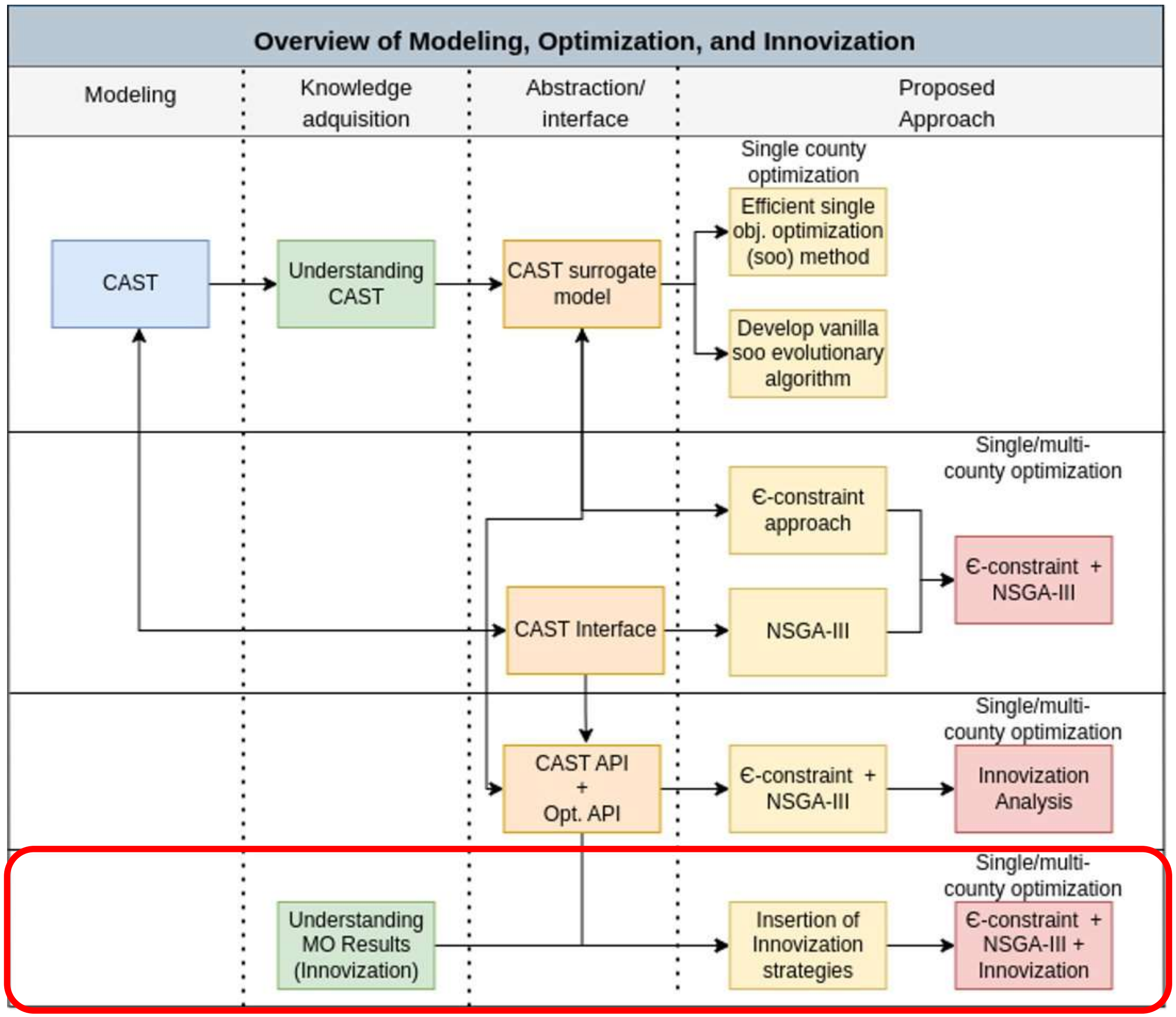


Not much change in 27 variables

Large change in one variable



Deb, K. and Srinivasan, A. (2006). *Innovization*: Innovating design principles through optimization. *Proceedings of the Genetic and Evolutionary Computation Conference (GECCO2006)*, New York: Th Association of Computing Machinery (ACM), (pp. 1629–1636)



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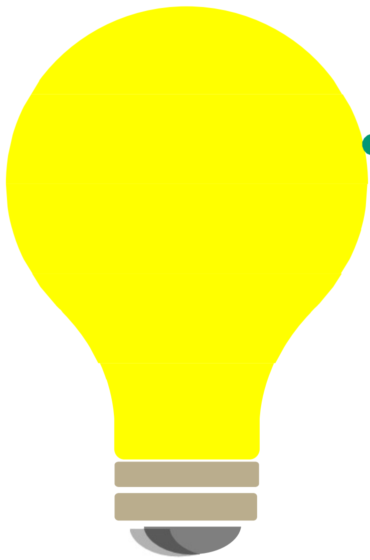
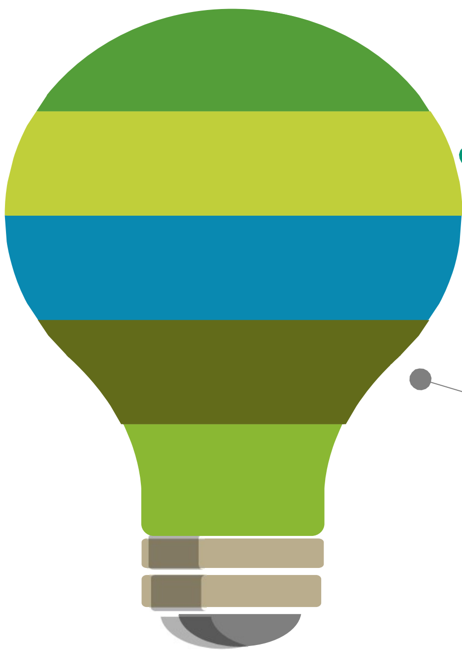
Knowledge Discovery Using Optimization



What are the benefits of optimization?

- Identify the **best solutions** for the problem in hand.
- **Generating knowledge** to solve future problems.

Innovization Analysis



1

- **What is innovization?**

Learning from optimization results and introducing new ideas, products, and services different from the existing ones.

2

What innovization can do to CBPO?

- Provide information for better decision-making for BMP selections **(farmers)**
- Identify the high priority areas for BMP implementation **(regulators)**
- Help with resources allocation **(policymakers)**

Methodology

BMP Selection ranking methodology based on Land use:

- ***Overall goal:*** learn from optimization results to

1. Examine different ranking methodologies to **identify the top BMPs**,
2. Identify the **similarities and differences** between top-ranked BMPs,
3. Provide recommendations to **reduce the optimization time**

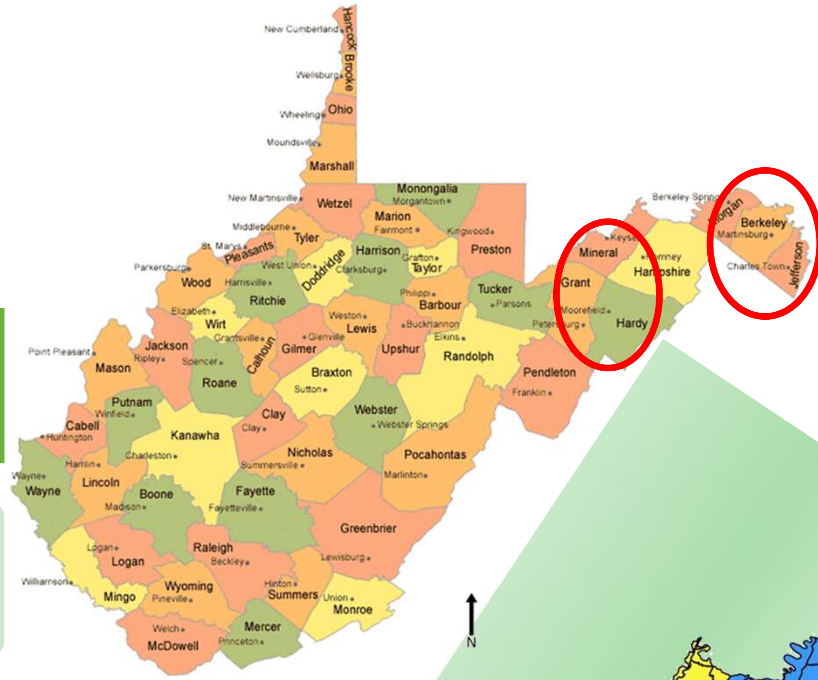
Methodology

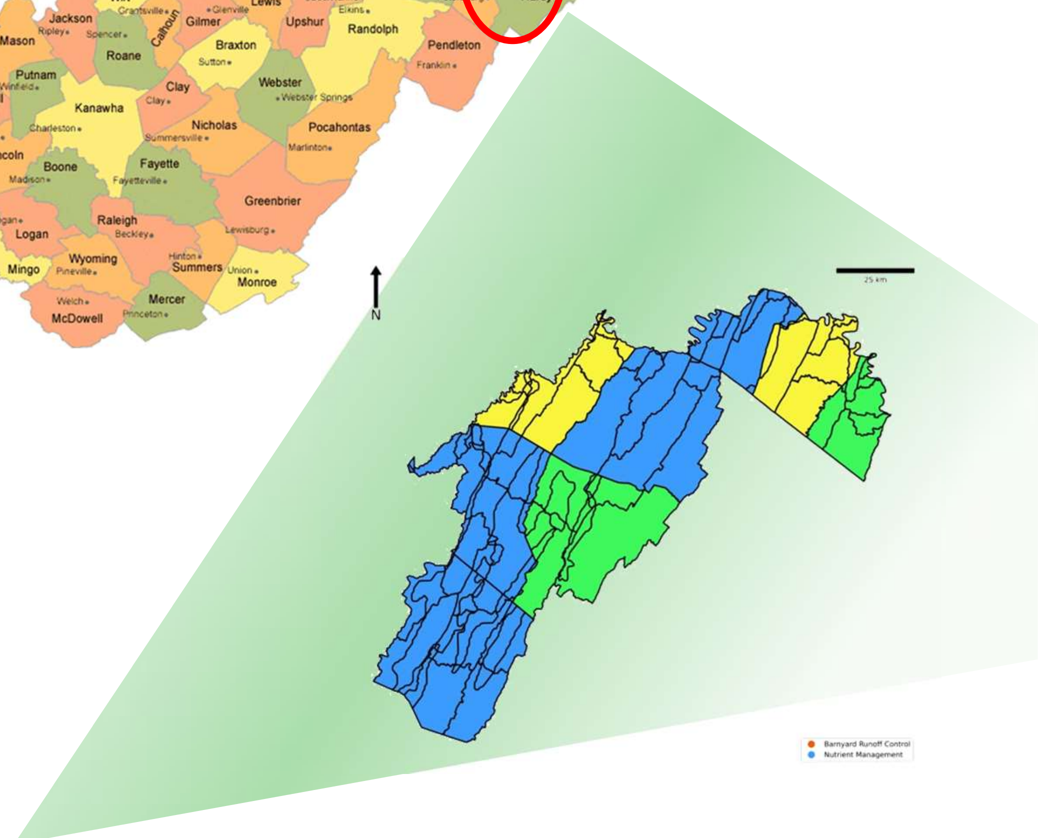
BMP Selection ranking methodology based on Land use:

In **West Virginia**, we identified the top two counties with the highest areas of urban and agricultural land uses.

(**Berkeley** and Mineral): Urban dominated

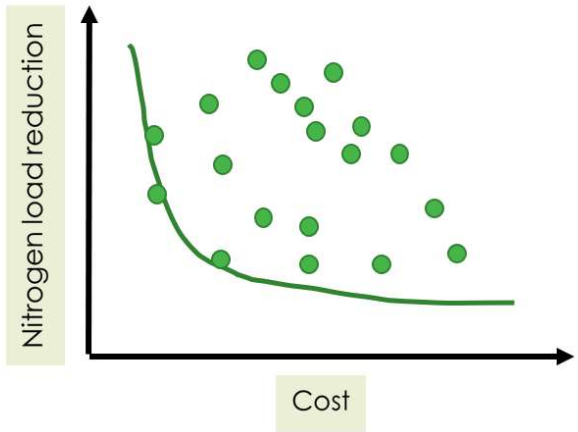
(Jefferson and Hardy): Agricultural dominated





Methodology

BMP Selection ranking methodology based on Land use:



1

Running CAST-optimization algorithm resulted in 220 solutions for **each county**

2

2420 solutions for 11 counties in about thousands land river segments.

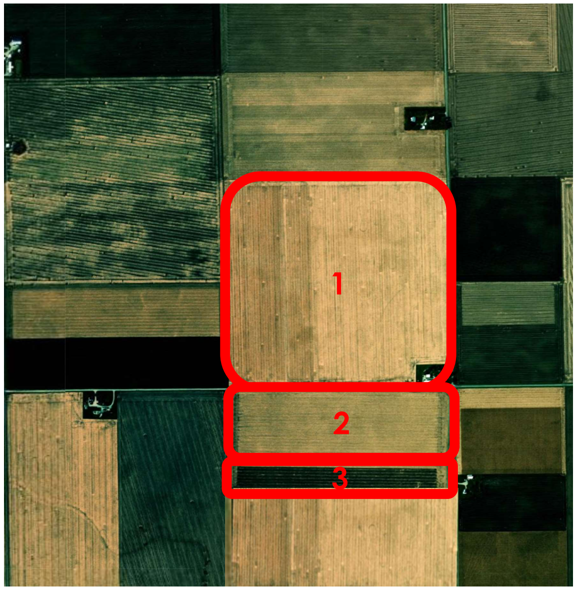
3

Identified the **best solutions from optimization**.

Methodology

1 Examine different ranking methodologies to **identify the top BMPs**,

- **Ranking methodology 1)** rank the top BMPs based on the **implementation acreages**;
- **Ranking methodology 2)** rank the top BMPs based on the percentage of **maximum allowable** acreages;
- **Ranking methodology 3)** rank the top BMPs based on the amount of **nitrogen reduction per dollar spent.**



Methodology

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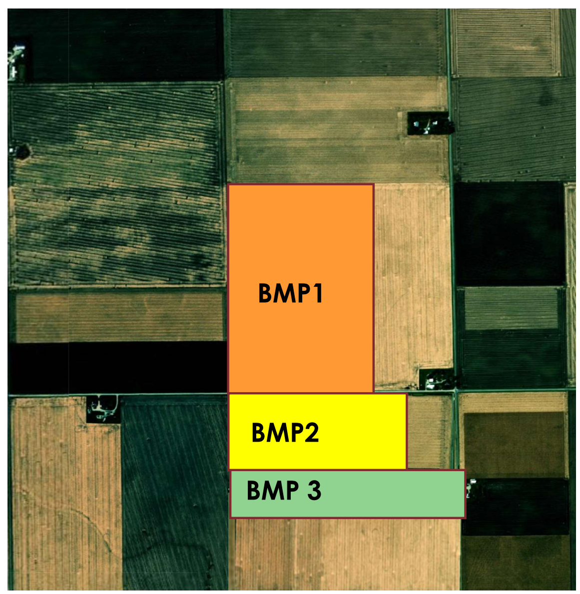
Ranking methodology1):

BMP1
BMP2
BMP3



Methodology

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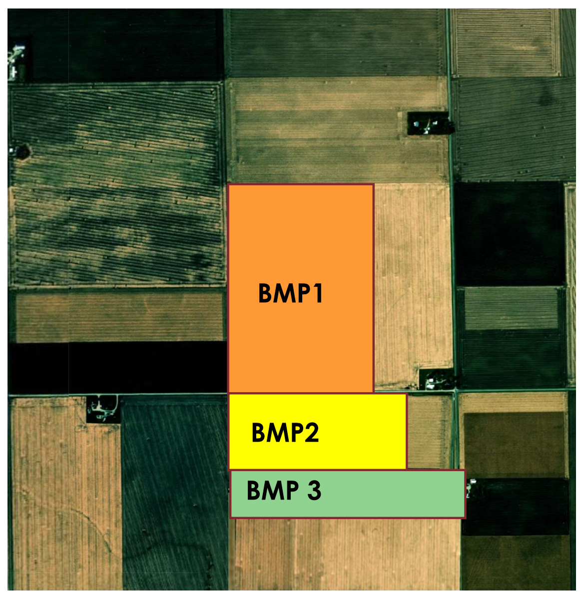
Ranking methodology 2):

BMP3
BMP2
BMP1



Methodology

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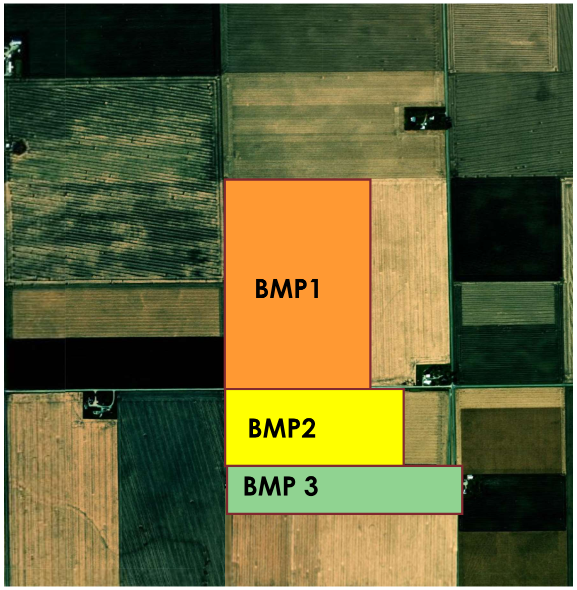
- **Ranking methodology 3)** rank the top BMPs based on the amount of **nitrogen reduction per dollar spent.**

Ranking methodology3):

BMP2 ($12/lb N)
BMP3 ($15/lb N)
BMP1($24/lb N)



Methodology

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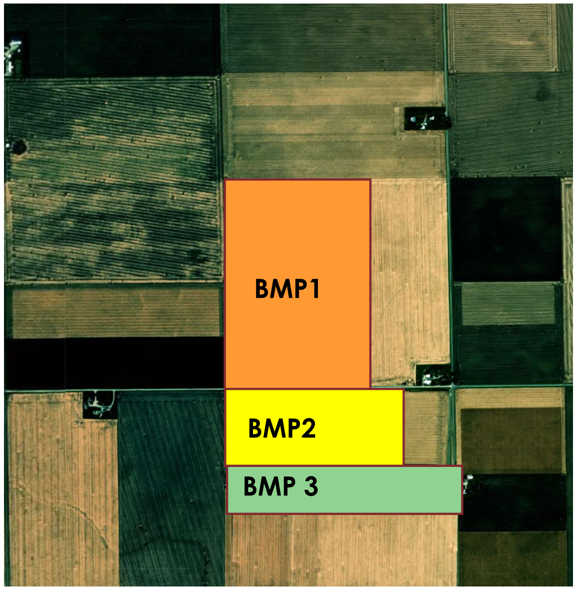
Ranking methodology1):
BMP1
BMP2
BMP3

Ranking methodology2):
BMP3
BMP2
BMP1

Ranking methodology3):
BMP2 ($12/lb N)
BMP3 ($15/lb N)
BMP1($24/lb N)



Results:

2

Identify the **similarities and differences** between top-ranked BMPs,

All three-ranking methodologies:

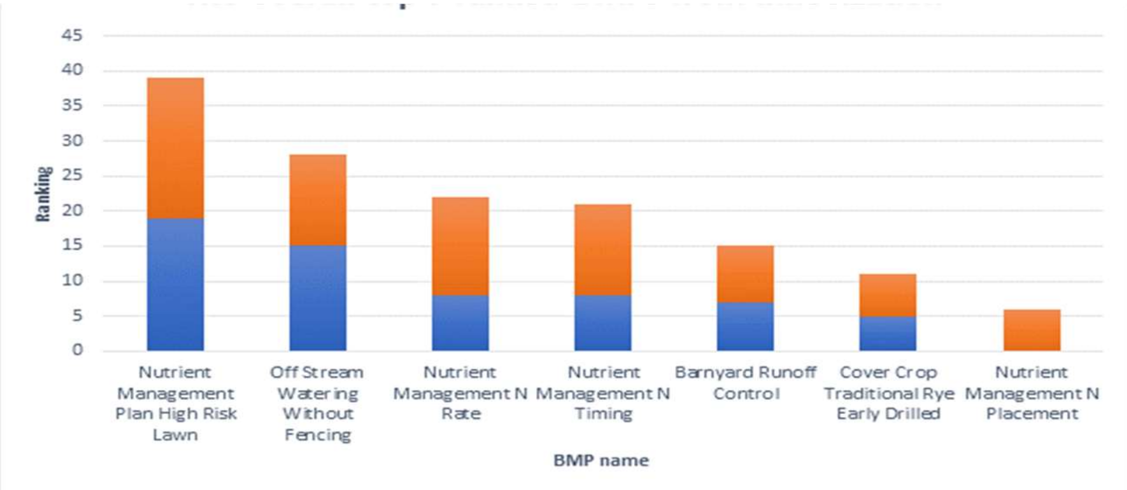
Table: Top choice BMPs based on the all three-ranking methodology

Urban Top-Ranked Counties			Agricultural Top-Ranked Counties		
Strategy 1	Strategy 2	Strategy 3	Strategy 1	Strategy 2	Strategy 3
Nutrient Management Plan High-Risk Lawn	Barnyard Runoff Control	Nutrient Management Plan High-Risk Lawn	Nutrient Management Plan High-Risk Lawn	Barnyard Runoff Control	Nutrient Management Plan High-Risk Lawn
Off Stream Watering Without Fencing	Agricultural Stormwater Management	Off Stream Watering Without Fencing	Off Stream Watering Without Fencing	Nutrient Management Plan High-Risk Lawn	Off Stream Watering Without Fencing
Nutrient Management N Timing	Nutrient Management Plan High-Risk Lawn	Nutrient Management N Rate	Nutrient Management N Timing	Nutrient Management N Rate	Nutrient Management N Rate
Precision Intensive Rotational/Prescribed Grazing	Soil Conservation and Water Quality Plans	Forest Harvesting Practices	Nutrient Management N Rate	Nutrient Management N Timing	Nutrient Management N Timing
Cover Crop Traditional Rye Early Drilled	Off Stream Watering Without Fencing	Nutrient Management N Timing	Cover Crop Traditional Rye Early Drilled	Agricultural Stormwater Management	Cover Crop Traditional Rye Early Drilled
Nutrient Management N Rate	Nutrient Management N Placement	Cover Crop Traditional Rye Early Drilled	Nutrient Management N Placement	Nutrient Management N Placement	Nutrient Management N Placement
Nutrient Management N Placement	Nutrient Management N Rate	Nutrient Management N Placement	Barnyard Runoff Control	Off Stream Watering Without Fencing	Cover Crop Traditional Rye Early Other

Results:

3 Provide recommendations to **reduce the optimization time**

Obtaining the total ranking of each BMP by adding the associated ranking to induvial BMPs.



Results:

2

Identify the **similarities and differences** between top-ranked BMPs,

Similarities:

Top BMP choice: Nutrient management lawn or farm
The pasturelands: Off-stream watering facilities

Differences:

More diversity in BMP types was in agricultural settings compared to urban ones.

“Innovization” Study on CBW Problem
Variable Reduction

1
- Pareto solutions spilt for **rural and urban** counties

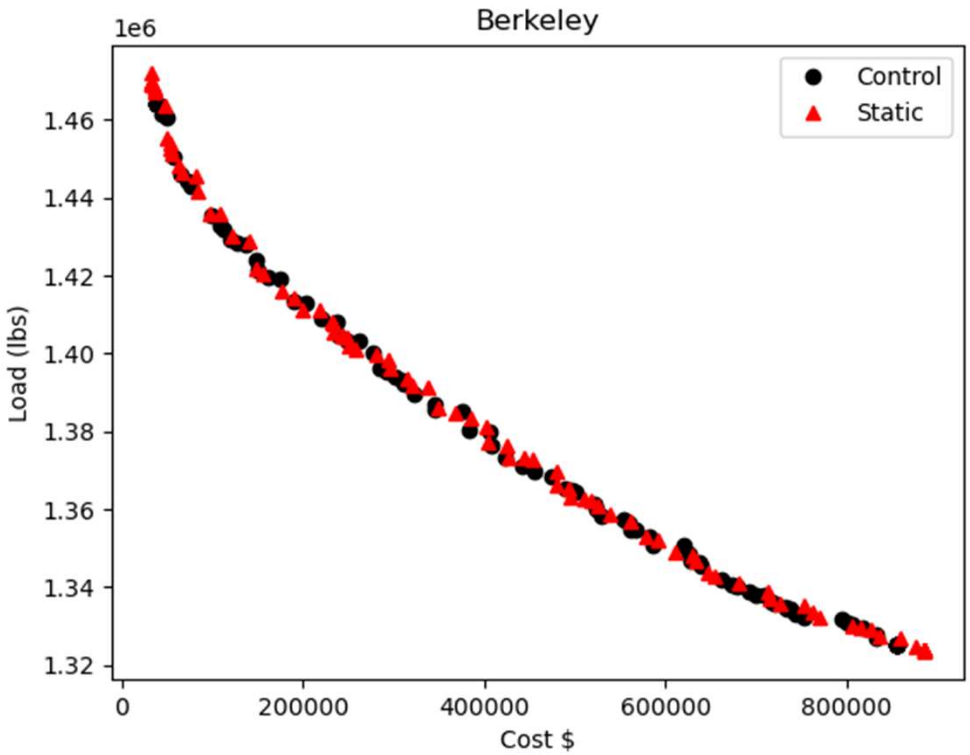
2
- **Frequency** of BMPs extracted

3
- **7 out of 200 BMPs** are frequently used in Pareto solutions

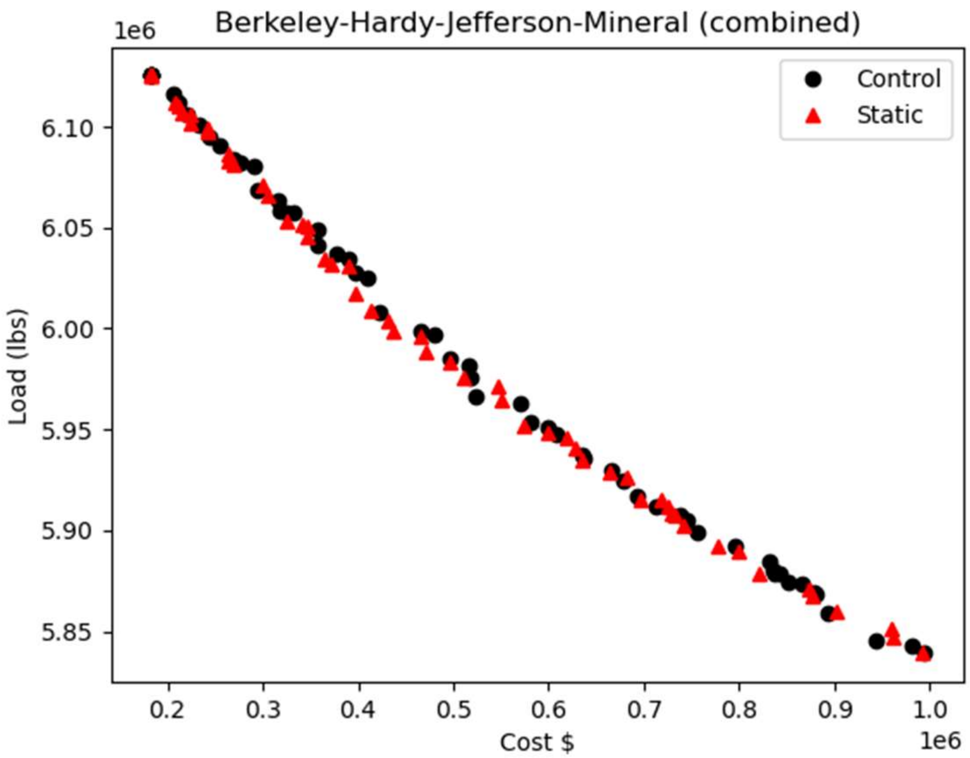
4
- **Re-optimize** using only 7 BMPs

	Control	Static
Berkeley	14,090	510 (3%)
Hardy	18,607	725 (3%)
Jefferson	12,303	456 (3%)
Mineral	20,260	765 (3%)

Reoptimization Using Innovization Results on Berkeley County



Reoptimization Using Innovization Results on Berkeley, Hardy, Jefferson, and Mineral Counties (Combined)



Results:

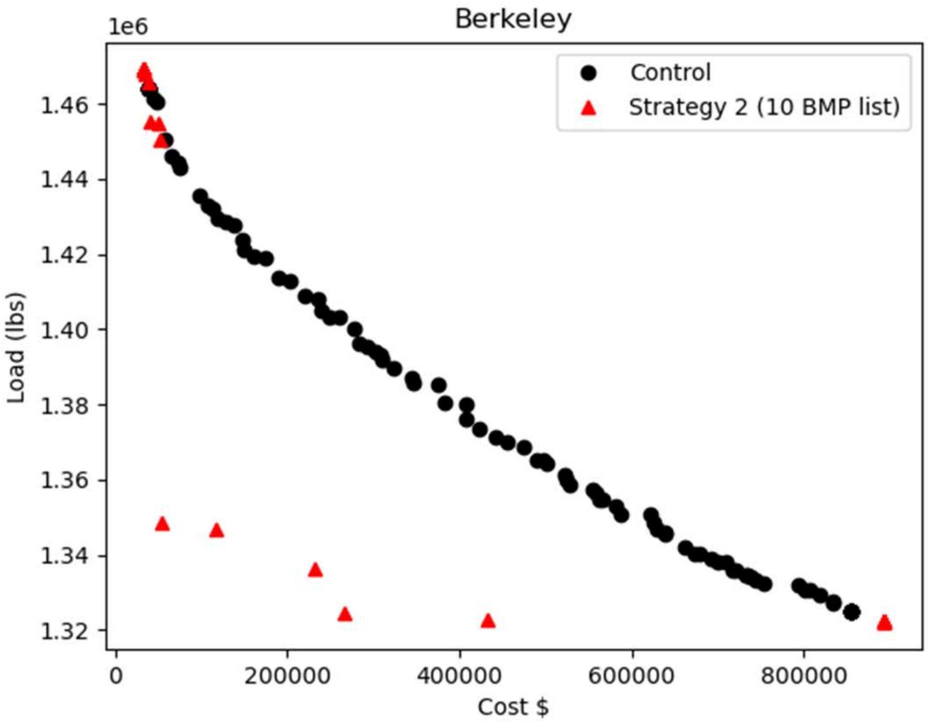
3 Provide recommendations to **reduce the optimization time**

Recommend the selection of **the top seven BMPs from the overall column** for optimization.

Can be used in developing the initial population in other counties within the state of West Virginia.

Hypothesis: this approach could significantly reduce the **optimization processing time** while producing more cost-effective BMP implementation plans.

Reoptimization Using Innovization Results on Berkeley County



Prototype Interactive Web Tool

1

- Input-output through **the web portal** (Done)

2

- Collects scenario for optimization (Done)

3

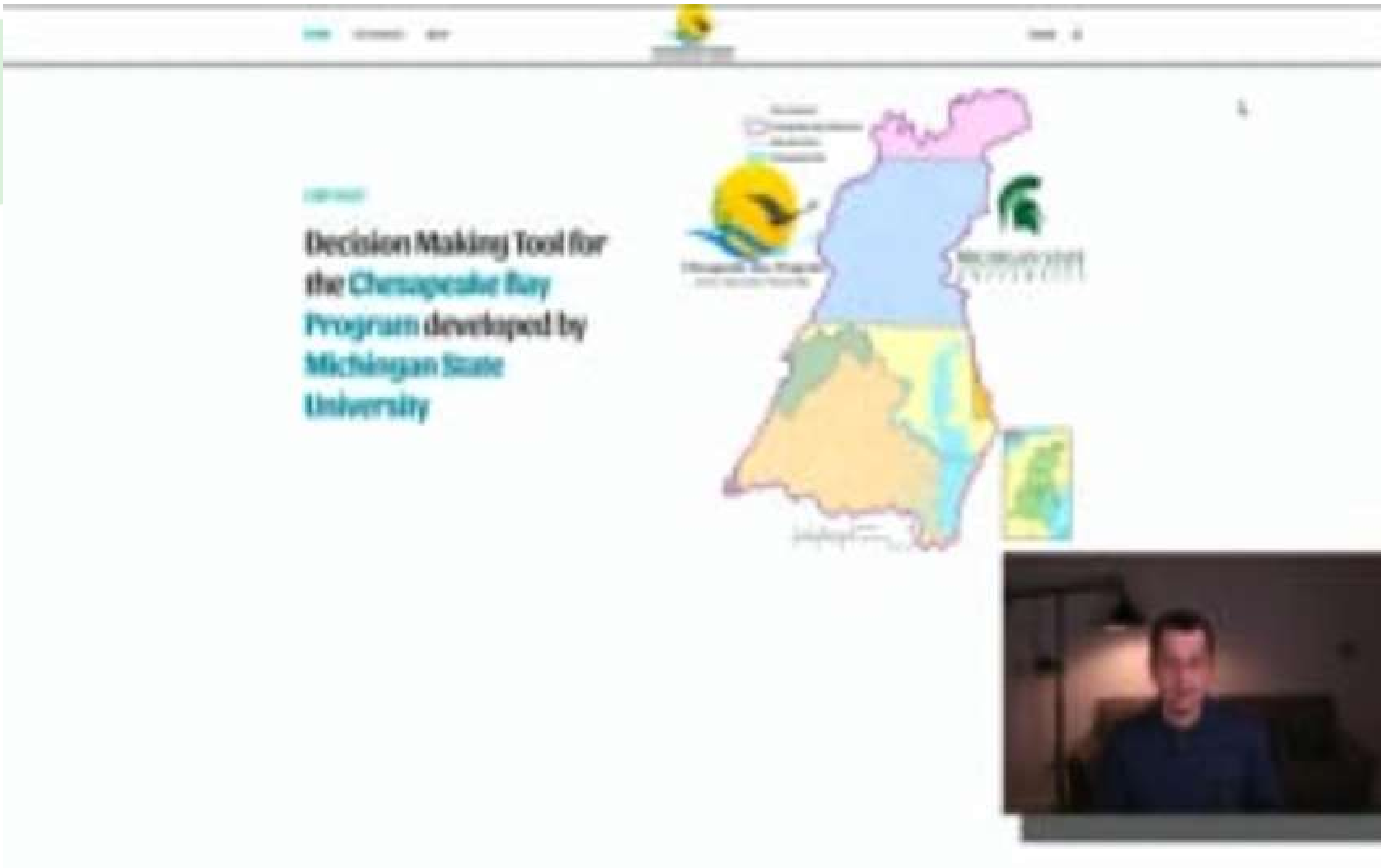
- NSGA-III is invoked and calls CAST for evaluation (Done)

4

- Calls Decision-making Dashboard for analysis of Pareto solutions (Remaining)

5

- Re-optimize using "**Innovized**" principles until satisfied (Partially Done)

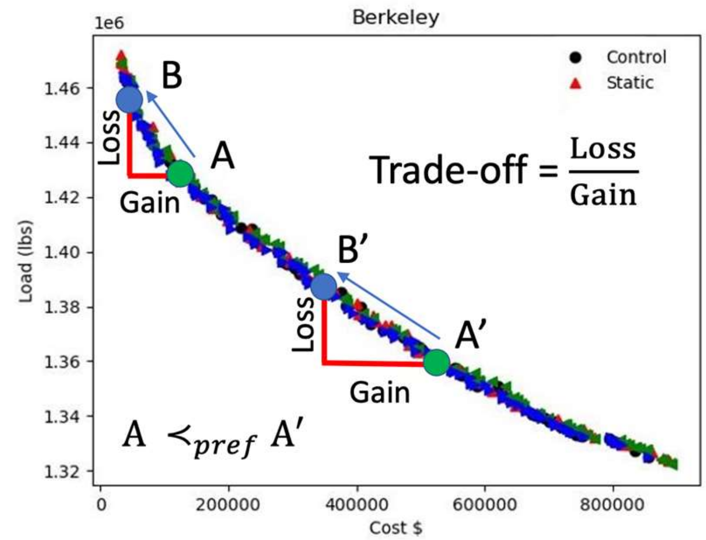

Decision Making Tool for the Chesapeake Bay Program developed by Michigan State University

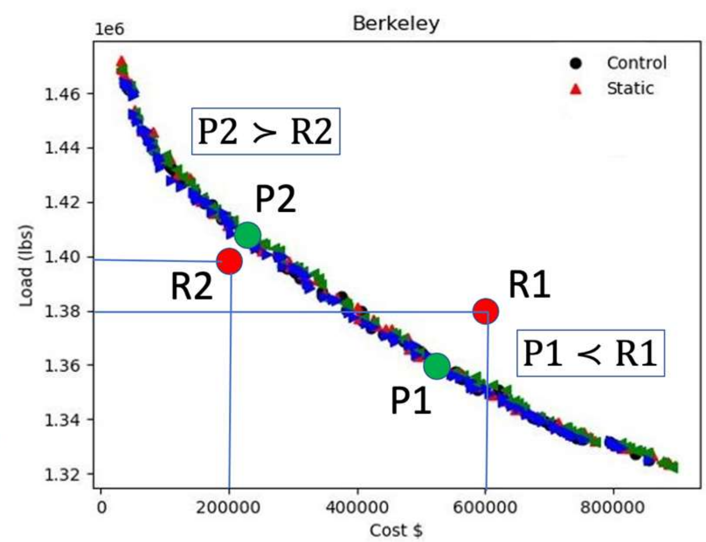
Decision-Making Methods

Decision-making:

A systematic approach to pick a preferred solution

A-posteriori Trade-off analysis
A-priori Aspiration based approach
Interactive EMO-MCDM
DM provides preference information during optimization





Deb, K., Sundar, J., Reddy, Uday, B., and Chaudhuri, S. (2006). Reference point bas multi-objective optimization using evolutionary algorithms. *International Journal of Computational Intelligence Research (IJCIR)*, 2(6), 273–286.

Remaining Tasks

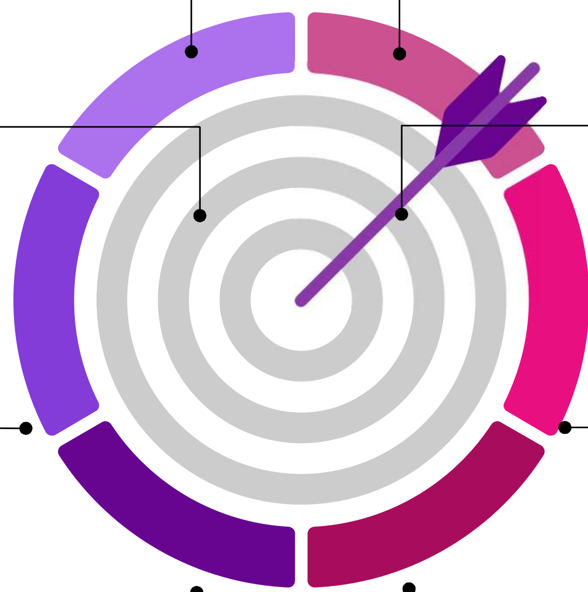
Completion of all BMP types: **Land conversion, Animal, Manure transport, etc.**

Multi-criterion Decision-making (MCDM) to choose a single solution

Converted Oxygen optimization to combine **multiple loadings**

Dashboard for interactive applications

- A partial framework is completed



More than two-objective optimization

Harnessing hardware parallelism

Scale-up study to multi-state and watershed level optimization

Demonstration through workshops and tutorials

MICHIGAN STATE UNIVERSITY

Computational Optimization and Innovation

Thank you

C-ECO

Computational Ecohydrology