

Scenario Optimization Tool for CAST

(the time-averaged Phase 6 watershed model)

12 September 2018 – STAC Quarterly Meeting

Danny Kaufman

Project Goal: Investigate, develop, test, and implement an optimization system for the Chesapeake Assessment Scenario Tool (CAST) that will facilitate identification of more cost-effective and otherwise optimal approaches to pollutant load reduction for CBP partners.

Current system

Best
Management
Practices
(BMPs)



Chesapeake
Assessment
Scenario Tool
(CAST)



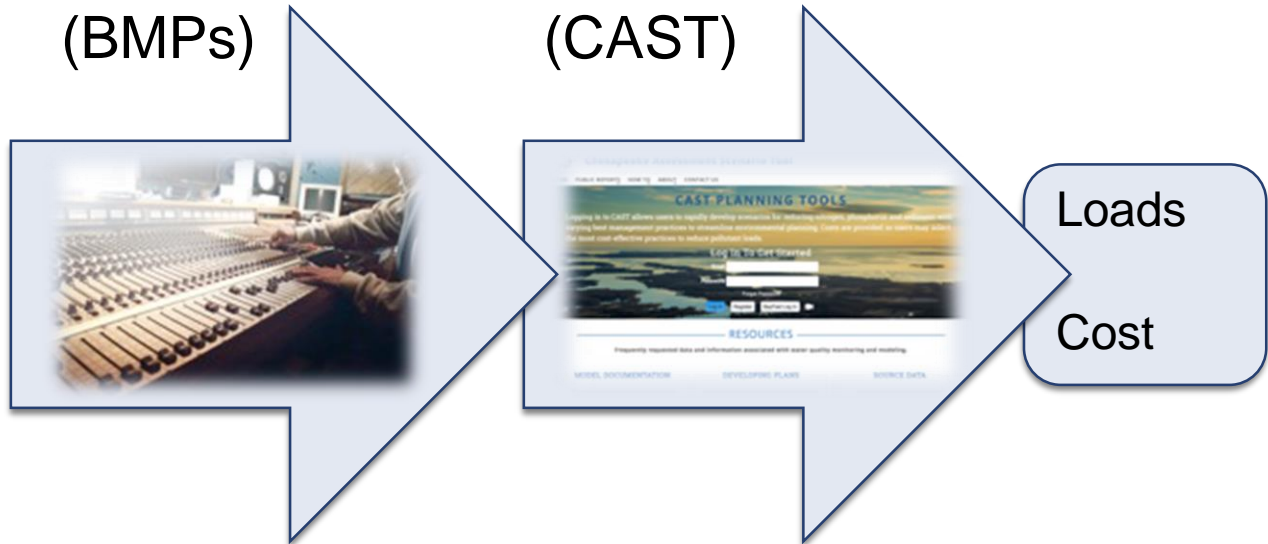
Loads
Cost

Current system

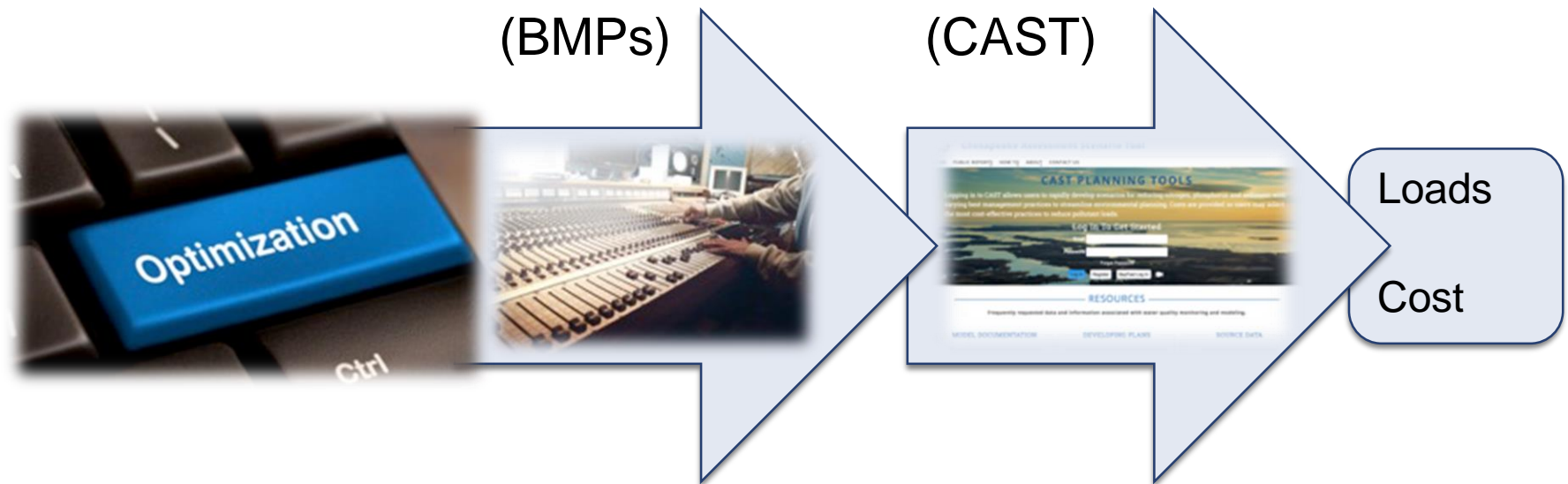
Best
Management
Practices
(BMPs)

Chesapeake
Assessment
Scenario Tool
(CAST)

Not feasible to
exhaustively try
potential strategies



Scenario Optimization System



Analyze potential BMP options and identify low-cost strategies

To help the Chesapeake Bay Program and its Partners restore the Bay and its watershed

Why this update? (outline)

From STAC Workshop to Now

Current working prototype and progress

Next steps

STAC Workshop

“...[m]odels that can identify potential strategies for efficiently advancing multiple goals and objectives of the broader Chesapeake Bay Watershed Agreement are needed.”

Workshop goal(s)

- review and examine optimization modeling approaches / applications in a water quality context
- examine capacity to integrate an optimization engine with existing tools developed by the CBP to guide WIP development

Goals of a Bay optimization system:

- Objectives:
 - Minimizing total costs
 - Maximizing co-benefits
 - Maximizing load reduction reliability
- Equitable distribution of effort among jurisdictions / source sectors
- Limits on retirement of agricultural land
- Ability to use the tool at various scales (county -> baywide)

Stepwise approach, and incorporate into CAST (the Bay Watershed Model)

Up to December, 2017

Highlights

Workshop held

STAC Workshop held on Feb 17-18

ASC Established

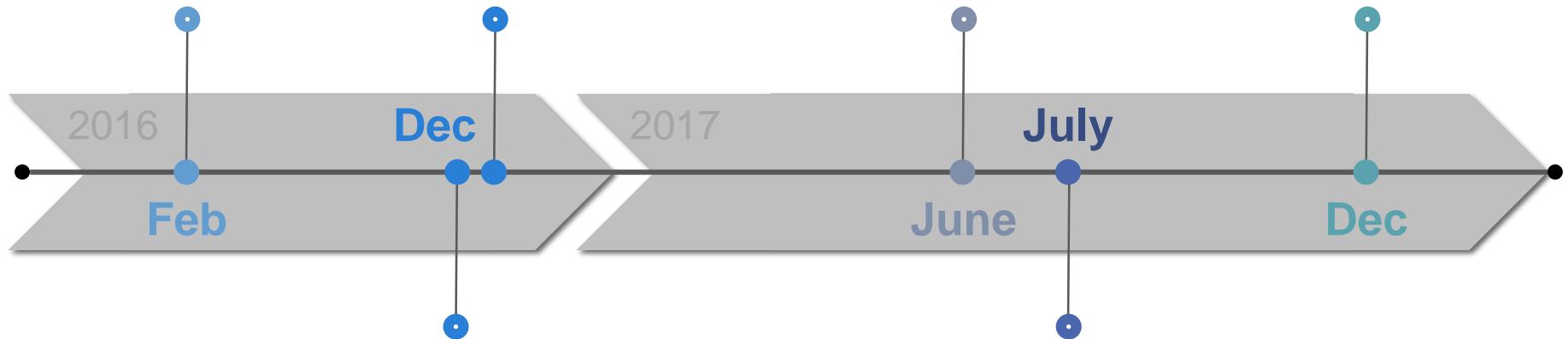
Advisory and Support Committee formed to provide guidance

Report Published

STAC Workshop Report published

R.S. Hired

Research Scientist hired to work full-time at the Chesapeake Bay Program Office on Optimization Tool Development



Grant Awarded

Grant for optimization tool development awarded to Chesapeake Research Consortium (CRC)

Preliminary Work

Dr. Stuart Schwarz of UMBC worked on Phase 1 activities in June and July of 2017, and proposed a recursive greedy algorithm for adding improved feasible choices to an optimization solution set.

Since December, 2017 (nine months)

Highlights

Programmatic

Meetings with:

- Advisory and Support Committee (~Quarterly)
- Dr. Hugh Ellis, at Johns Hopkins (~monthly)
- CBPO technical teams (regularly)

Presentations and feedback gathered from:

- Water Quality Goal Implementation Team (WQGIT)
 - Workgroups
 - Watershed Technical
 - Modeling
 - Urban Stormwater
 - Wastewater Treatment
 - Scientific, Technical Assessment, and Reporting (STAR) team
 - Chesapeake Research & Modeling Symposium
-
- Response to STAC workshop drafted for CBP Management Board
 - Project workplan updated, and no-cost extension granted (to March 31, 2020)

Since December, 2017 (nine months)

Highlights

Technical

Pre-prototype software created for on-the-fly generation of Best Management Practice (BMP) scenario files for use with CAST.

Two prototype optimization models for efficiency BMPs (a sub-population of all BMPs) have been developed for cost and load reduction objectives.

Analyses of the efficiency BMP optimization model results have provided insight into problem characteristics

Main Takeaways from recent optimization ASC meeting

(Monday, 20 Aug 2018)

Working prototype, using subset of BMPs, is well formulated:

- convexity and starting point analyses were useful
- and there are not any fatal flaws

Key elements to build on:

- larger geographic scales
- compare prototype results to 'optimal solutions' obtained by both CAST experts and other users
- include additional BMPs
- other operational issues

Post-ASC meeting discussions

Focus the CBPO “operations research department” on merging ASC ideas with the need to develop a working prototype in 2019

Utilize working prototype to gather feedback and collaboratively build in features desired by users

- Actively engage users that have not been previously engaged
- Work with folks (could be you!) to construct and explore case studies

Concurrent long-term strategizing:

- Algebraically formulating additional BMPs
- Testing heuristic and/or model-based optimization strategies

Working Prototype

Problem description

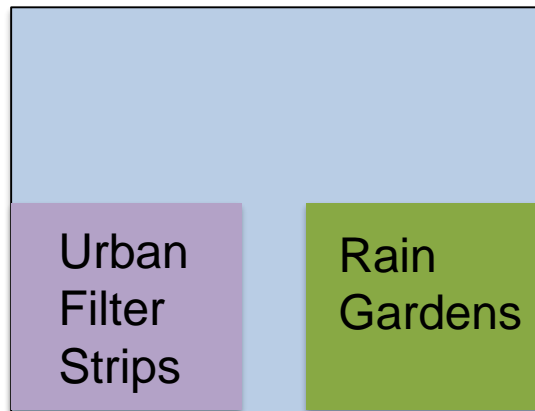
Optimization model

- two forms
- example results – land river segment
- example results – county

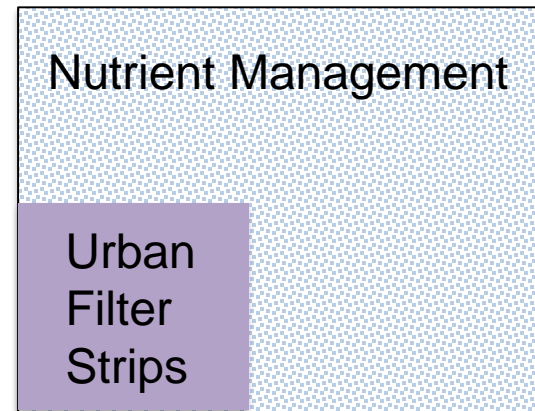
Challenges and long-term tests

Efficiency BMPs

Mutually Exclusive
(aka Additive)

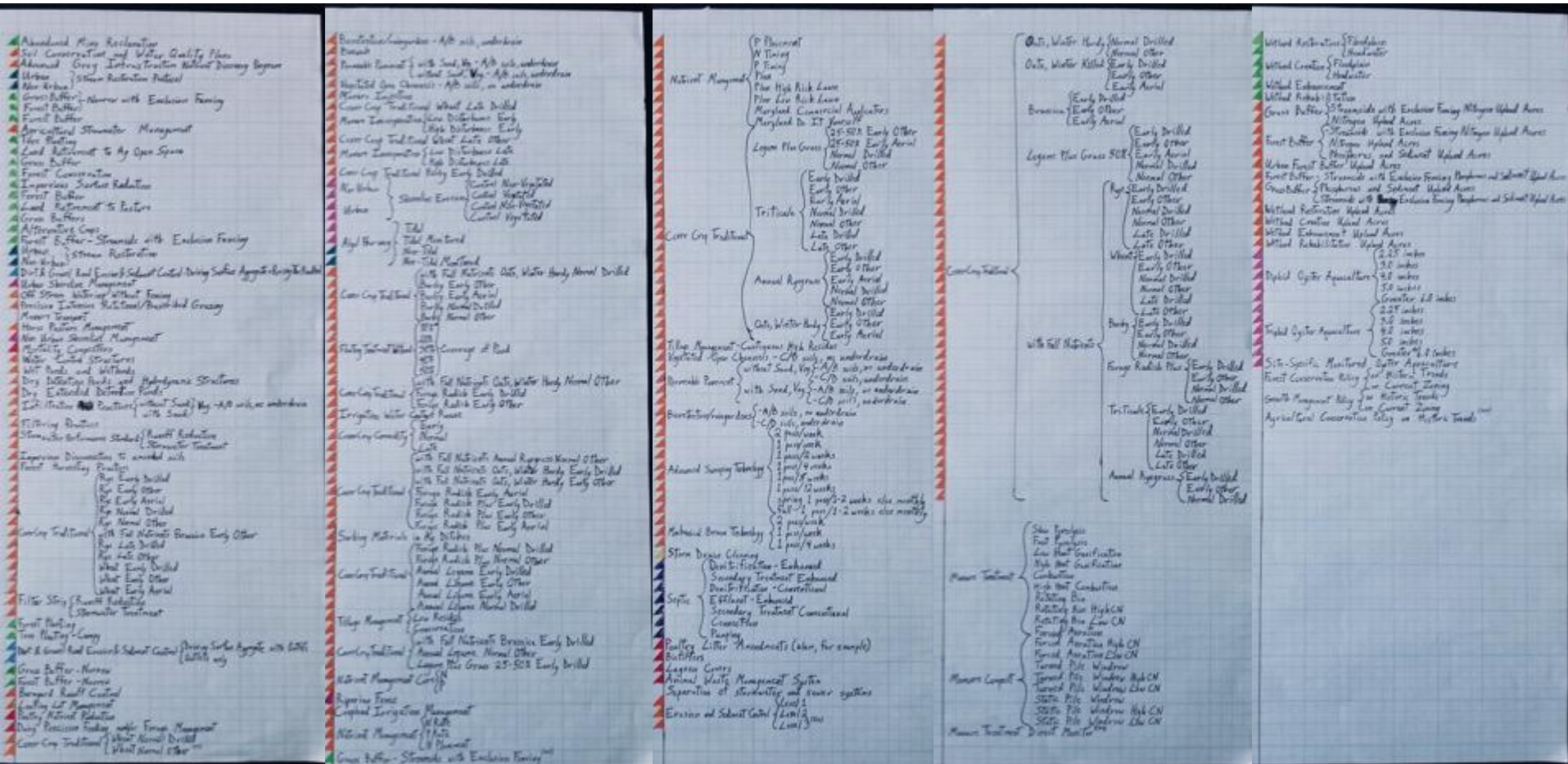


Overlapping
(aka Multiplicative)



What's the optimal (lowest-cost) implementation of these BMPs for a given geographical area?

BMPs and their simulation rules



Orange - Efficiency Purple – Septic efficiency Yellow – Load reduction Light blue – dirt and gravel
 Green – Land use change Brown – Septic connections Pink – shore Teal – stream Red - animal

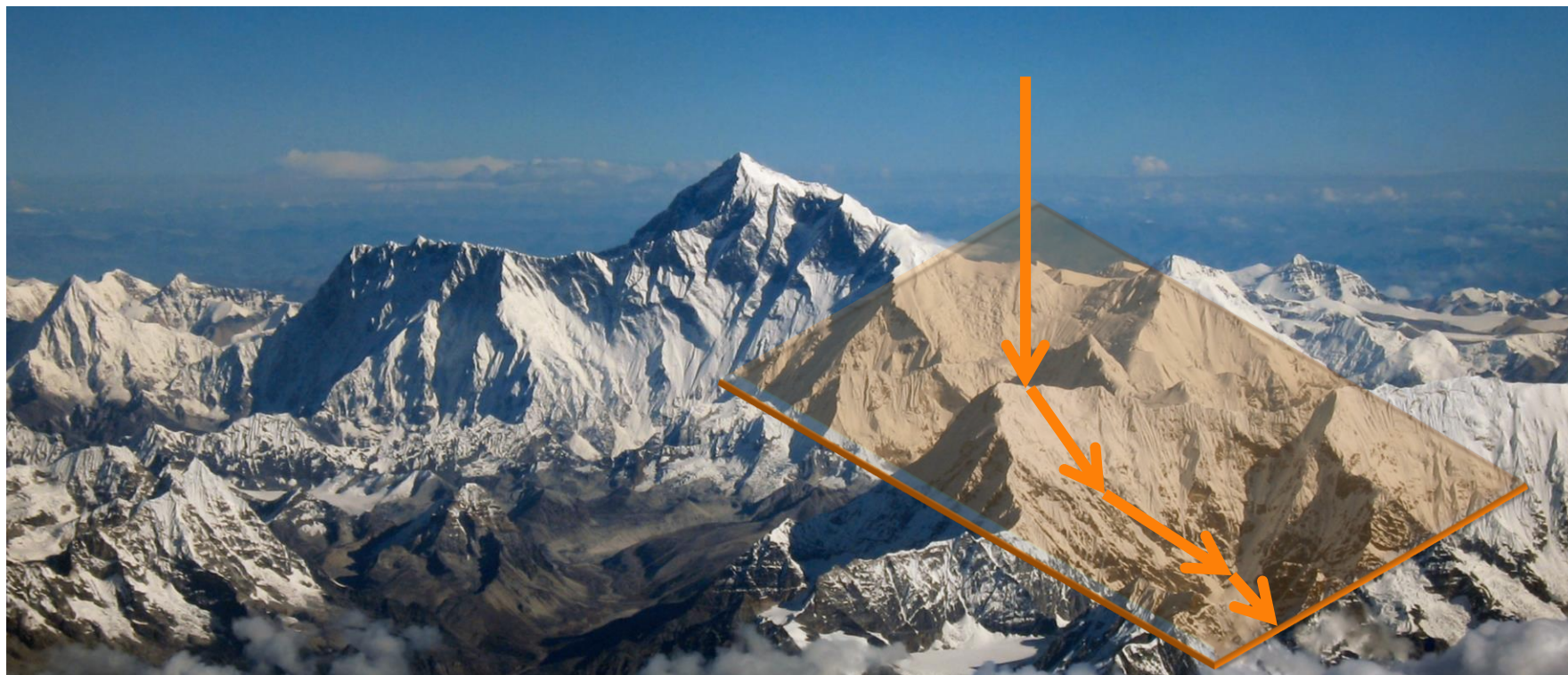
Optimization as search

How would you go about finding the lowest point? Without GPS :



Optimization as search

Move in the direction of the steepest slope, towards a minimum



Efficiency BMP prototype



total cost

$$\sum_{\substack{\text{Segments} \\ \text{BMPs} \\ \text{LoadSources}}} (\text{cost} * \text{BMPacres})$$

load reduction

$$\% \text{LoadReduction}_{\substack{\text{segment} \\ \text{pollutant}}}$$

available acreage

$$\sum_{\substack{\text{BMPs} \\ \text{in} \\ \text{Groups}}} \text{BMPacres} \leq \text{AvailableAcres}$$

The same calculations as in CAST

Efficiency BMP prototype



Two Versions

Minimize
(total cost)




$$\sum_{\substack{\text{Segments} \\ \text{BMPs} \\ \text{LoadSources}}} (\text{cost} * \text{BMPacres})$$

Constrained by:
(Target load)

Efficiency BMP prototype




Two Versions

Minimize
(total cost) 

$$\sum_{\substack{\text{Segments} \\ \text{BMPs} \\ \text{LoadSources}}} (\text{cost} * \text{BMPacres})$$

Constrained by:
(Target load)

Maximize
(load reduction) 

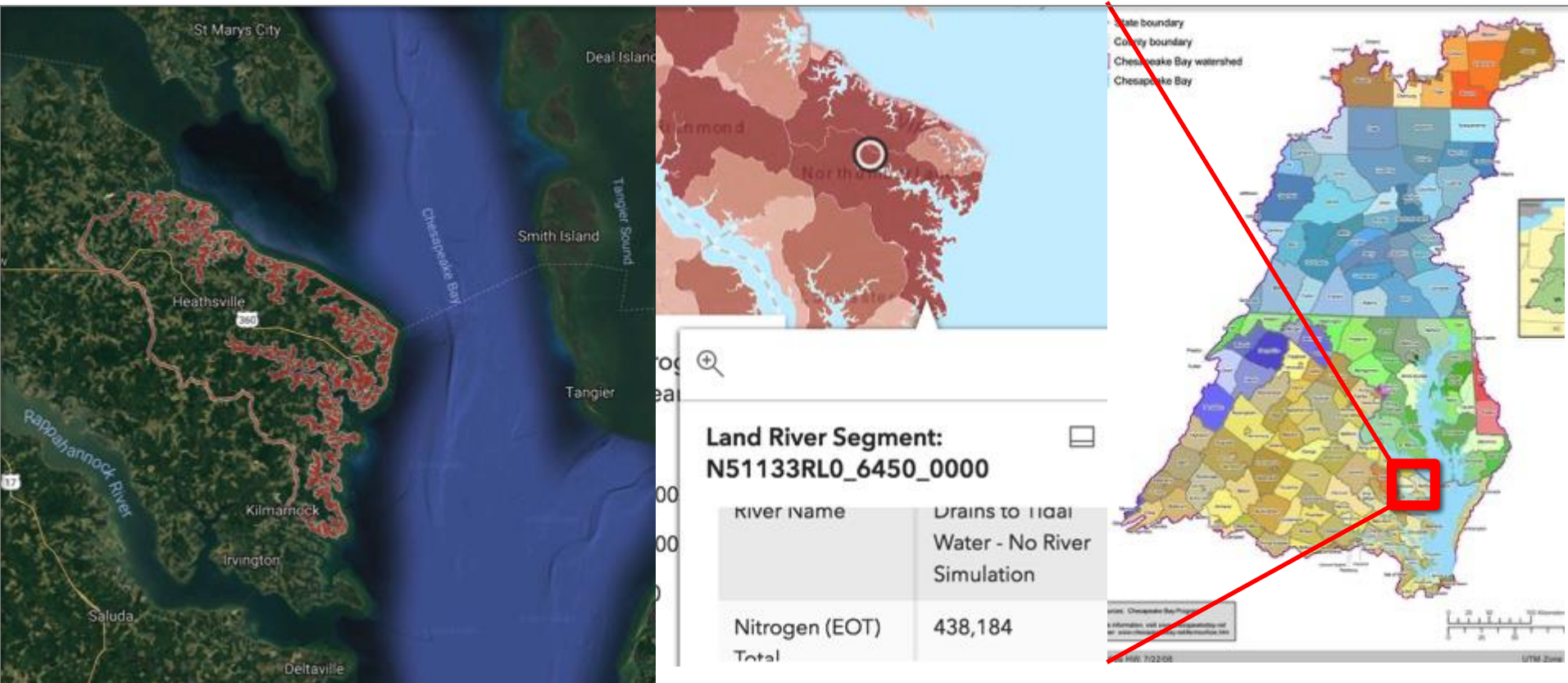
$$\% \text{LoadReduction}_{\substack{\text{segment} \\ \text{pollutant}}}$$

Constrained by:
(Cost bound)

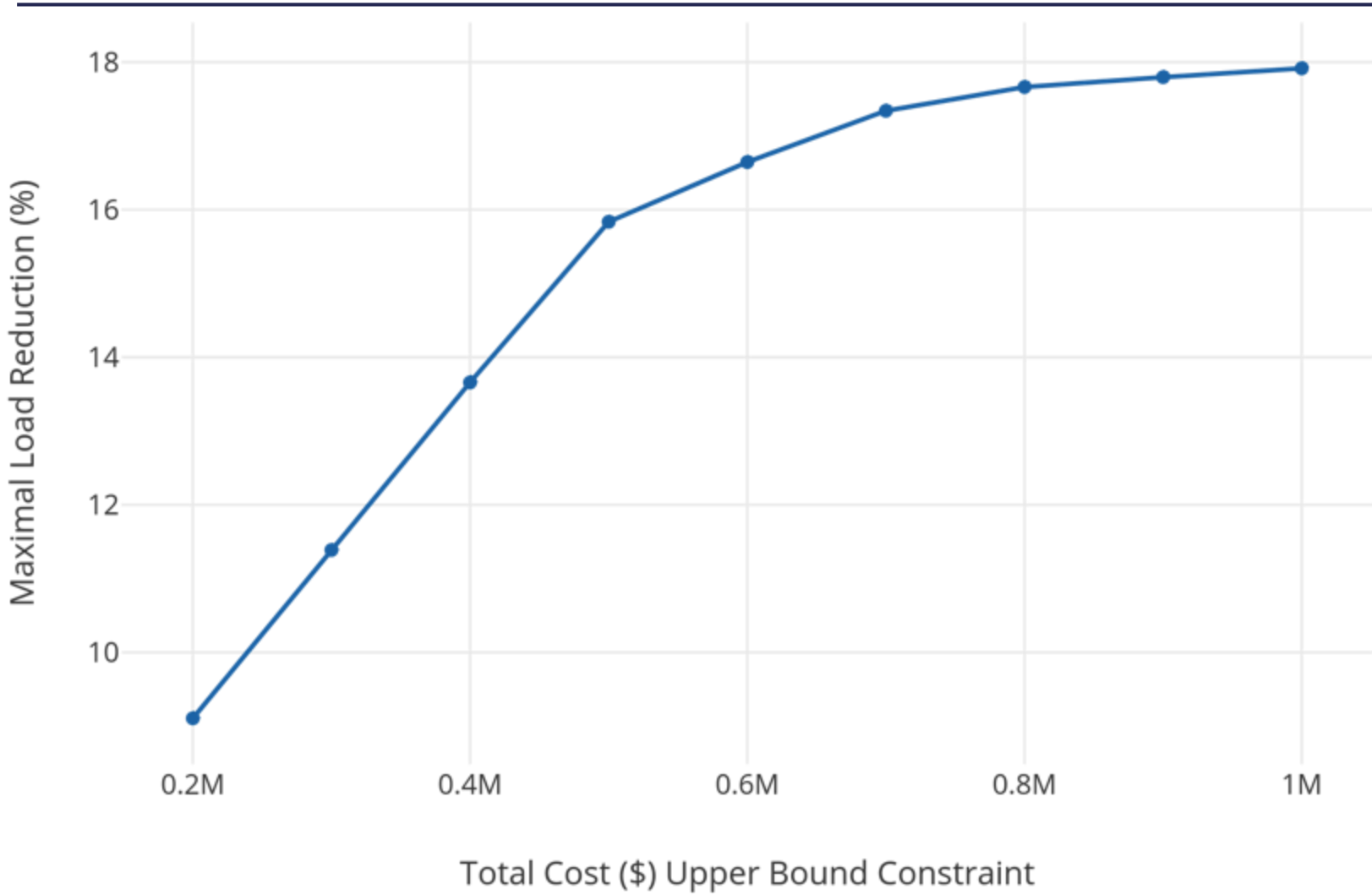
Results

Northumberland county, VA - Land River Segment N51133RL0_6450_0000

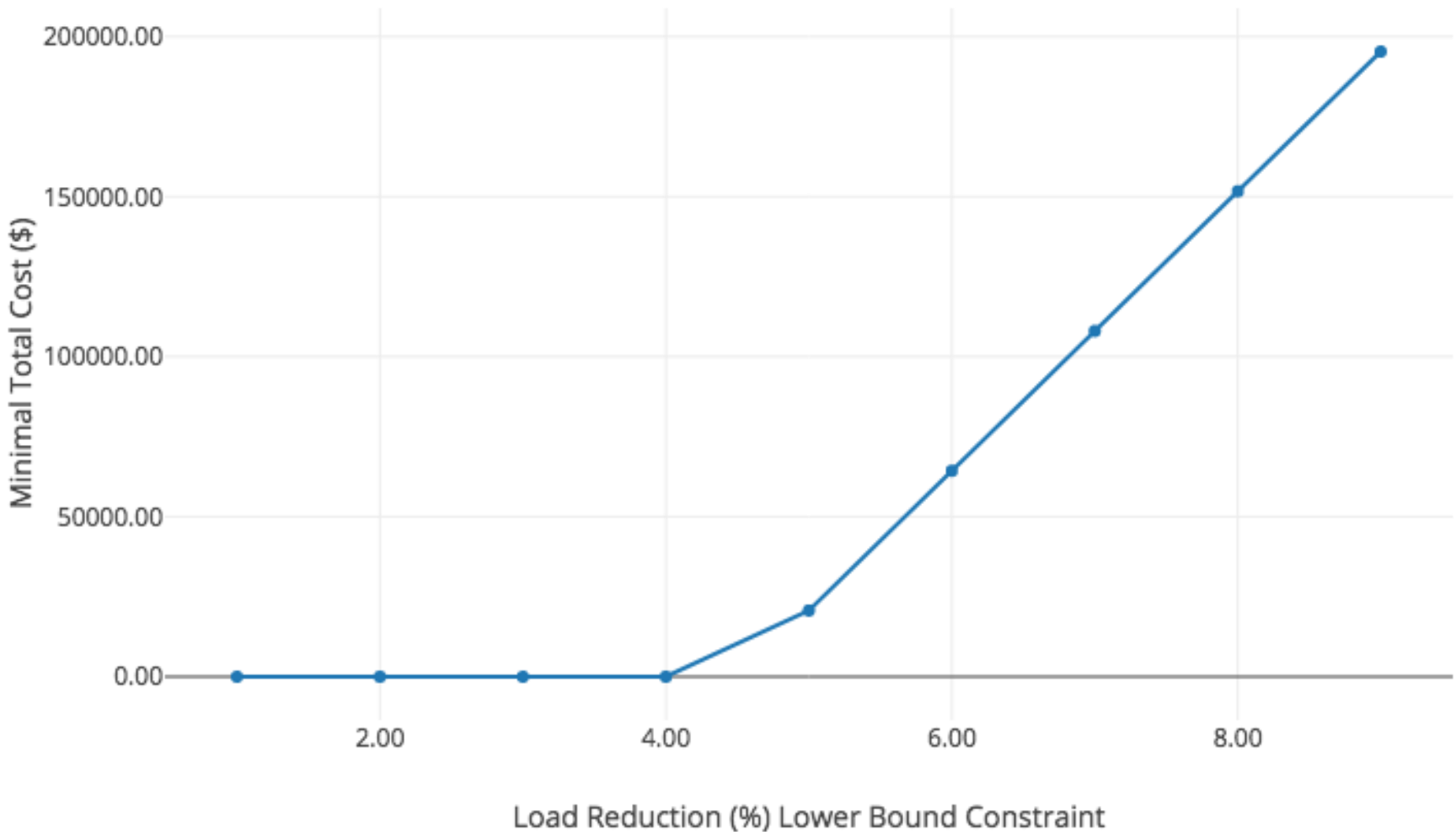
total acres = 58,040.90



Objective: Maximize **Load Reduction (%)**



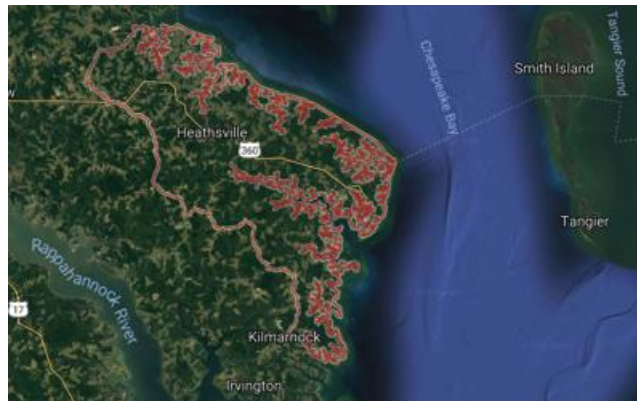
Objective: Minimize Total Cost (\$)



County-level

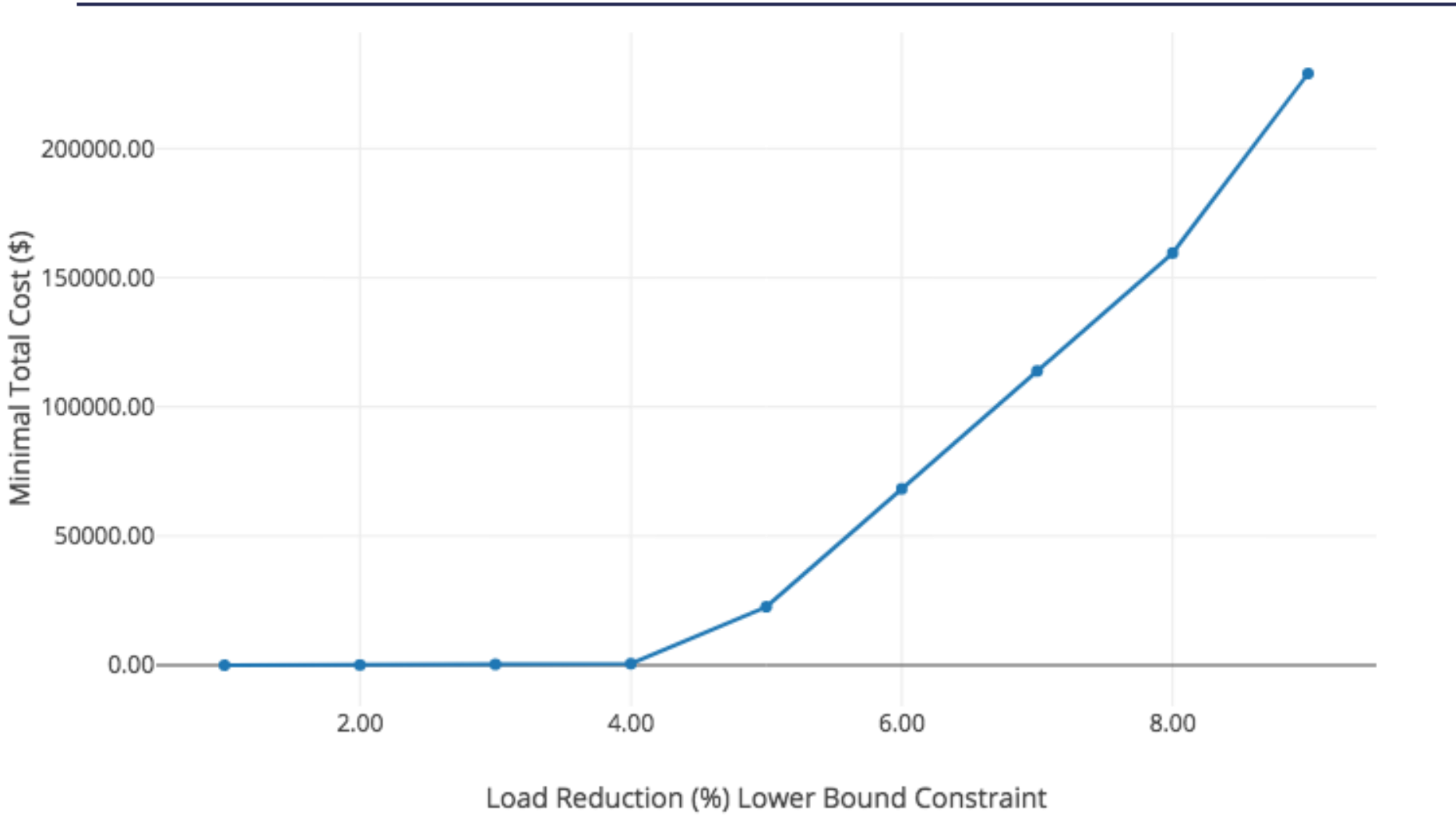
- Total cost summed over all land river segments
- Separate target load reduction constraint for each land river segment

Northumberland county, VA

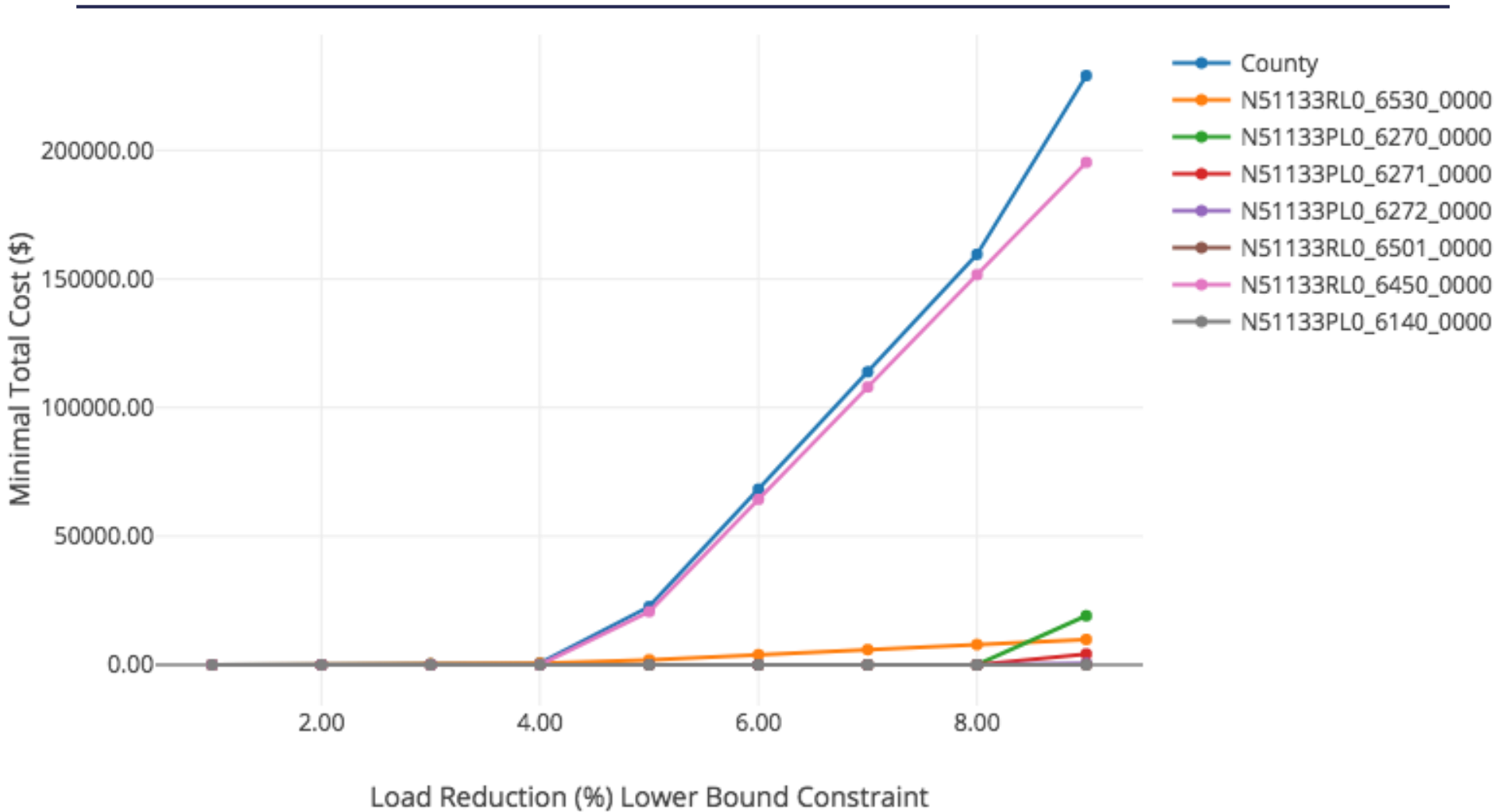


7 land river segments

Objective: Minimize Total Cost (\$)



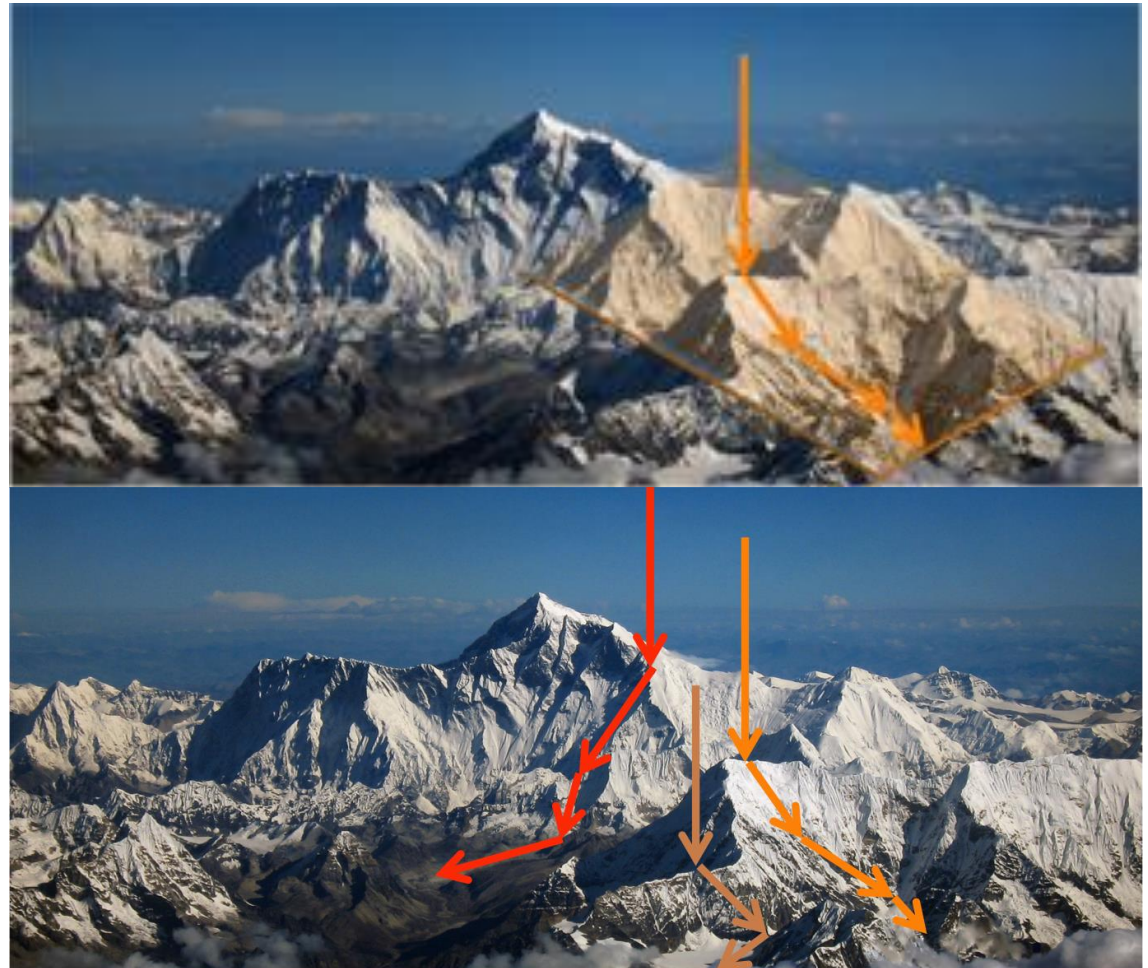
Objective: Minimize Total Cost (\$)



Starting point analysis

Why?

There may be starting point dependence, because load reduction function is non-convex.



(a local optimum may not be a global optimum)

Starting point analysis

Completed 10 runs for each formulation, for which the variable values were all drawn from a uniform distribution spanning 0 - 6000 (acres). *Note: this means that the initial points were not feasible.*

- Same solution was found each time.
- Numbers of iterations taken to find the solution, and the trajectories, were different for the trials.
- Upper bound (6000 acres) used for randomizing start points was never a binding constraint.

Solution was robust to changing the solver starting point

Next steps

Efficiency BMP optimization model:

- Using oxygen damage units to consolidate N & P
- Ensuring robust solutions for more geographic regions
- Accounting for existing constraints, structural BMPs
- Testing county-level targets / unequal target loads between land river segments within a county
- “John Henry” test

Feedback

Concurrent discovery for incorporating other BMPs

What are others thinking?

Feedback from Presentations

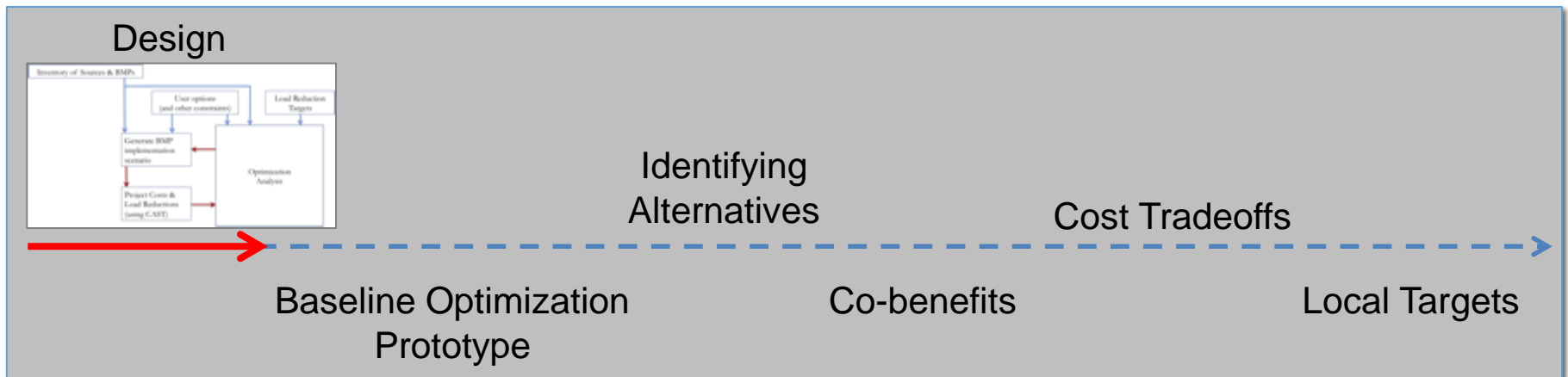
- Built-in cost profiles may not be representative (zeros are strange)
- This is going to be a very useful tool
- Going to make a big difference in conjunction with co-benefit quantification (current GIT proposed funding)

Will be shaped by feedback

Actively searching for ways to engage local decision makers at county and municipal scales for their guidance and feedback on prototype design.

Your area (county, sub-watershed) can be an early case study

Email me (Danny) at: dkaufman@chesapeakebay.net



**EXTRA SLIDES
FOLLOW**

Fine print



“Straw-arm” prototype
(Part of straw-man)

- Prototype is unlikely to be ready in time for Phase III WIP development.
- Beta version prototype will likely not include BMPs other than efficiencies. There are other BMPs, e.g. Buffers, that are important for reducing load.

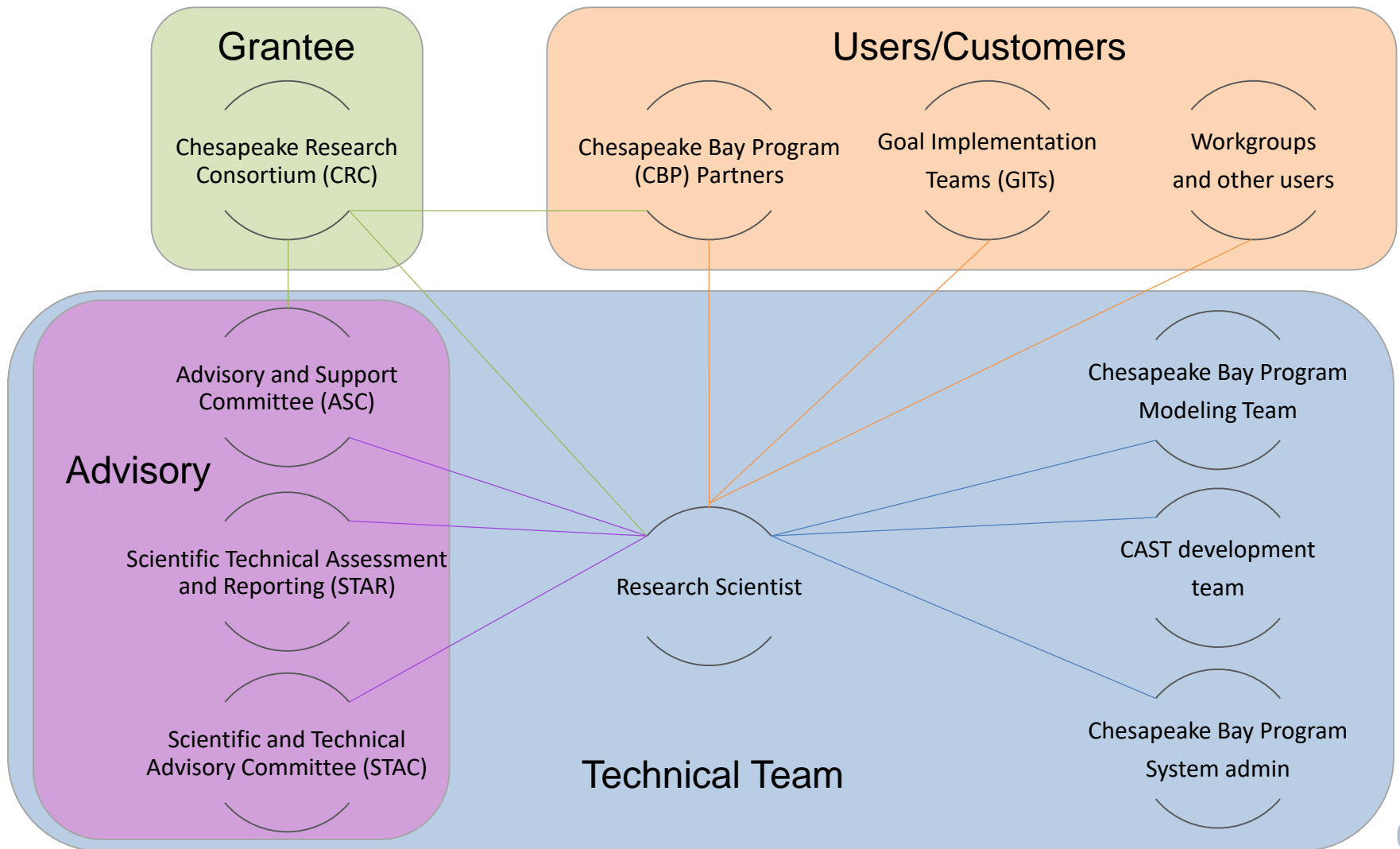
“Straw-arm”

(Part of a straw-man prototype)



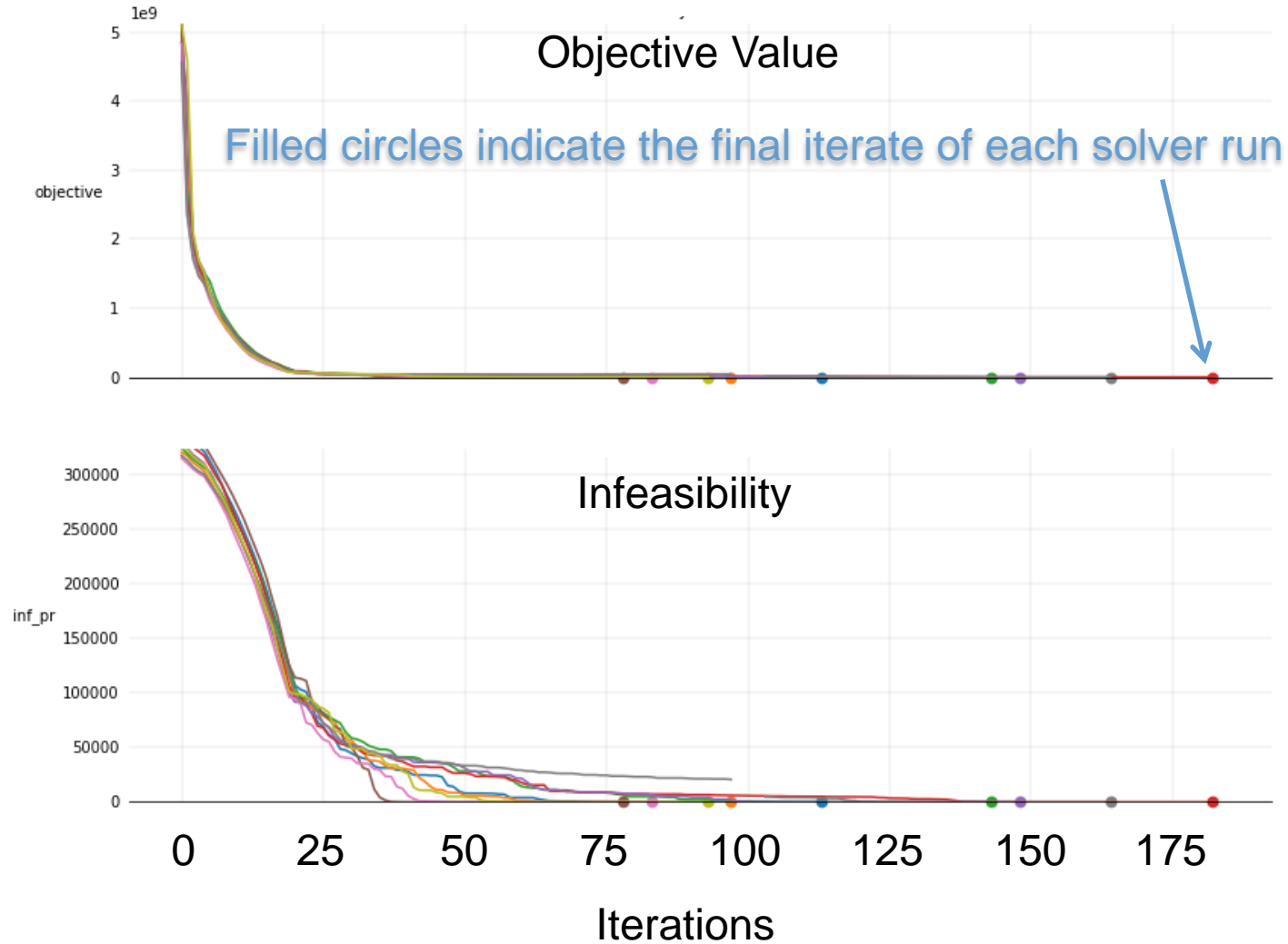
Cast of characters

Project Organization



Starting point analysis

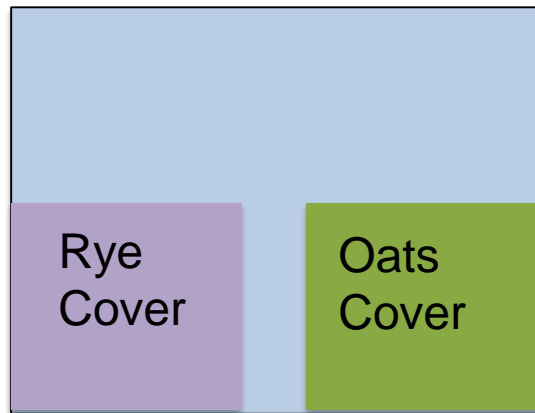
The objective and primal infeasibility follow similar trends for each of the randomized starting point trials.



Objective:
Minimize
Total Cost (\$)

Efficiency BMPs

Mutually Exclusive
(aka Additive)



Overlapping
(aka Multiplicative)



What's the optimal (lowest-cost) implementation of these BMPs for a given geographical area?

Prototyping Experiments

Search Space Investigations

Fine-tuned sub-problem

Next steps

Conceptual

- Investigate solutions in more depth
 - Look at z_L , dual outputs at the solution
 - Look at Pynumero gradient results
- Sensitivity analyses
 - Test other randomized start pt. ranges (0-100,000; 0-100; etc.)

Practical

- Solving NLP for multiple land-river segments simultaneously
- Solve cost min. objective formulation with only N constraint to parallel load objective
- Use oxygen damage units to consolidate N & P
- Many more geographic regions
- Feedback!

Heatmap

- for county BMPs (aggregated by land river segment?)
- and then on the next slide (aggregated by load source?)

Efficiency BMP prototype



Two Versions

Minimize
(total cost)

$$\sum_{\substack{\text{Segments} \\ \text{BMPs} \\ \text{LoadSources}}} (\text{cost} * \text{BMPacres})$$

Maximize
(load reduction)

$$\% \text{LoadReduction}_{\substack{\text{segment} \\ \text{pollutant}}}$$

Cost objective



↓ Minimize:
(total cost)

$$\sum_{\substack{\text{Segments} \\ \text{BMPs} \\ \text{LoadSources}}} (\text{cost} * \text{BMPacres})$$

Subject to:
(Target load)

$$\% \text{LoadReduction}_{\substack{\text{segment} \\ \text{pollutant}}} \geq \text{TargetLoadReduction} \quad (\text{e.g. } 10\%)$$

(Availability)

$$\sum_{\substack{\text{BMPs} \\ \text{in} \\ \text{Groups}}} \text{BMPacres} \leq \text{AvailableAcres}$$

Load objective



↑ Maximize:
(load reduction) $\% LoadReduction_{\substack{segment \\ pollutant}}$

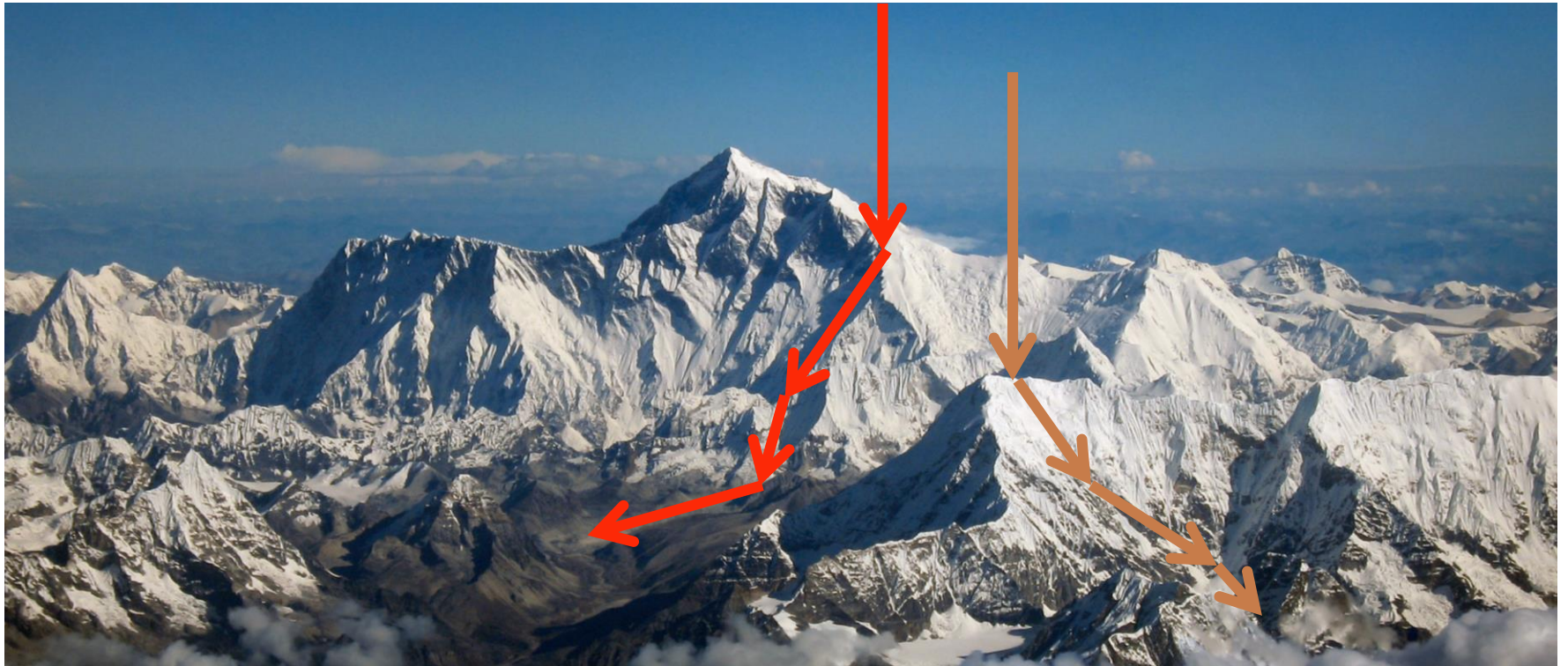
Subject to:
(Cost bound) $\sum_{l \in L} \sum_{b \in B} \sum_{\psi_b^\lambda \in \Psi_b^*} (c_b * X_{b,l,\psi_b^\lambda}) \leq C$ (e.g. \$500,000)

(Availability) $\sum_{\substack{BMPs \\ in \\ Groups}} BMPacres \leq AvailableAcres$

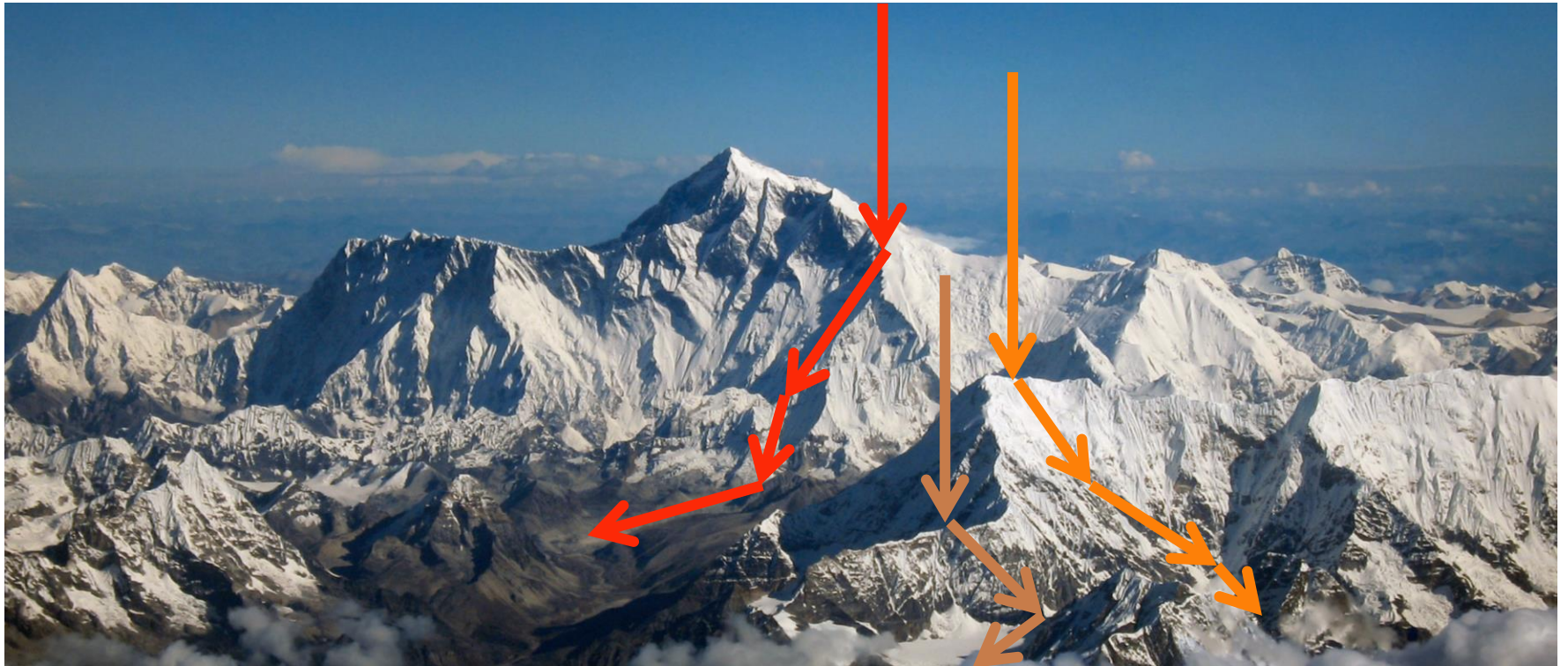
Efficiency BMP prototype



Efficiency BMP prototype



Efficiency BMP prototype



Summary of starting point analysis

- Results for 10 runs for each formulation are shown, for which the variable values were all drawn from a uniform distribution spanning 0 - 6000 (acres). *Note: this means that the initial points are almost assuredly not feasible.*
- Overall, these results are showing that the same solution is being found each time (so far).
- The number of iterations it takes to find the solution, and the trajectory of points through which it travels, is different for the various trials.
- The upper bound (*6000 acres*) used for randomizing the start points never appears to be a binding constraint

Details

<p>Setting up parameters & variables</p>	<p><u>Sets:</u></p> <ul style="list-style-type: none"> - Land River Segments, Pollutants - BMPs (type = efficiency) - BMP groups - Load Sources - (BMP, BMP group) - (BMP, Load Source) - (BMP group, Load Source) 	<p>Solved using</p>
<p>Query CAST source data</p>		<p>Pyomo (algebraic modeling language library for python)</p>
<p>Build variables [lrseg, agency, load source, bmp, unit]</p>	<p><u>Parameters</u></p> <ul style="list-style-type: none"> - Costs - Load Reduction Efficiencies - Base loading - Pre-bmp Acres for load sources 	<p>developed by Sandia National Laboratories</p>
<p>Get parameters (costs, efficiency values, base loading, acres)</p>	<p><u>Variables</u></p> <ul style="list-style-type: none"> - Acres per (LRseg, Loadsource, BMP) 	<p>IPOPT (interior point / barrier method solver)</p>

Why analyze different starting points?

Non-convex load reduction function

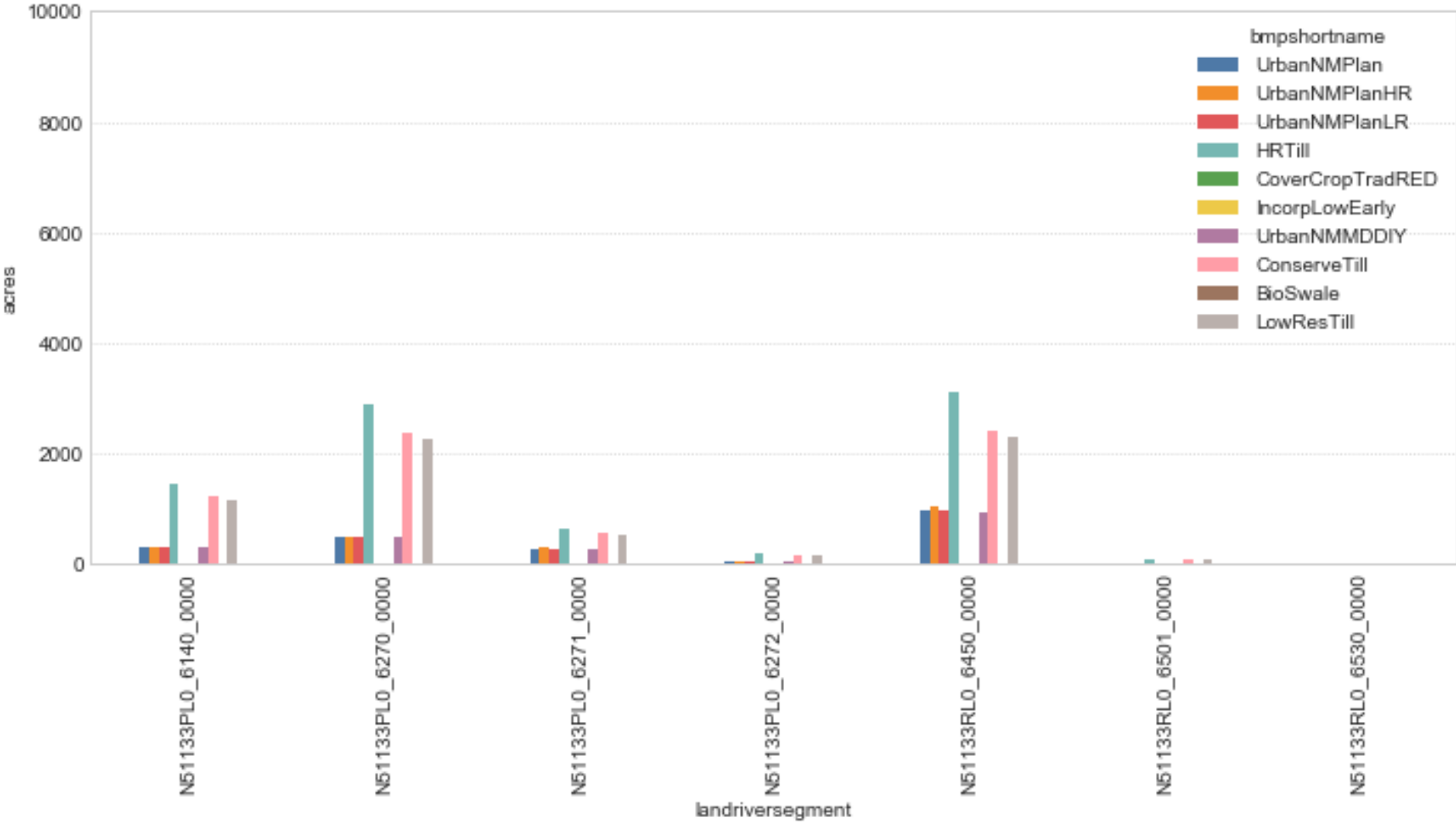
Local optimum may not be global optimum

Means that there may be starting point dependence

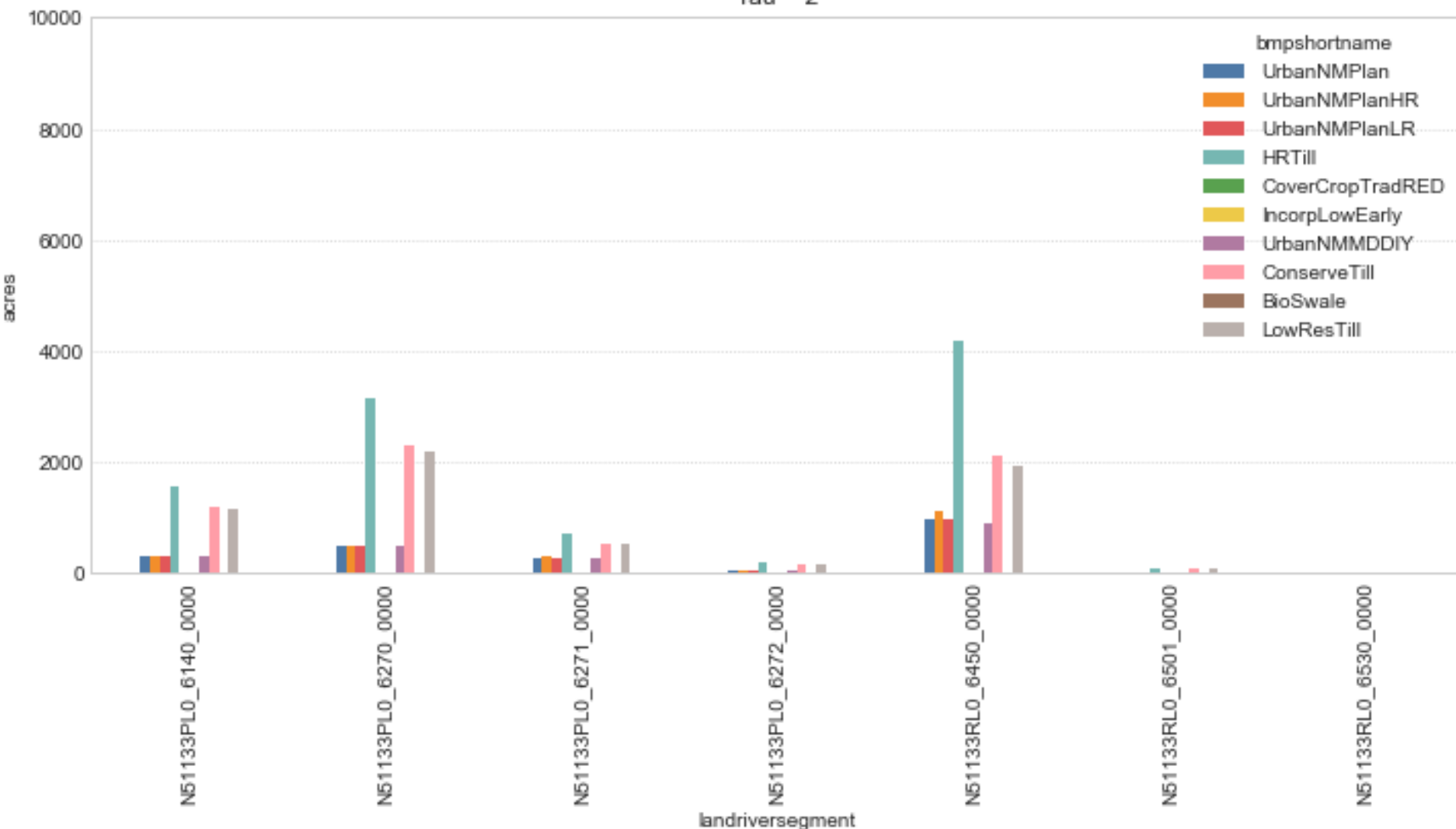
$$\text{eig}(H) = \begin{bmatrix} \emptyset & \emptyset \\ \alpha_1 \sqrt{(\beta_1^2 + \beta_2^2)(\beta_3^2 + \beta_4^2)} \\ -\alpha_1 \sqrt{(\beta_1^2 + \beta_2^2)(\beta_3^2 + \beta_4^2)} \end{bmatrix}$$

Hessian is not positive definite, therefore, $f(x)$ is not convex

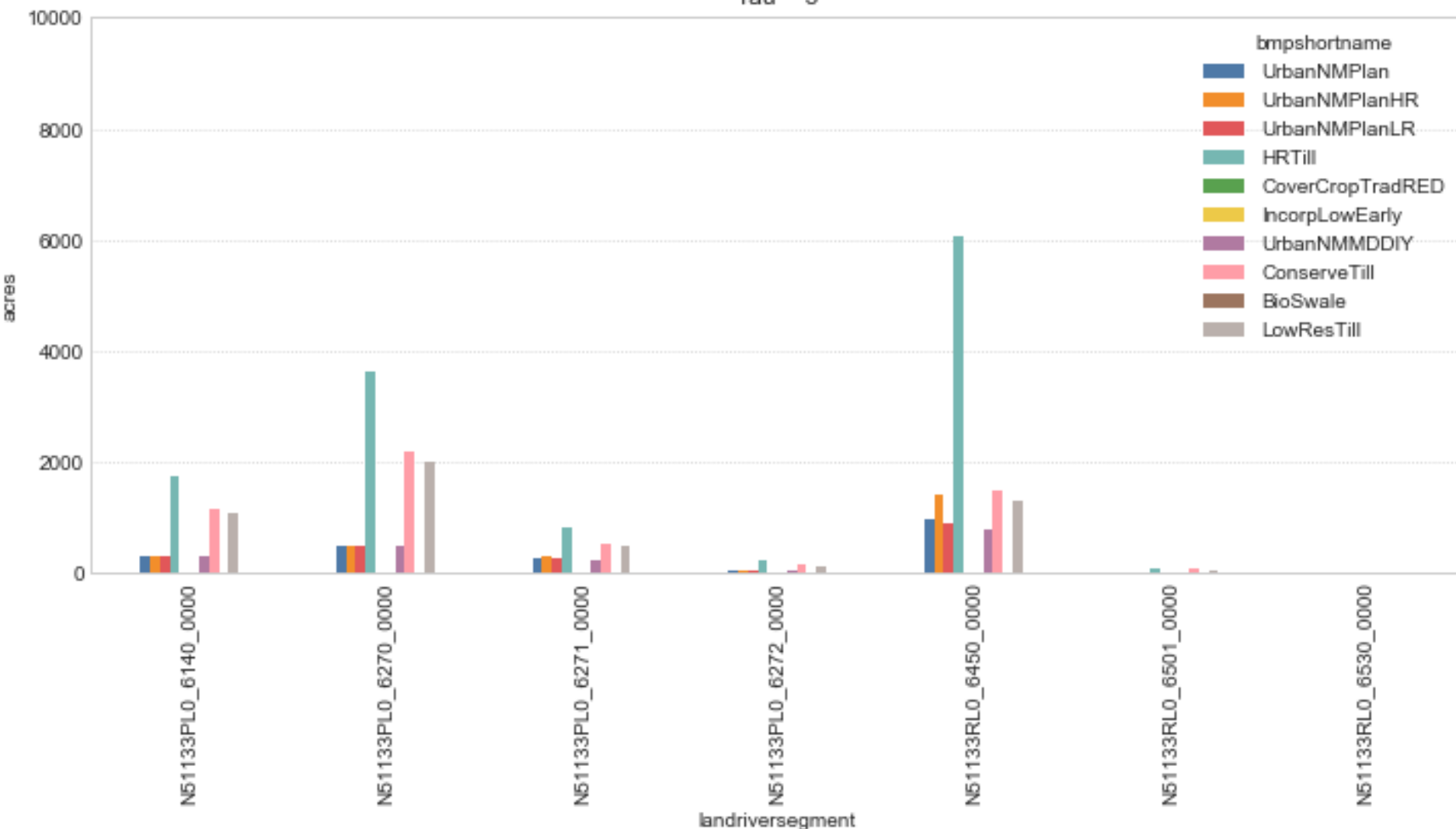
Tau==1



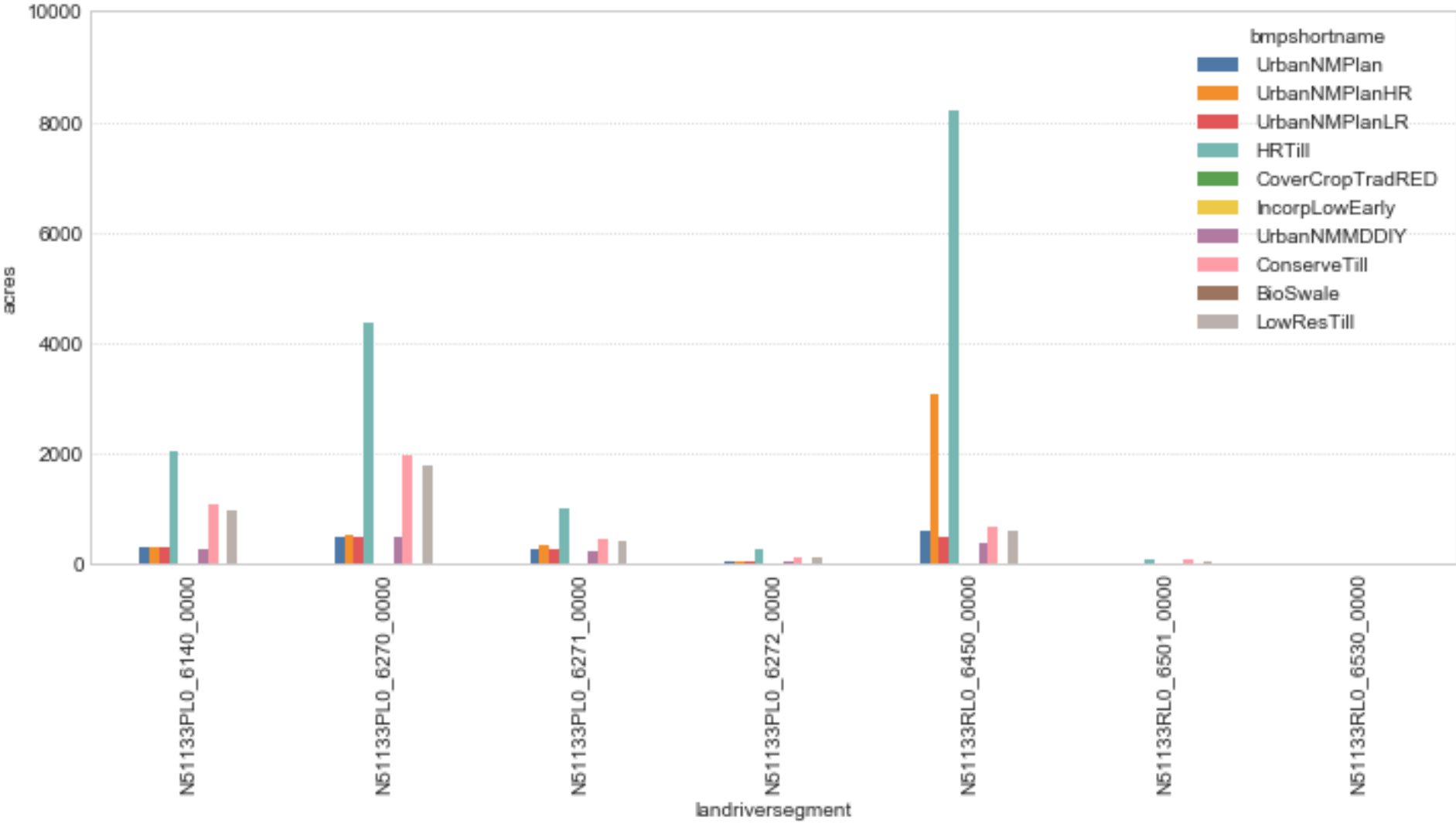
Tau==2



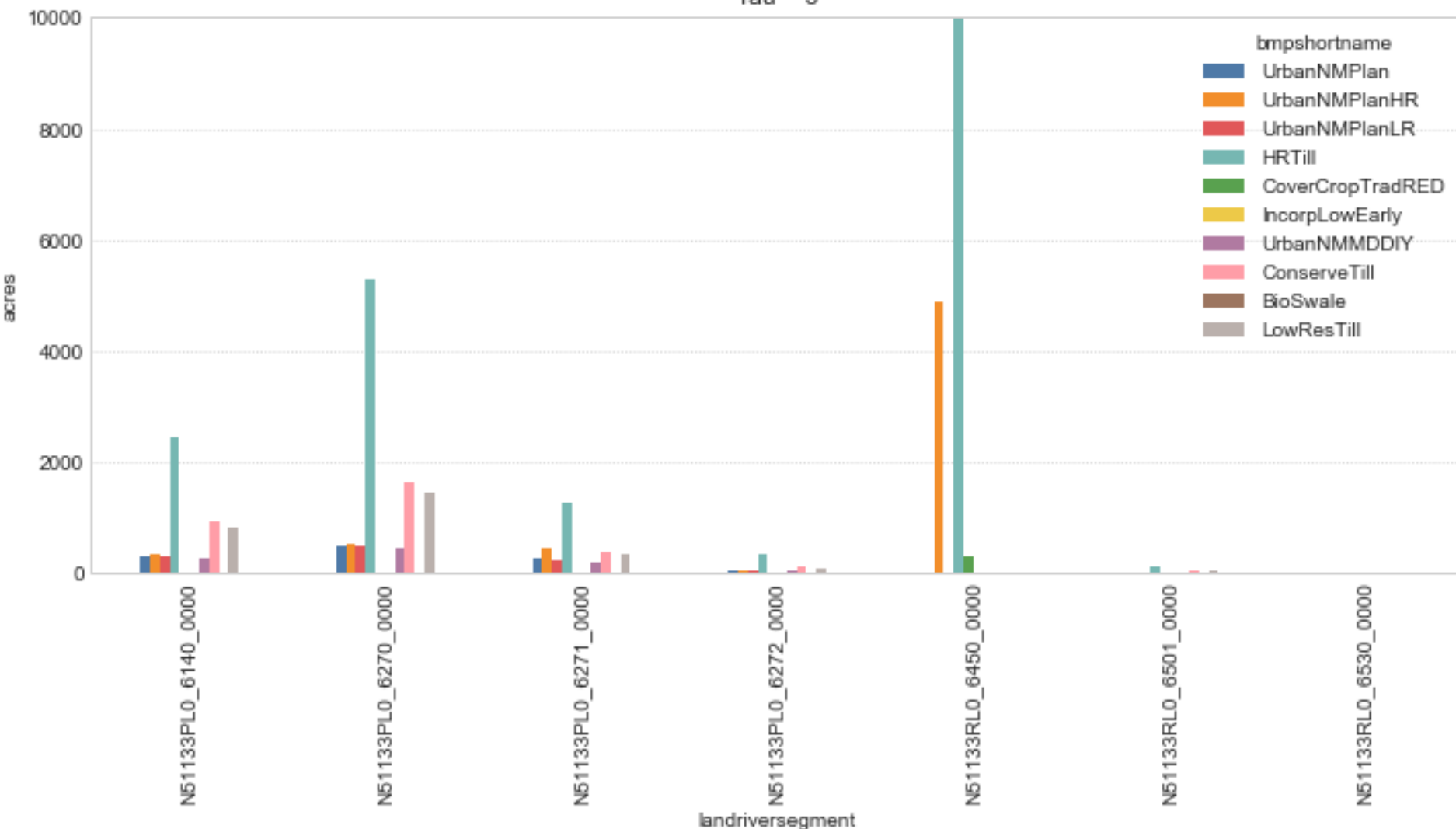
Tau==3



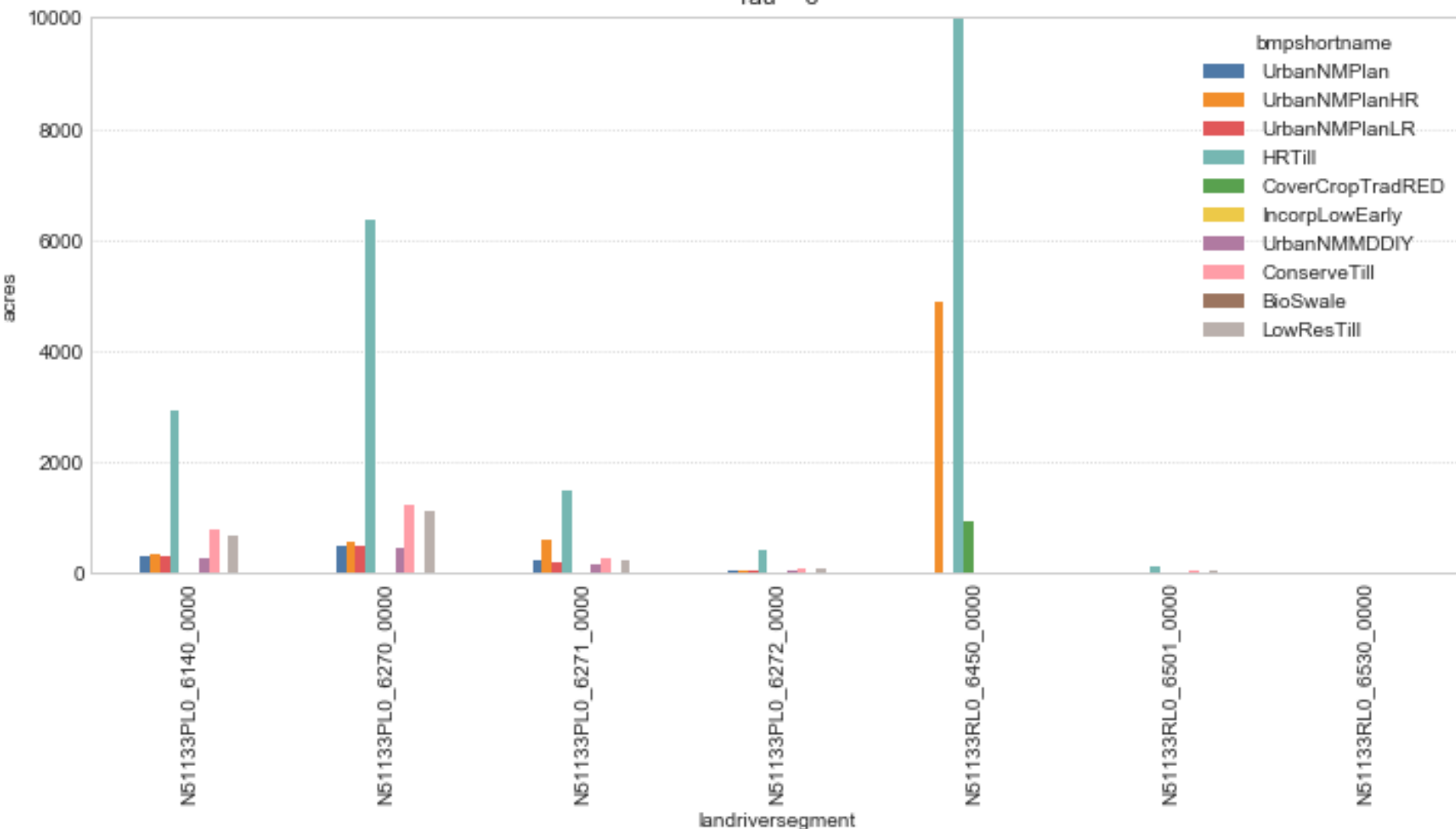
Tau==4



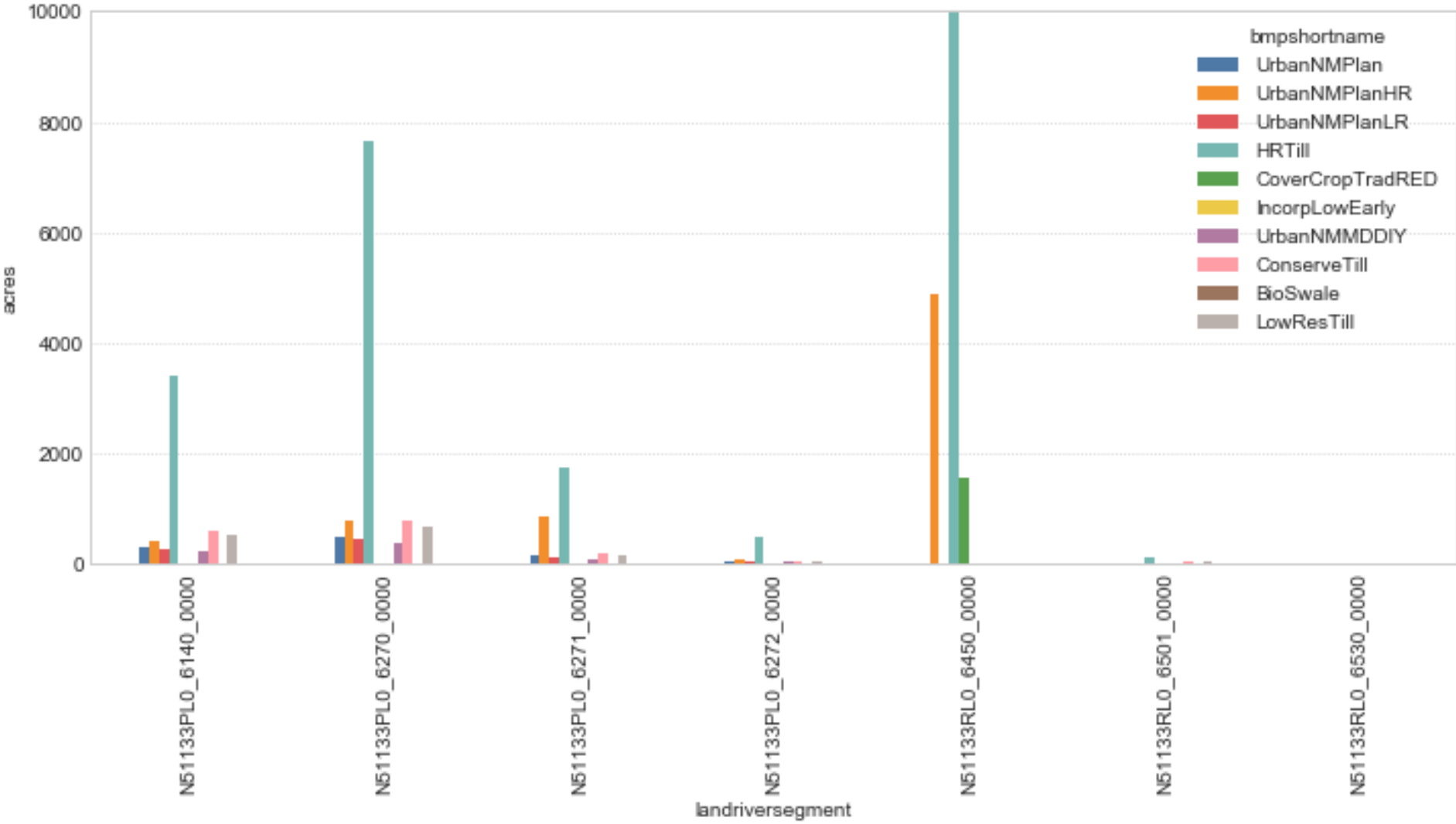
Tau==5



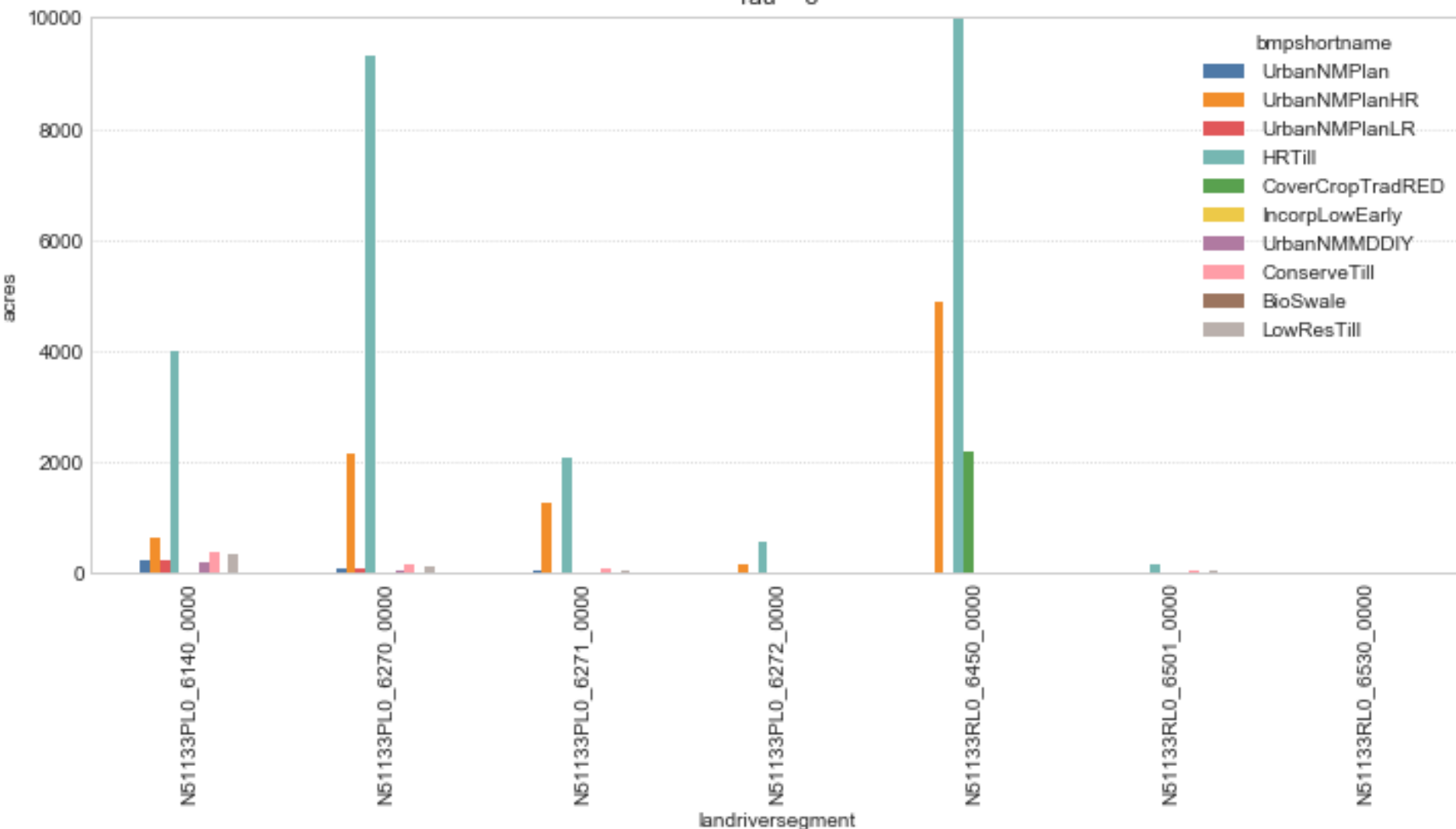
Tau==6



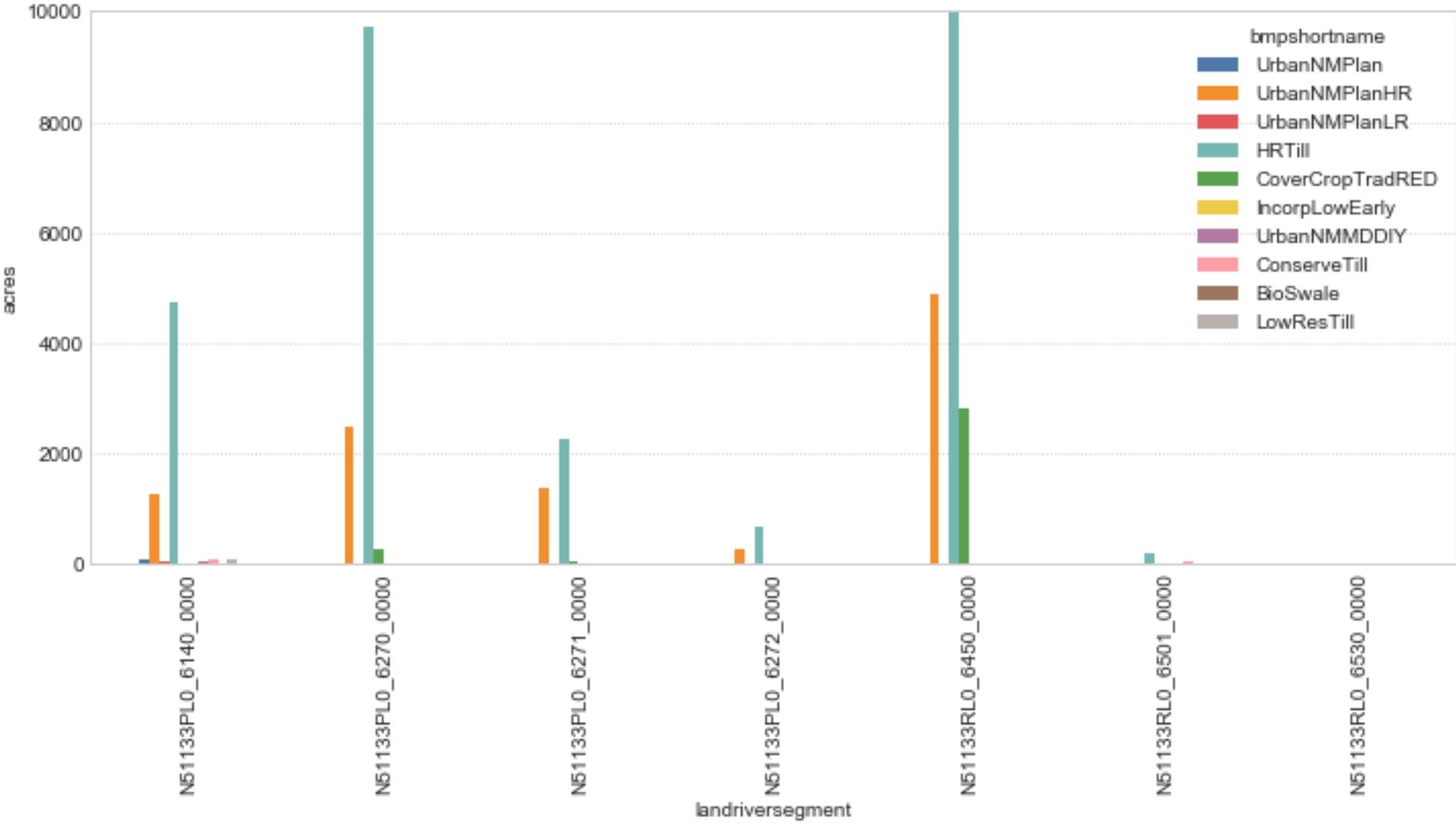
Tau==7

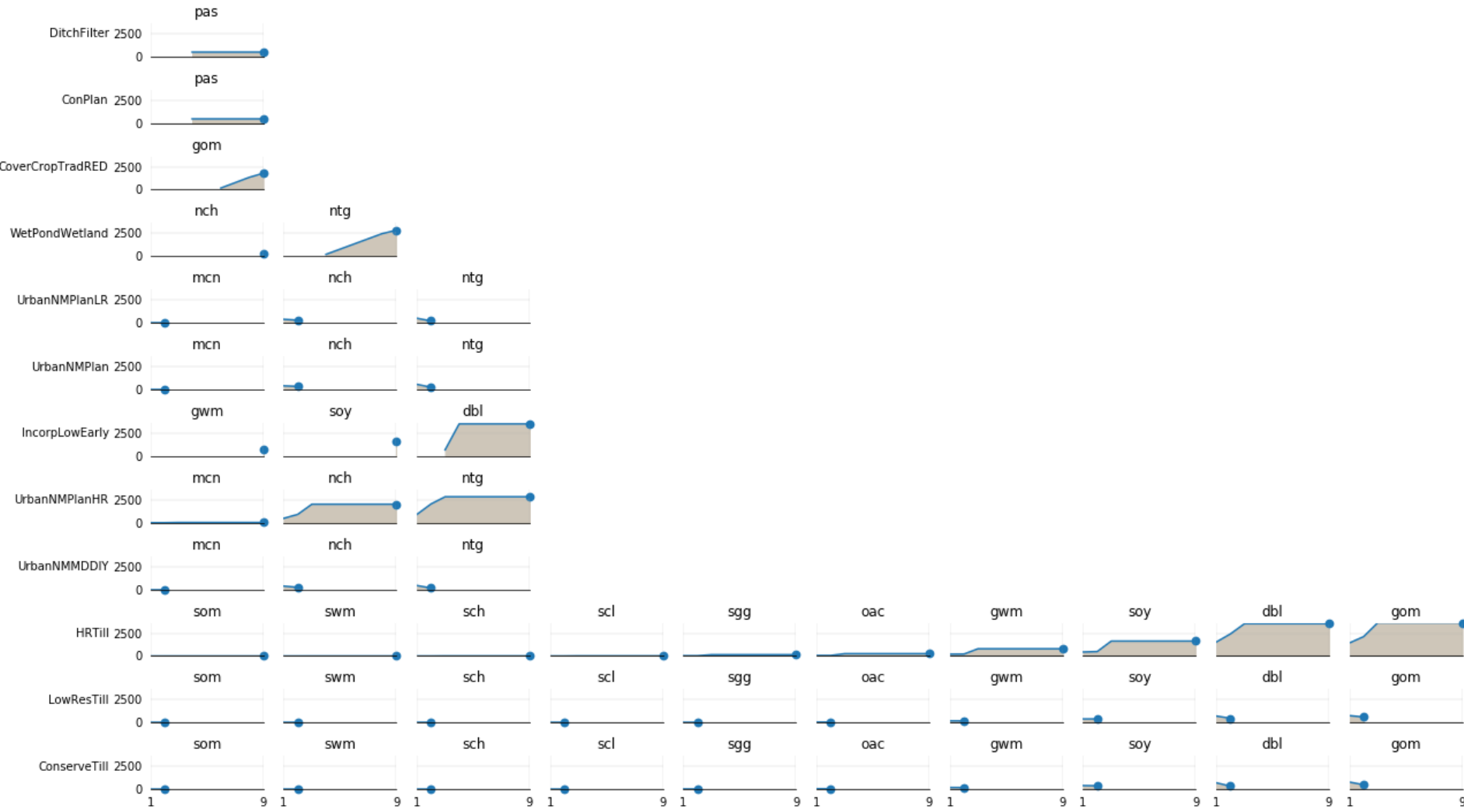


Tau==8



Tau==9

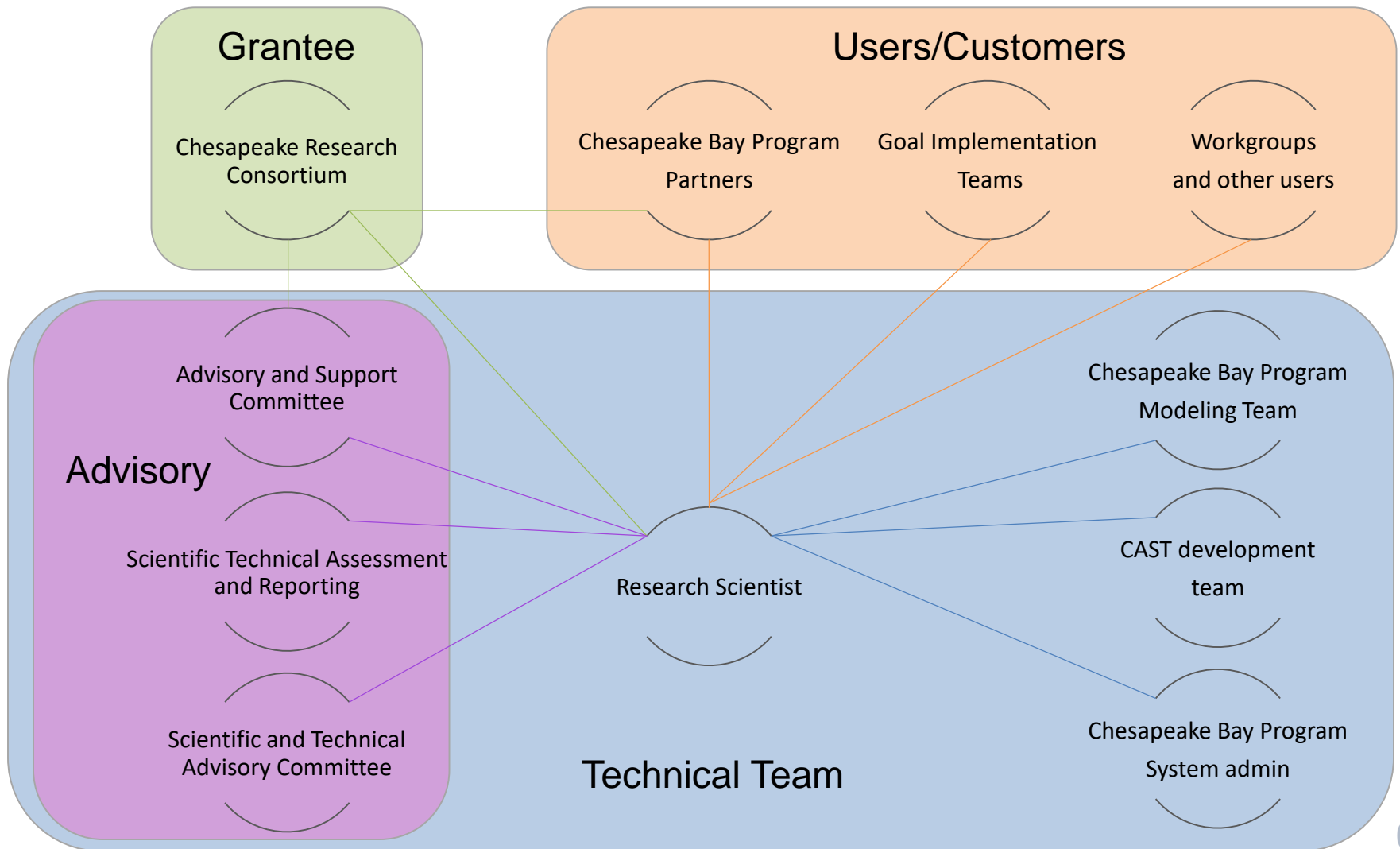




Percent Load Reduction Lower Bound

Objective:
Minimize Total Cost (\$)

Project Organization



Current system

Best
Management
Practices
(BMPs)



Chesapeake
Assessment
Scenario Tool
(CAST)



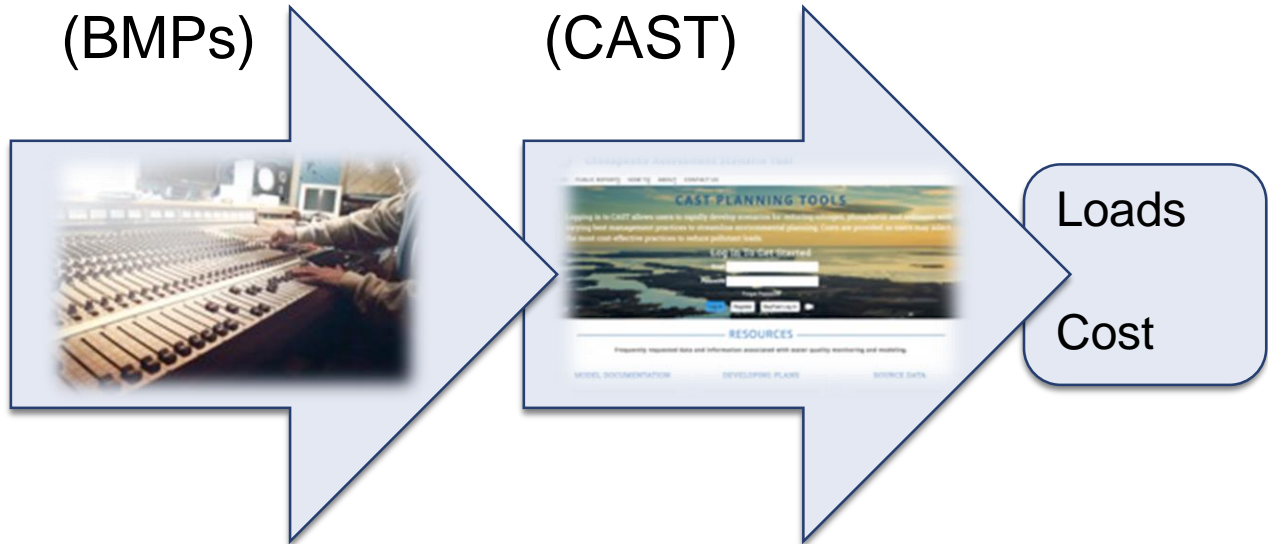
Loads
Cost

Current system

Best
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Chesapeake
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Not feasible to
exhaustively try
potential strategies



Scenario Optimization System

Best
Management
Practices
(BMPs)

Chesapeake
Assessment
Scenario Tool
(CAST)

Loads

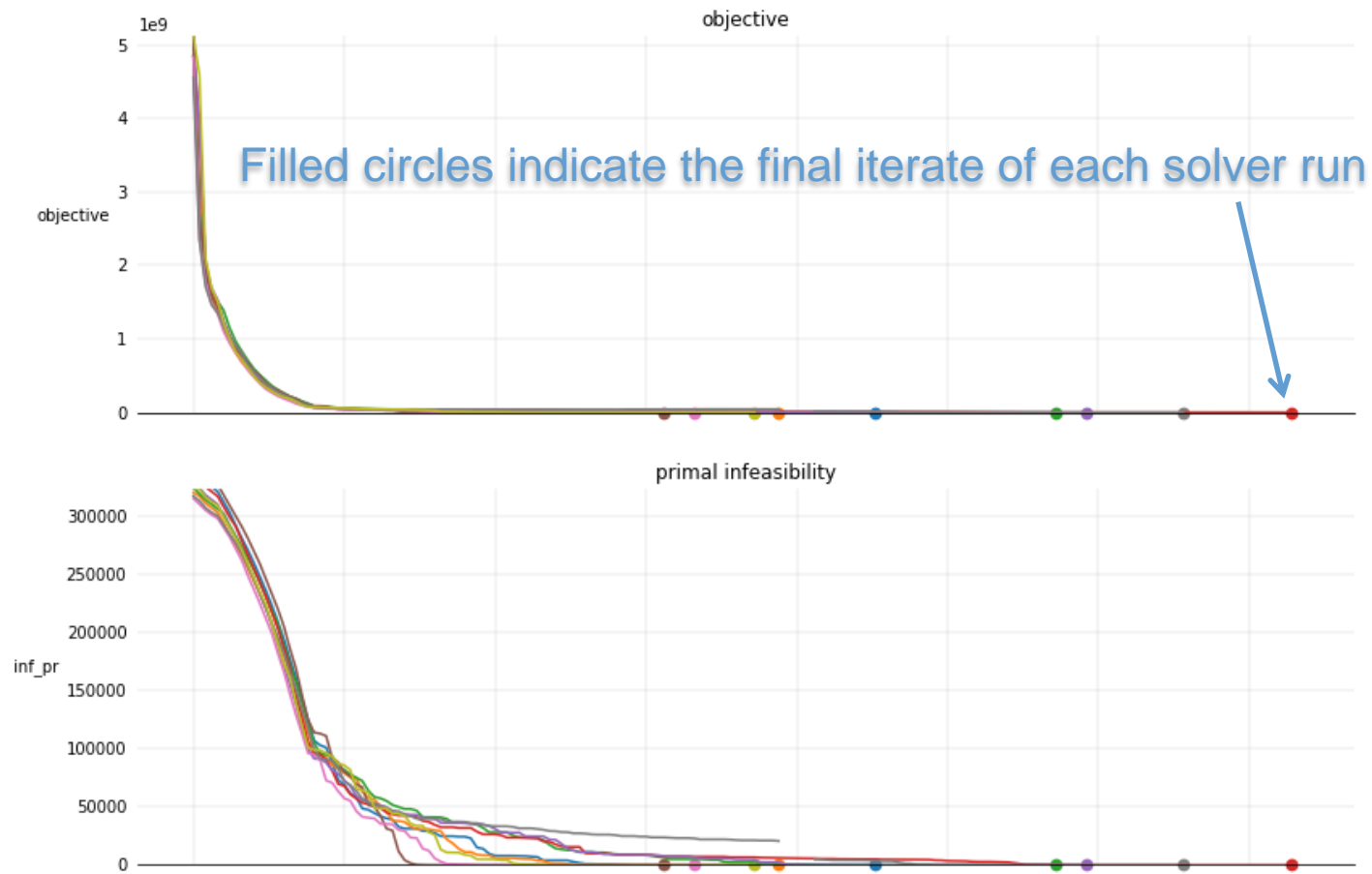
Cost

Analyze potential BMP options and identify low-cost strategies

To help the Chesapeake Bay Program and its Partners restore the Bay and its watershed

Multiple Runs

The objective and primal infeasibility follow similar trends for each of the randomized starting point trials.



Objective:
Minimize
Total Cost (\$)

Why analyze different starting points?

$f(x) =$ (load reduction) $\alpha_1 \left(1 - \beta_3 x_3 + \beta_4 x_4 - \beta_1 x_1 + \beta_2 x_2 + \beta_1 \beta_3 x_1 x_3 + \beta_1 \beta_4 x_1 x_4 + \beta_2 \beta_3 x_2 x_3 + \beta_2 \beta_4 x_2 x_4 \right)$

$H =$

\emptyset	\emptyset	$\alpha_1 \beta_1 \beta_3$	$\alpha_1 \beta_1 \beta_4$
\emptyset	\emptyset	$\alpha_1 \beta_2 \beta_3$	$\alpha_1 \beta_2 \beta_4$
$\alpha_1 \beta_1 \beta_3$	$\alpha_1 \beta_2 \beta_3$	\emptyset	\emptyset
$\alpha_1 \beta_1 \beta_4$	$\alpha_1 \beta_2 \beta_4$	\emptyset	\emptyset

$\text{eig}(H) =$

\emptyset
\emptyset
$\alpha_1 \sqrt{(\beta_1^2 + \beta_2^2)(\beta_3^2 + \beta_4^2)}$
$-\alpha_1 \sqrt{(\beta_1^2 + \beta_2^2)(\beta_3^2 + \beta_4^2)}$

Cross products of the form $x*y$

Hessian is not positive definite, therefore, $f(x)$ is not convex

Objective: Maximize Load Reduction (%)

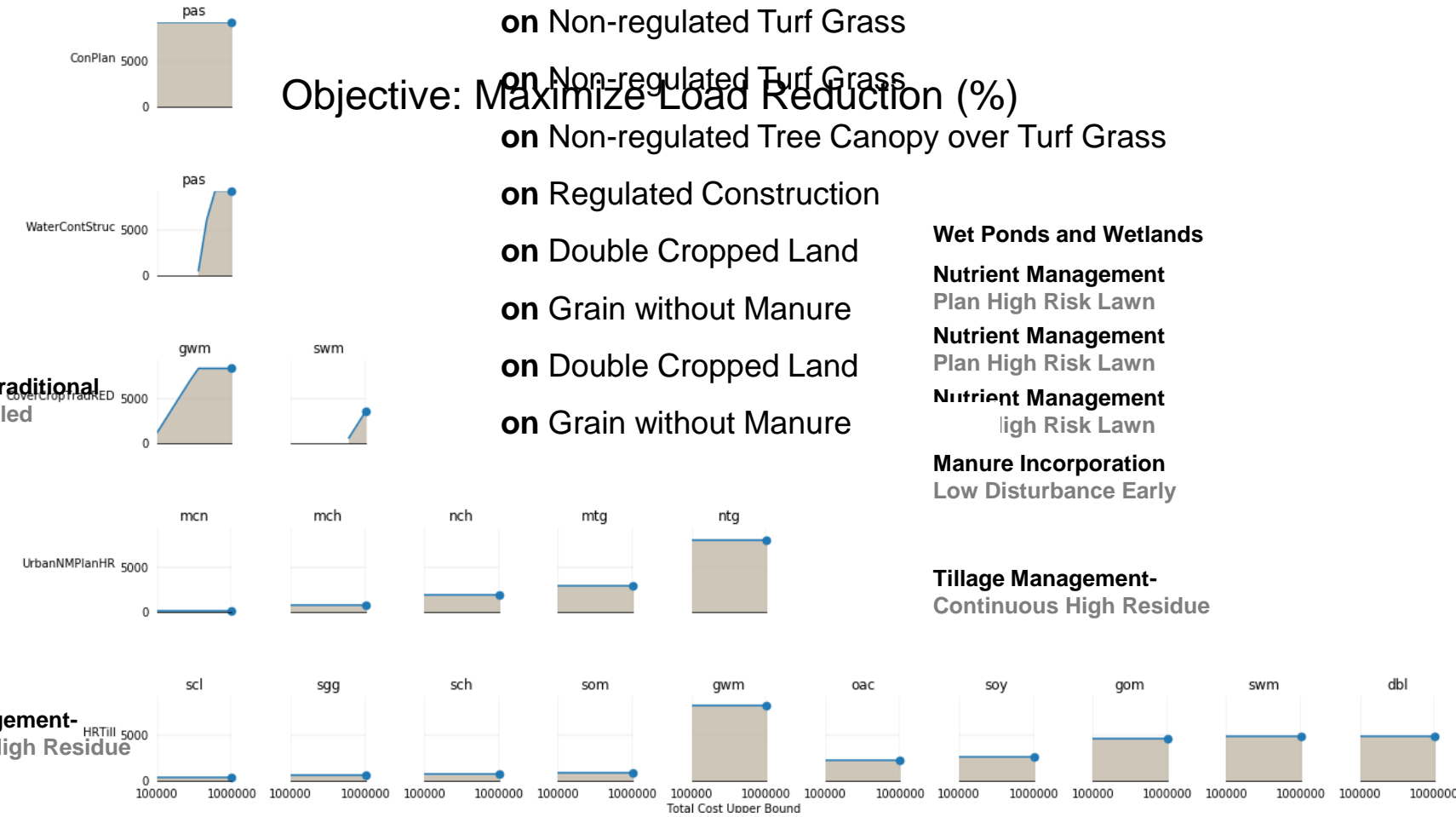
- on Non-regulated Turf Grass
- on Non-regulated Turf Grass
- on Non-regulated Tree Canopy over Turf Grass
- on Regulated Construction
- on Double Cropped Land
- on Grain without Manure
- on Double Cropped Land
- on Grain without Manure

Wet Ponds and Wetlands
 Nutrient Management
 Plan High Risk Lawn
 Nutrient Management
 Plan High Risk Lawn
 Nutrient Management
 High Risk Lawn
 Manure Incorporation
 Low Disturbance Early

Tillage Management-
 Continuous High Residue

Cover Crop Traditional
 Rye Early Drilled

Tillage Management-
 Continuous High Residue



Total Cost Upper Bound
 (\$ 200,000 to \$ 1,000,000)

RESULTS

Land River Segment N51133RL0_6450_0000

(in Northumberland, VA)

totalacres=58,040.90

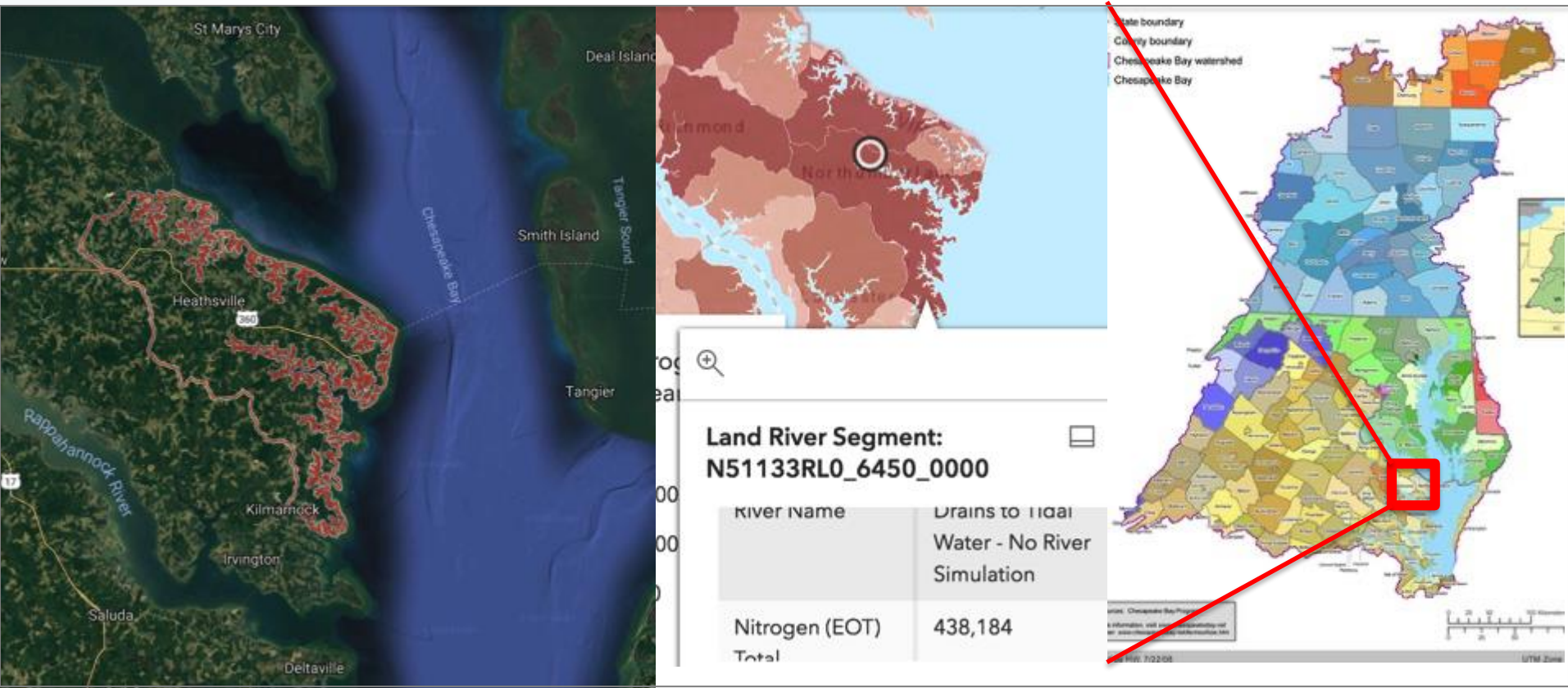
totalacresincludingtidalwetlands=60,642.83

BaseYear=2010 (Baseconditionid=29)

CostProfile=Watershed (costprofileid=4)

Agencies present (Only one!) : agencyid=9 (NONFED), with 58,040.90 acres

So we're not including an AGENCY set for now



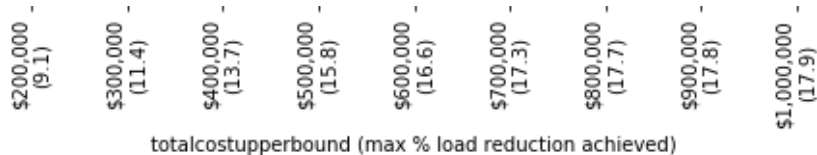
$X_{b,l,\psi}$

('ConPlan', 'N51133RLO_6450_0000', 'pas', 1.94) ·
('CoverCropTradRED', 'N51133RLO_6450_0000', 'dbl', 68.94) ·
('CoverCropTradRED', 'N51133RLO_6450_0000', 'gom', 68.94) ·
('CoverCropTradRED', 'N51133RLO_6450_0000', 'gwm', 68.94) ·
('CoverCropTradRED', 'N51133RLO_6450_0000', 'oac', 68.94) ·
('CoverCropTradRED', 'N51133RLO_6450_0000', 'sgg', 68.94) ·
('CoverCropTradRED', 'N51133RLO_6450_0000', 'soy', 68.94) ·
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('HRTill', 'N51133RLO_6450_0000', 'gwm', 0.0) ·
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('HRTill', 'N51133RLO_6450_0000', 'soy', 0.0) ·
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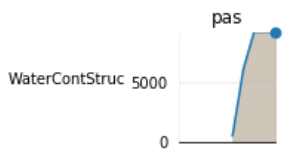
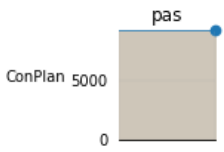
(BMP, LRSeg, LoadSource, \$/unit)

Cost Constraint,
Optimum Load Reduction

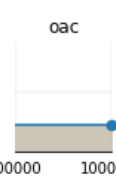
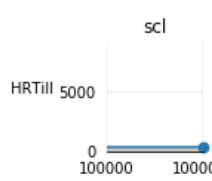
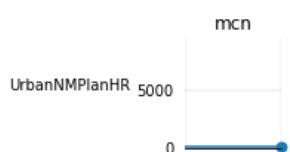
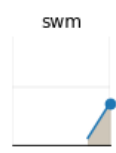
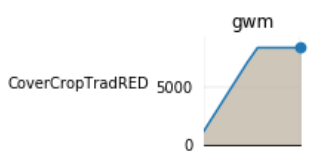
Objective:
Maximize Load Reduction (%)



acres



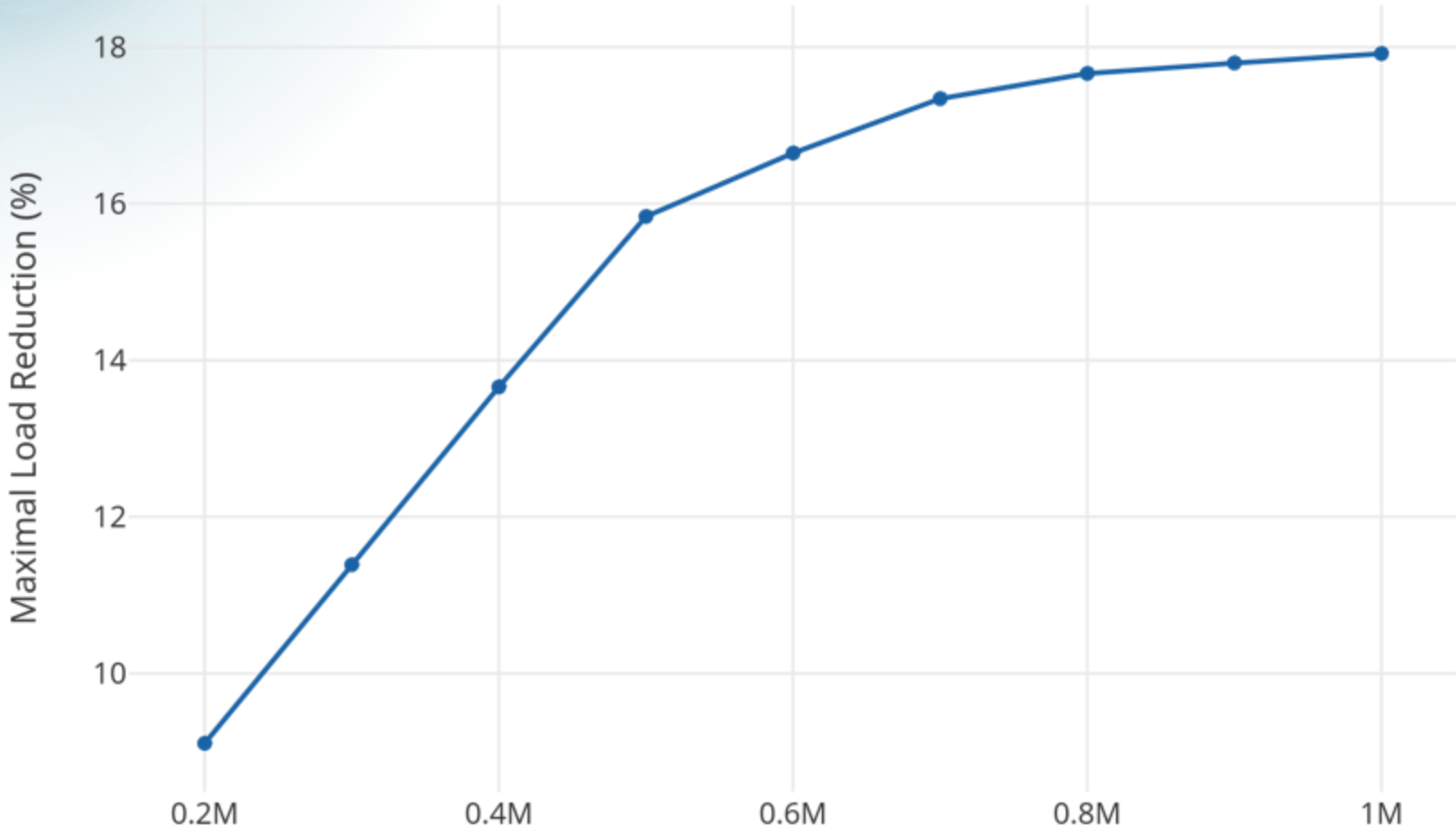
same as previous slide, but different graphic



Total Cost Upper Bound

Objective:
Maximize Load Reduction (%)

Max Load Reduction vs. Total Cost Constraint



Objective:
Maximize Load Reduction (%)

Total Cost (\$) Upper Bound Constraint

```

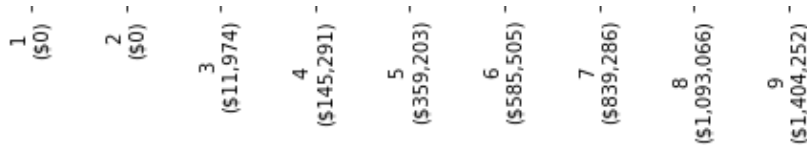
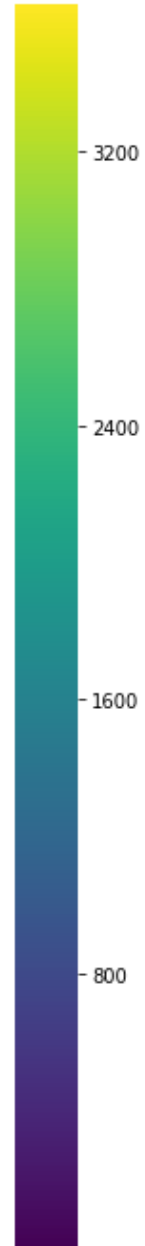
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$X_{b,l,\psi}$

(BMP, LRSeg, LoadSource, \$/unit)

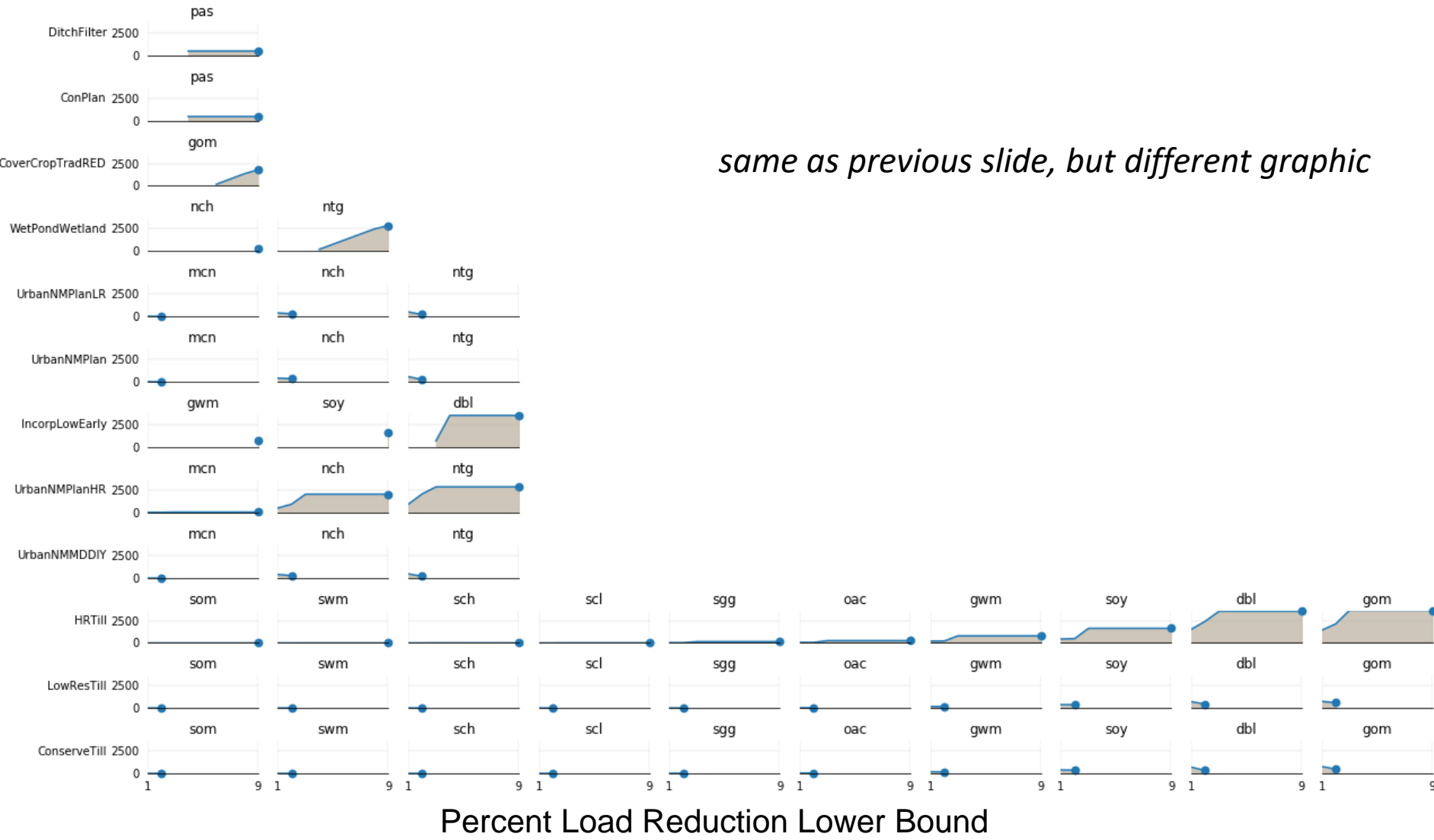
Load Reduction Constraint,
Optimum Minimum Cost



Objective:
Minimize Total Cost (\$)

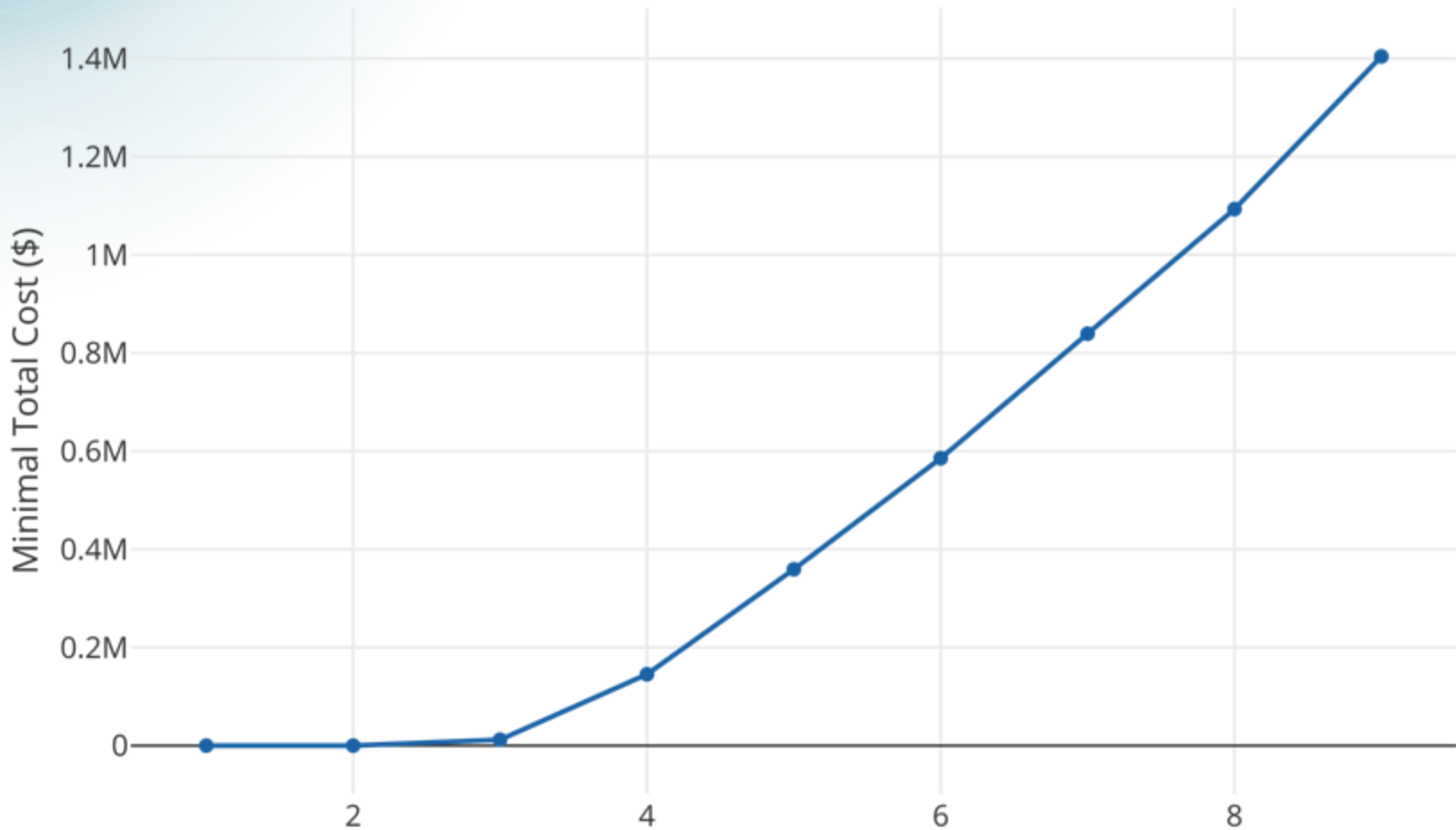
loadreductionlowerbound (min total cost achieved)

same as previous slide, but different graphic



Objective:
Minimize Total Cost (\$)

Minimal Total Cost vs. Load Constraint



Objective: Minimize Total Cost (\$)
Load Reduction (%) Lower Bound Constraint

Prototyping Experiments

Search Space Investigations

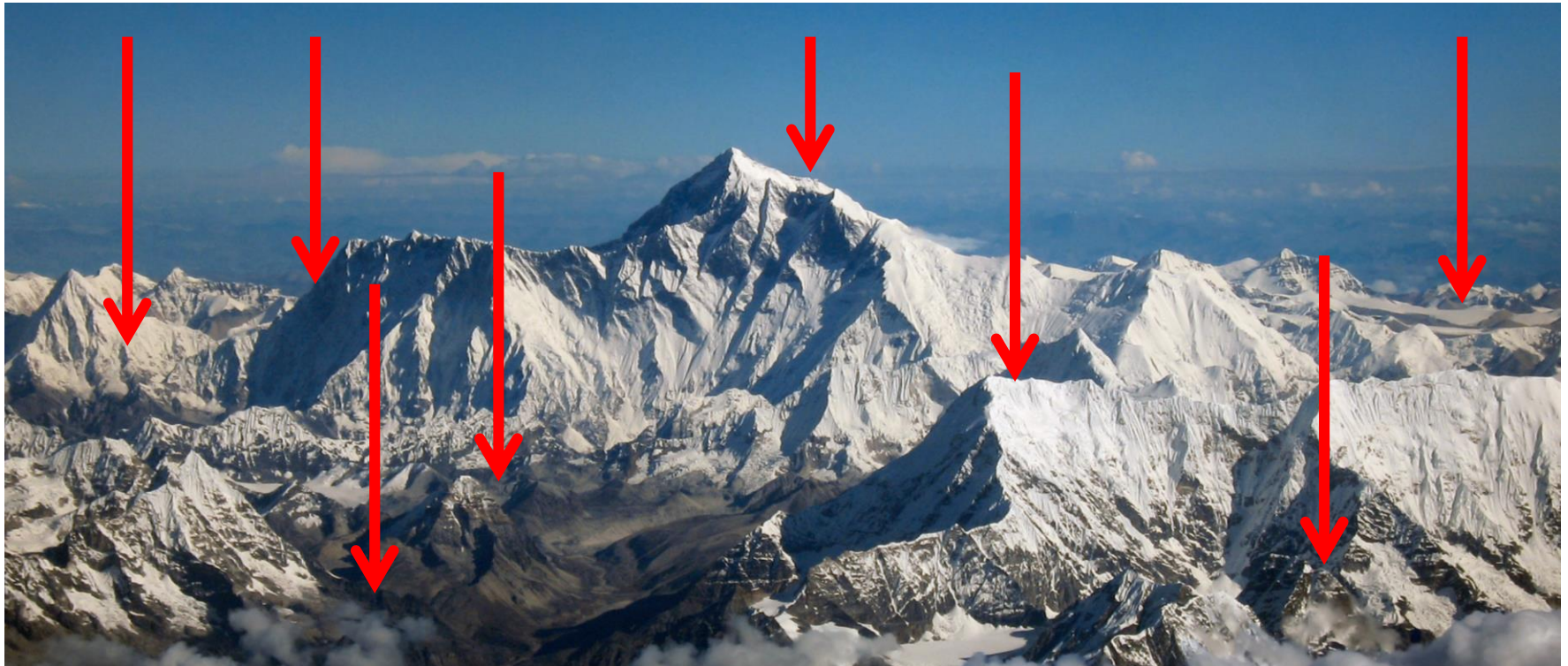
Fine-tuned sub-problem



Prototyping Experiments

Search Space Investigations

Fine-tuned sub-problem



What the future may hold...

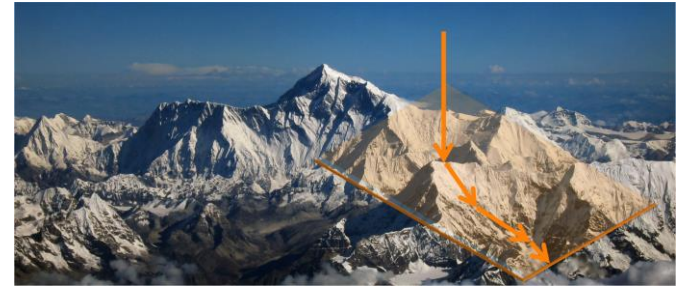
Two land-river segments

	Northumberland County, VA		Lancaster County, PA	
Objective:	Min. Cost ($\tau=12$)	Max Load Reduction ($C=100,000$)	Min. Cost ($\tau=12$)	Max Load Reduction ($C=100,000$)
# of variables	1339	1339	1339	1339
# of inequality constraints	1110	1108	1110	1108
# of nonzeros in inequality constraint Jacobian	3609	2628	3862	2628
# of nonzeros in Lagrangian Hessian	5575	5278	6058	5746
Iterations to solve	57	35	47	29

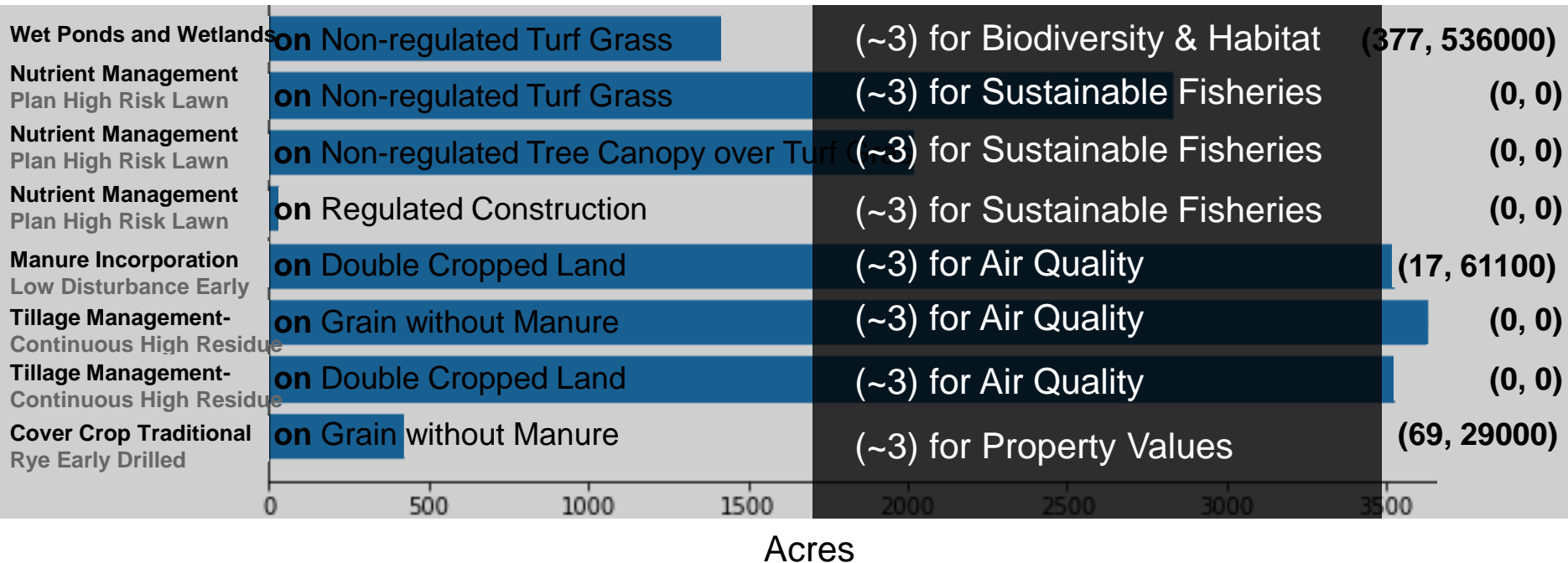
Experiments –

(2) Fine-tuned sub-problem

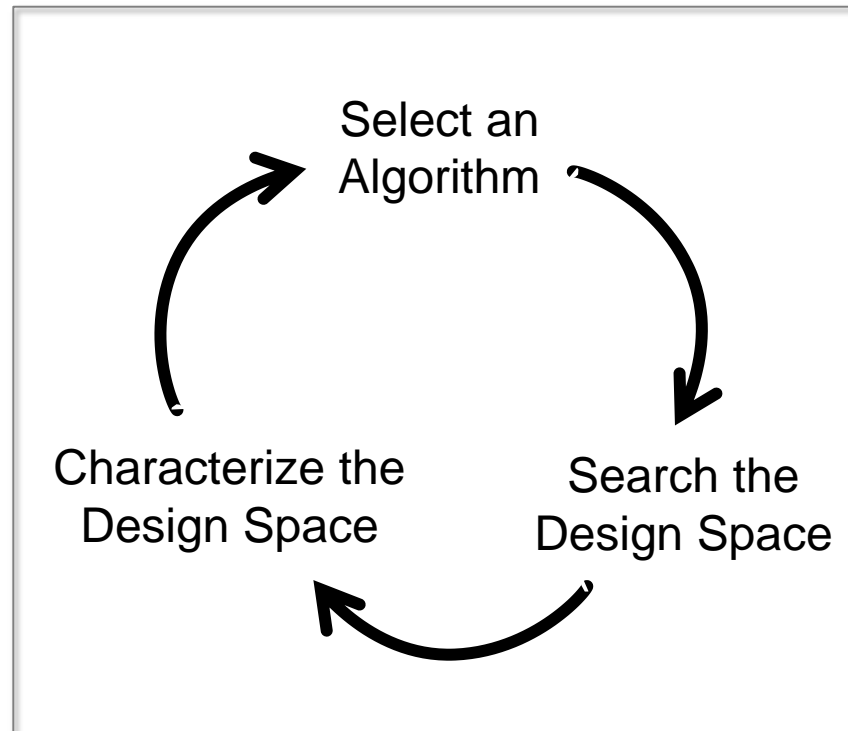
- Guide explorations of increasing complexity
- Solutions for select BMPs



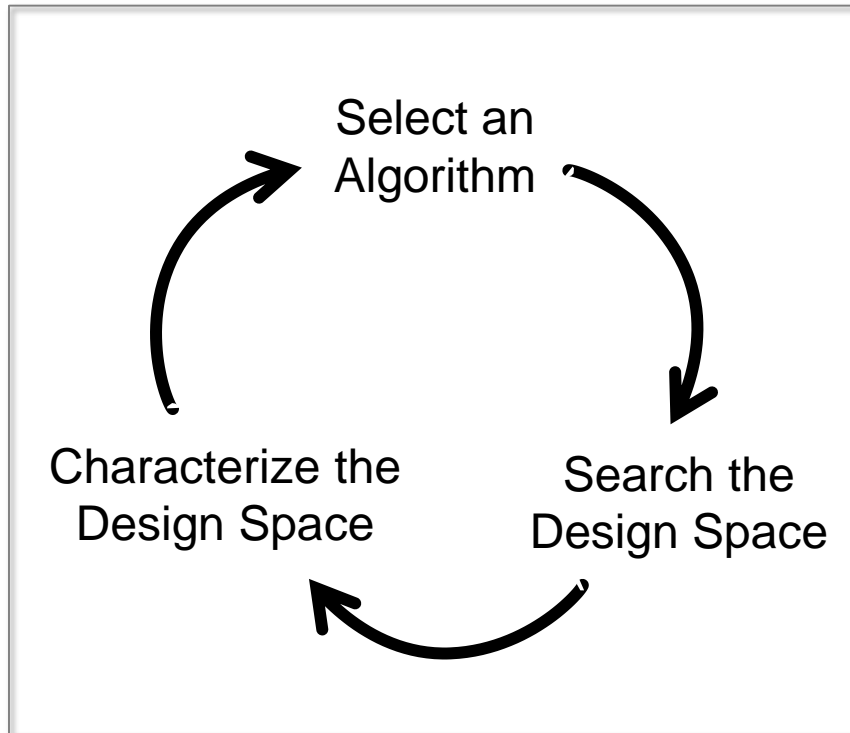
Example Results (6% Reduction Constraints)



Medium-term goals: Post Core-CAST approaches



After prototyping experiments...



Various Possible Approaches

- **Population-based stochastic search**
(e.g. Genetic algorithm)
- **Decomposing into sub-problems, with multiple algorithms**
 - *Population-based for land use change and/or manure transport*
 - *Greedy algorithm or nonlinear programming for efficiency*
BMPs
- **Model training**

Heuristic + NLP?

Pseudocode for Hybrid algorithm:

P <- Build population of non-efficiency-BMP scenarios

$Best$ <- \emptyset

repeat

for each individual P_i in P **do**

 Fitness(P_i) <- NLP solution (for efficiency-BMPs)

using P_i variables, costs, &
loads as starting point

if $Best = \emptyset$ or Fitness(P_i) > Fitness($Best$) **then**

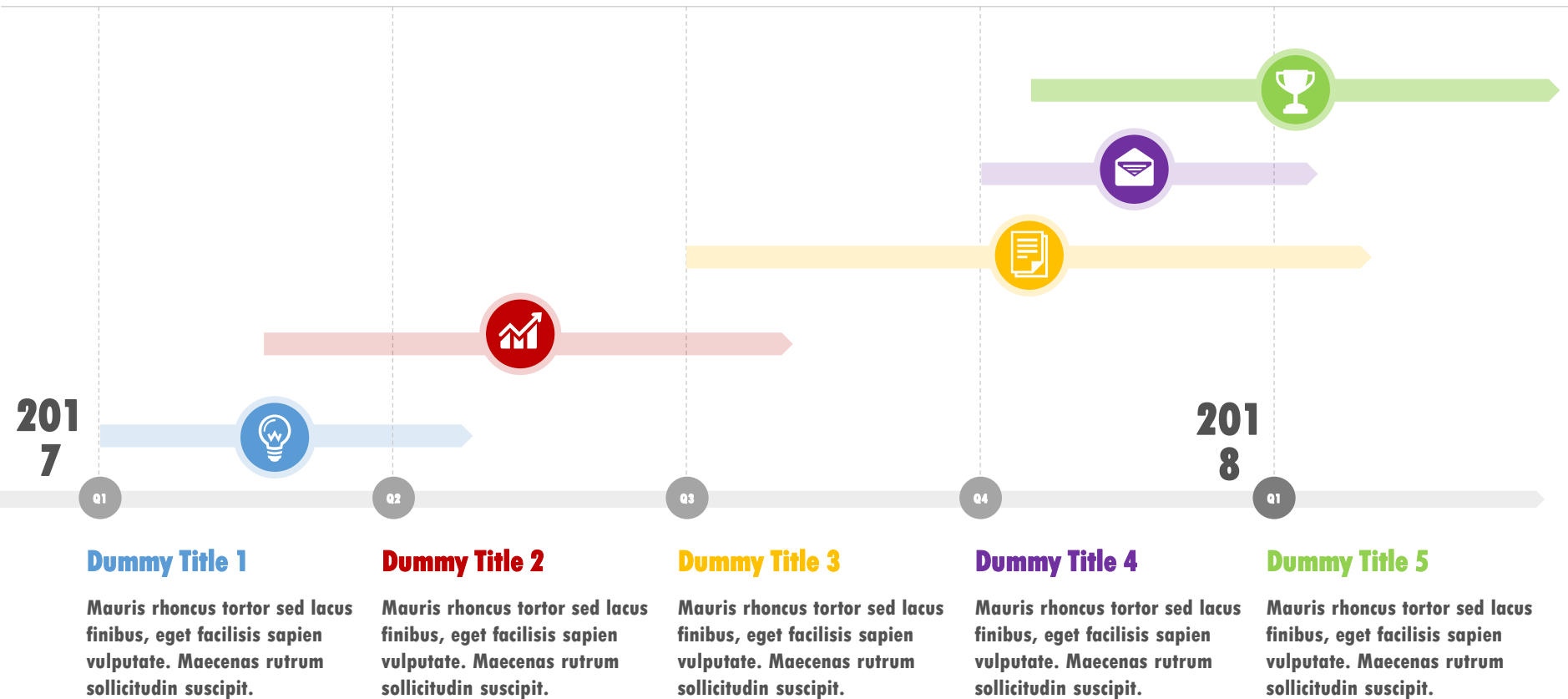
$Best$ <- P_i

P <- modified P using a heuristic (select, mutate, recombine,
 etc.) according to the fitnesses

until $Best$ is the ideal solution or we have run out of time

return $Best$

Project Timeline



Revised timeline

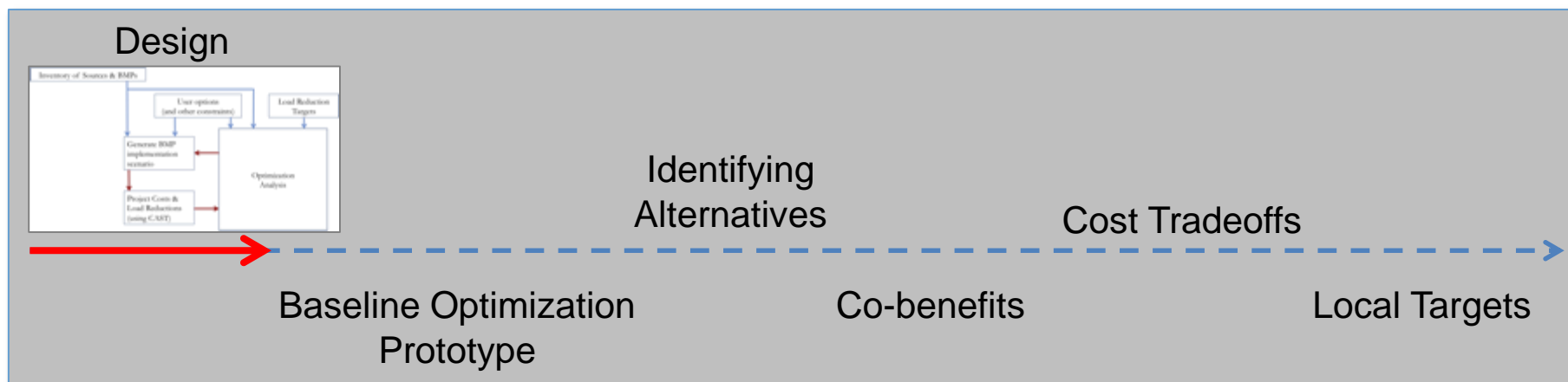
Date	CoreCAST Task	Optimization Task
May 2018	Detailed Design & Review with Jess and Dev Team	Formulate and code NLP sub-problem model
June - July 2018	CoreCAST Development	Conduct NLP sub-problem tests for efficiency BMPs
August 2018	CAST UI Integration & Performance Testing	Analysis of NLP sub-problem results
September 2018	CAST Master Processor Development	Analysis & visualization of batch scenario experiments
October 2018	Beta Testing / Results Verification; Integration with CAST UI	Scenario generator interfacing with CoreCAST Beta & Algorithm/package evaluation
November 2018	Performance Tuning	Design options for constraints and user interface
December 2018	CAST End User Testing	Beta Testing of version 0.1
January 1, 2019	Production Release	Beta Testing of version 0.1

Near-term Milestones

Date	Optimization Task
Summer 2018	Analyses of sampling experiments & sub-problem formulation
End of Summer	Scenario generator interfacing with CAST architecture update
Fall 2018	Algorithm/package evaluation
Winter 2018	Beta testing of version 0.1, constraints & user interface

Near-term Milestones & Looking Ahead

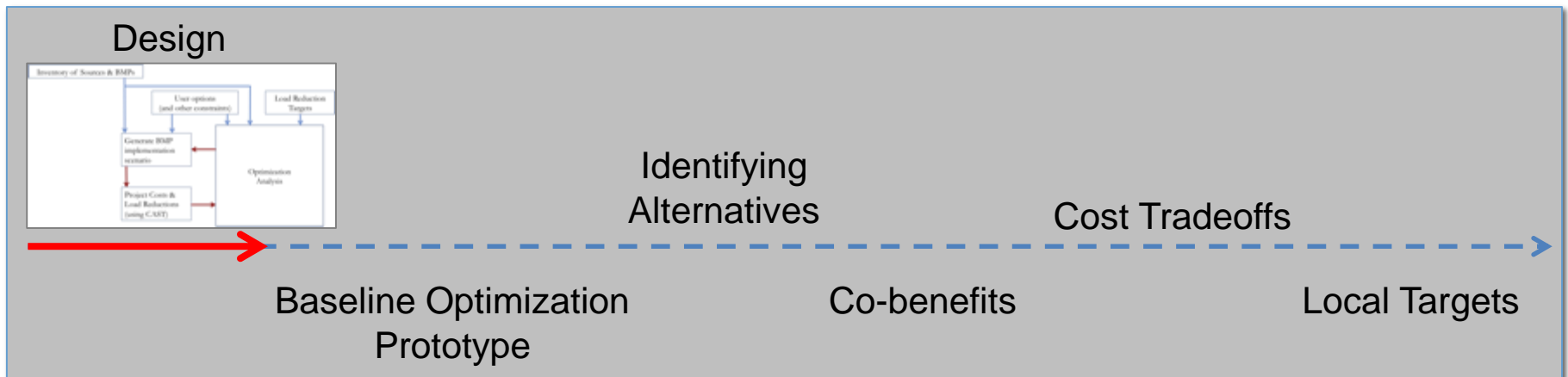
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Fall 2018	Algorithm/package evaluation
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Will be shaped by feedback!

Actively searching for ways to engage local decision makers at county and municipal scales for their guidance and feedback on optimization design.

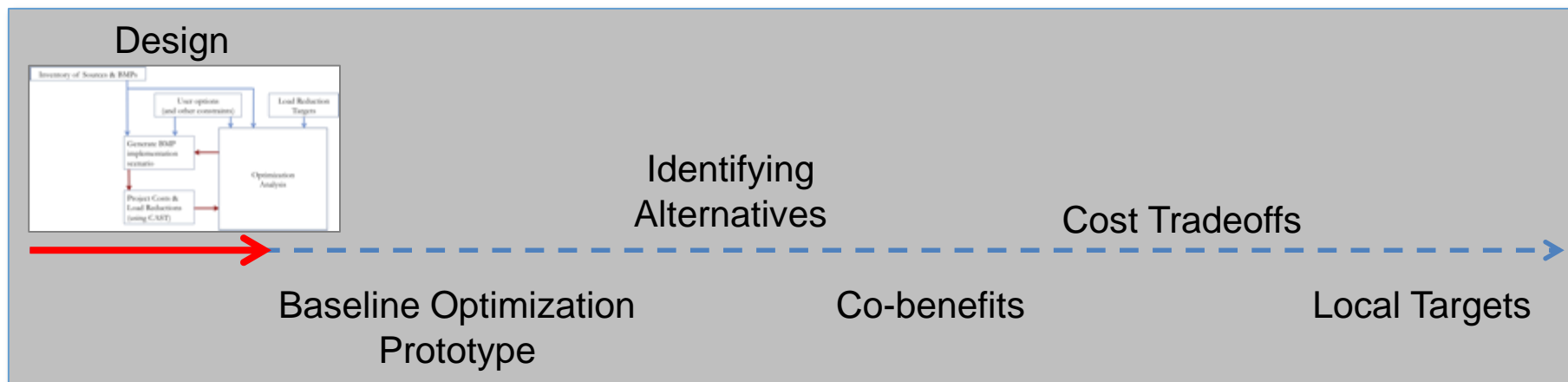
Email me (Danny) at: dkaufman@chESApeakebay.net



Will be shaped by feedback!

Actively searching for ways to engage local decision makers at county and municipal scales for their guidance and feedback on optimization design.

Email me (Danny) at: dkaufman@chesapeakebay.net



Extra Slides Follow

2016 to 2017

2016, February: STAC Workshop held

2016, December

- Grant for optimization tool development awarded to Chesapeake Research Consortium (CRC)
- Advisory and Support Committee (ASC) formed

2017, June

- STAC Workshop Report published
- Dr. Stuart Schwarz of UMBC worked on Phase 1 activities in June and July of 2017, and proposed a recursive greedy algorithm for adding improved feasible choices to a optimization solution set.

2017, December: Research Scientist hired

Optimization – from STAC to Development



Programmatic highlights since Dec, 2017

Meetings with:

- Advisory and Support Committee (~Quarterly)
- Dr. Hugh Ellis, at Johns Hopkins (~monthly)
- Modeling team (regularly)
- CBPO optimization technical team (modeling team, system administrators, CAST developers; monthly)
- CBPO cloud-computing group (~bi-weekly)
- CBPO User Experience team

Presentations and feedback gathered from:

- Water Quality Goal Implementation Team (WQGIT)
 - Workgroups
 - Watershed Technical
 - Modeling
 - Urban Stormwater
 - Wastewater Treatment
 - Scientific, Technical Assessment, and Reporting (STAR) team
 - Chesapeake Research & Modeling Symposium
-
- Response to STAC workshop drafted for CBP Management Board
 - Project workplan updated, and no-cost extension granted (to March 31, 2020)

Technical highlights since Dec, 2017

- Pre-prototype software for on-the-fly generation of Best Management Practice (BMP) scenario files for use with CAST.
- Two prototype optimization models for efficiency BMPs (a sub-population of all BMPs) have been developed for
 1. minimizing total scenario cost while achieving nonpoint source reduction, and
 2. maximizing total load reductions subject to a cost constraint
- Efficiency BMP optimization problem analyses established:
 - non-convexity of the load reduction function
 - negligible starting point sensitivity (for single land river segments)
 - results for constraint variations