Framing Decision Problems: Forecast Modeling & Optimization

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BREE Research Project
Vermont EPSCoR
PTAC Stakeholder Meeting
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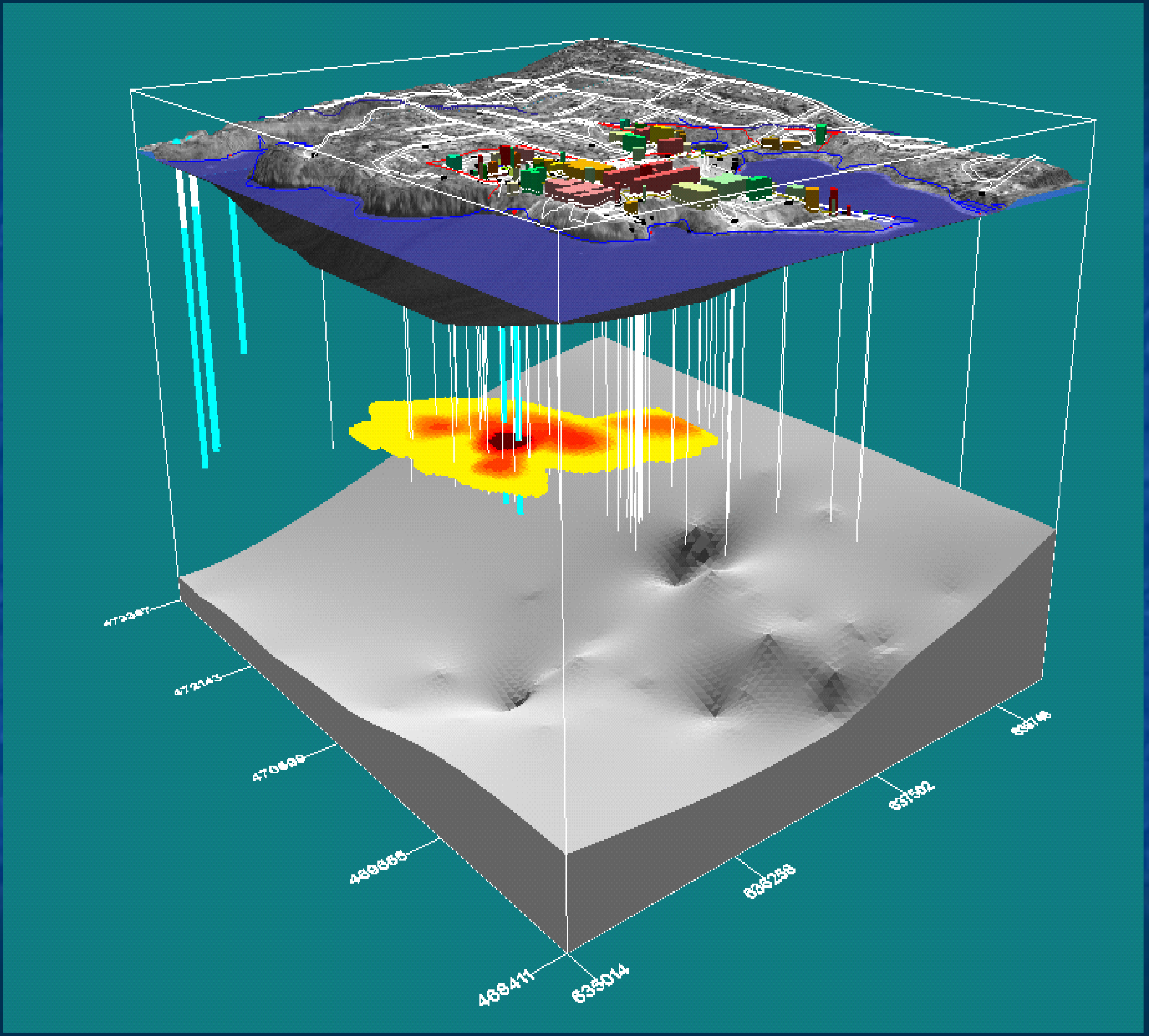
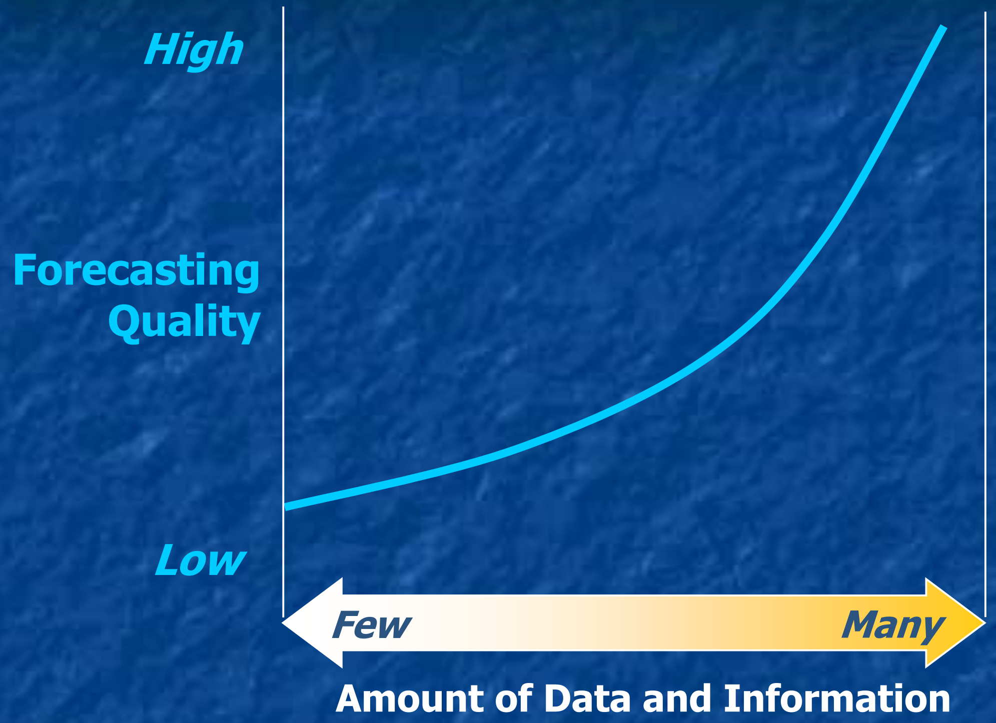
Forecast Modeling

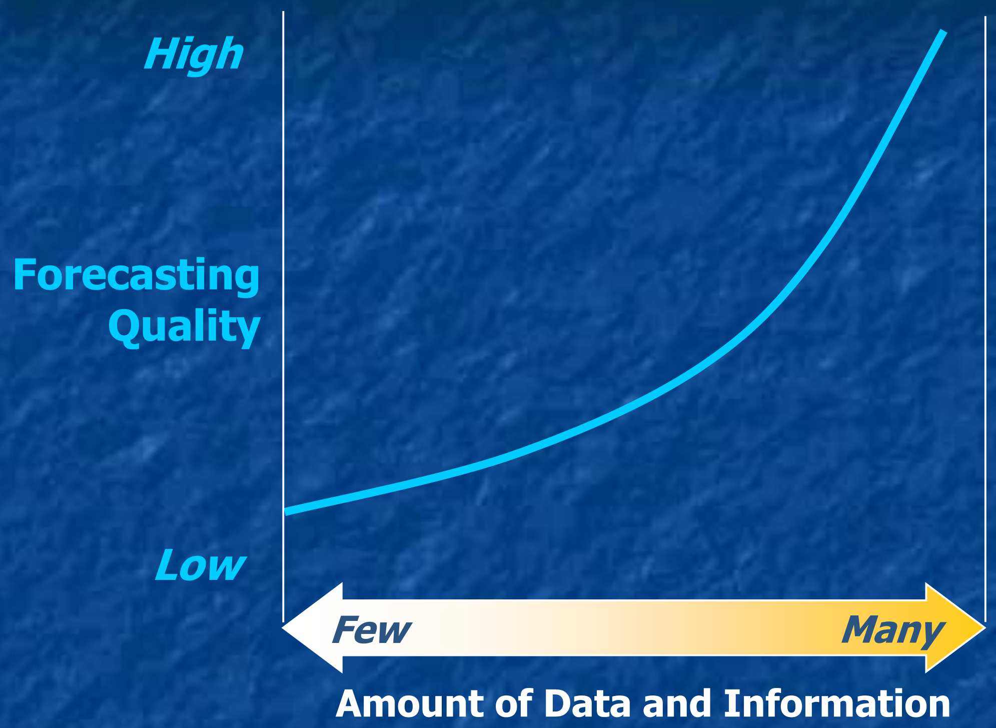


Rizzo and Dougherty, *Water Resources Research*, 30 (2), pp. 483-497, 1994.

Modeling & Maturity of Site Understanding



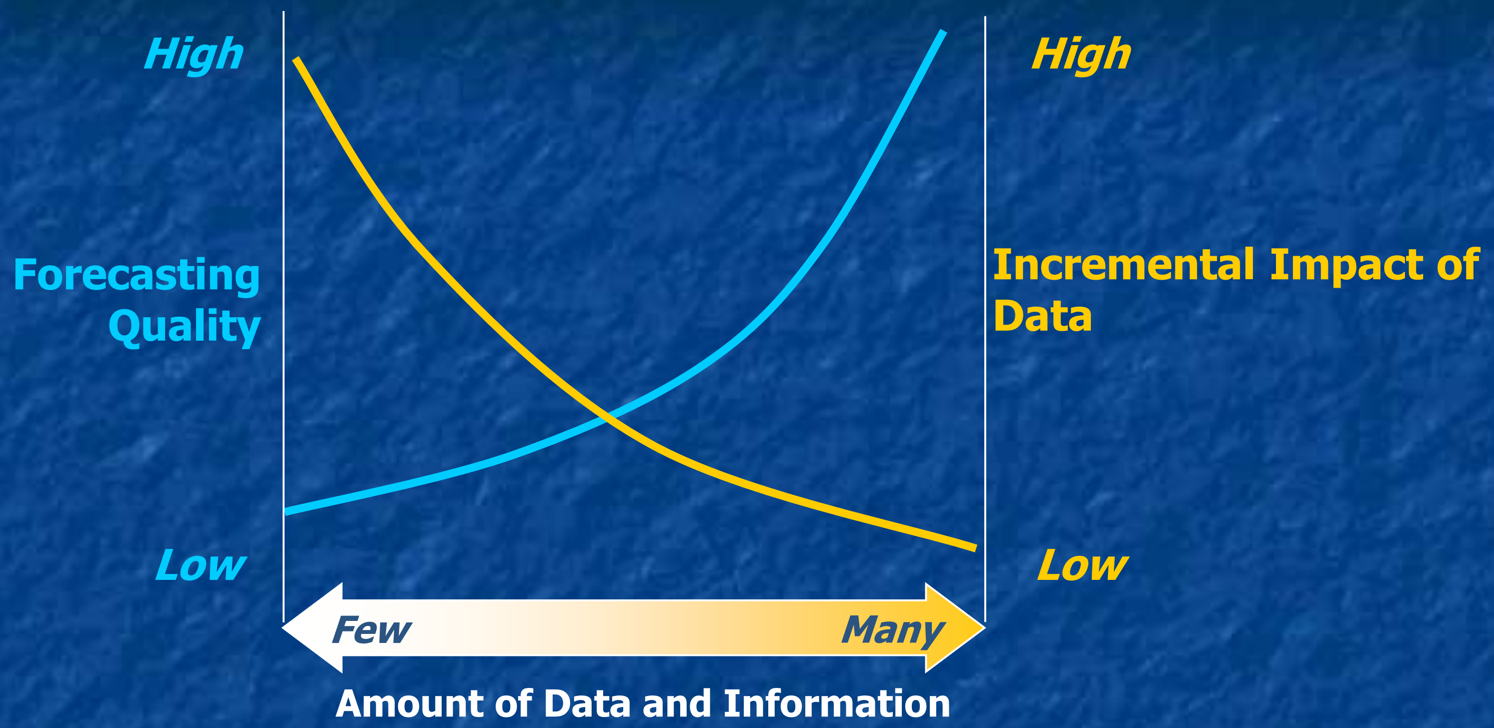
Modeling & Maturity of Site Understanding



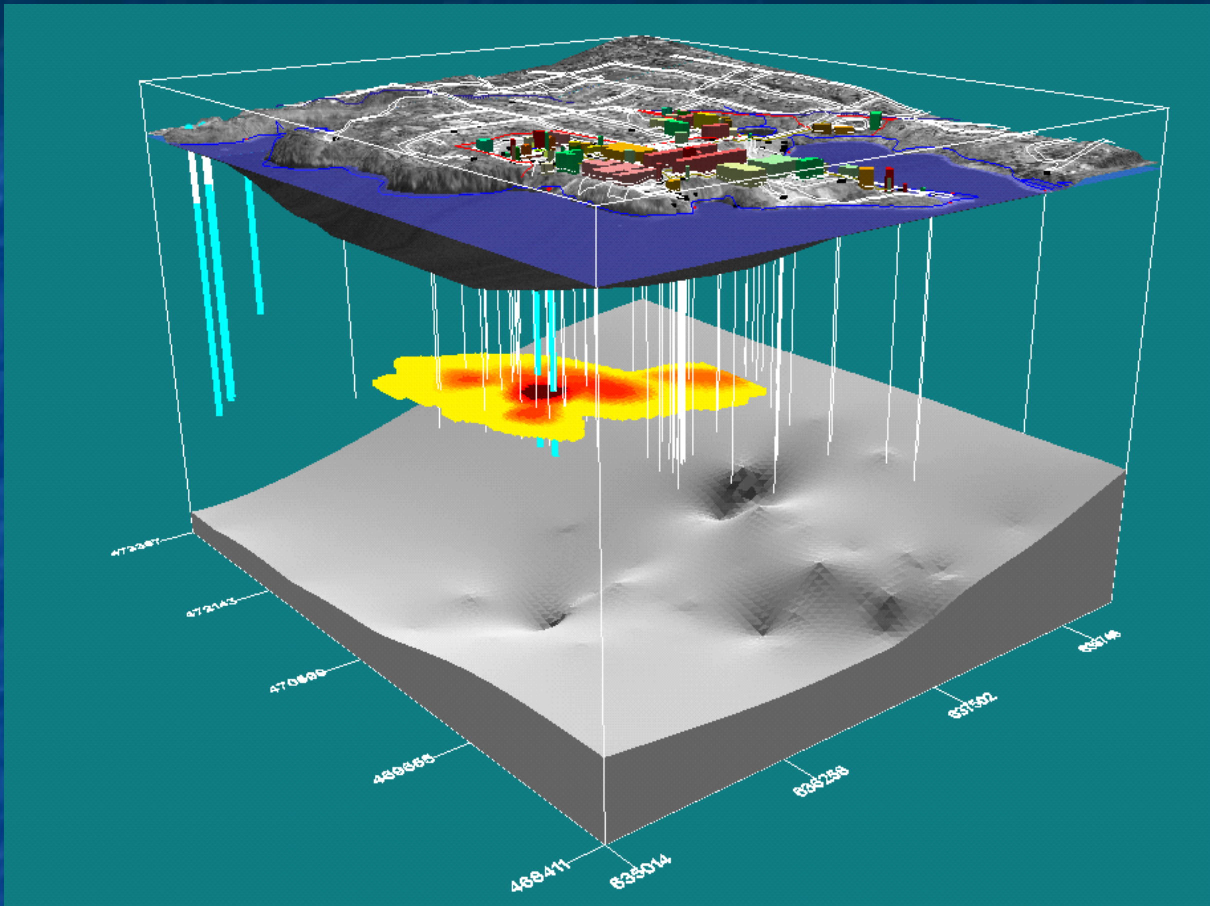
Model selection

Analytical	✓	✓	
2-D Numerical		✓	✓
3-D Numerical			✓
Statistical		✓	✓

Modeling & Maturity of Site Understanding



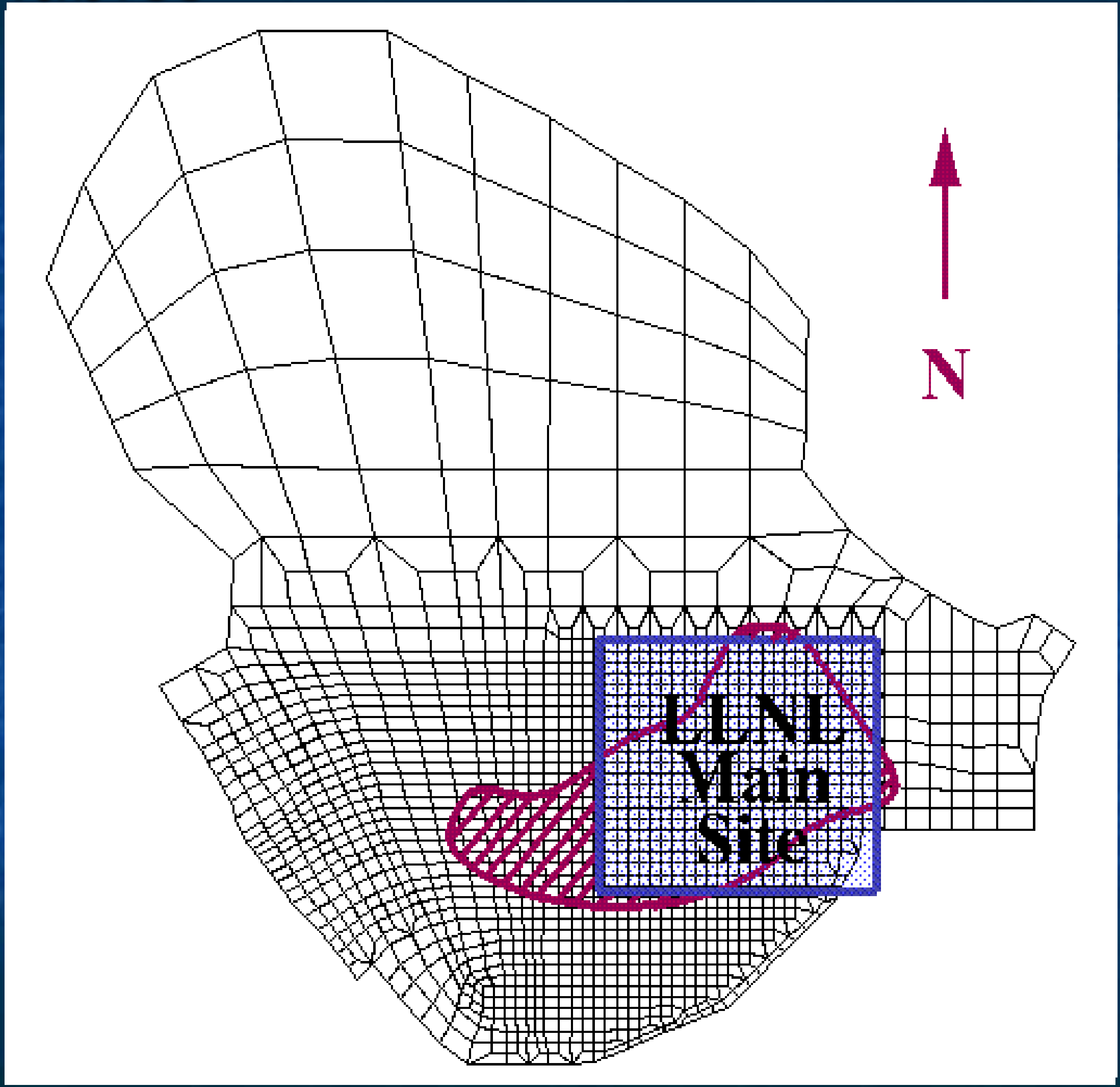
Multi-Objective Heuristic Optimization



"The **<u>extrapolations</u>** are the only things that have any real value.
… Knowledge is of no real value if all you can tell me is what happened yesterday….
you must be willing to stick your neck out."

R. P. Feynmann,
The Uncertainty of Science,
John Danz Lecture,
April 23, 1963

Decision Variables



Simplifications

Table 1. Remediation standards and State discharge limits for compounds of concern in ground water at the LLNL site.

	Concentration limit for drinking water[a]			
Constituent	Federal MCL (ppb)	California MCL (ppb)	Pre-remediation concentration range at LLNL March 1990–March 1991 (ppb)	Discharge limit[b] for treated water (ppb)
PCE	5	5	<0.1–1,050	4
TCE	5	5	<0.1–4,800	5
1,1-DCE	7	6	<0.5–370	5
cis-1,2-DCE	70	6	<0.5–24	5 (total 1, 2-DCE)
trans-1,2-DCE	100	10	<0.5–1	5 (total 1, 2-DCE)
1,1-DCA	—	5	<0.5–60	5
1,2-DCA	5	0.5	<0.1–190	5
Carbon tetrachloride	5	0.5	<0.1–91	5
Total THM[c]	100[c]	100[c]	<0.5–270	5
Benzene	5	1.0	<0.1–4,600	0.7
Ethyl benzene	700	680	<0.2–610	5
Toluene	1,000	—	<0.5–4,200	5
Xylenes (total)	10,000	1,750[d]	<0.5–3,700	5
Ethylene dibromide	0.05	0.02	<0.1–51	5
Total VOCs	—	—	up to 5,808	5
Chromium[+3 e]	50 (total Cr)	50 (total Cr)	<5–150 (total Cr)	50 (total Cr)
Chromium[+6 e]	50 (total Cr)	50 (total Cr)	<10–140	11
Lead	15[f]	50	<2–10	5.6
Tritium[g]	20,000 pCi/L	20,000 pCi/L	<200–33,100	(h)

[a] Human receptor. The more stringent concentration limits on this part of the table are shown in a larger typeface to illustrate that LLNL will comply with the most stringent requirements.

[b] From NPDES Permit No. CA0029289 (revised 8/1/90) and RWQCB Order No. 90-106. VOC-specific State discharge limits exist in RWQCB Order No. 90-106 only for PCE (4 ppb) and benzene (0.7 ppb). Other VOCs listed in this table are included in the 5 ppb total VOC limit. Discharge limits for metals differ slightly according to discharge location.

[c] *Total trihalomethanes (THMs); includes chloroform, bromoform, chlorodibromomethane, and bromodichloromethane* (California Drinking Water Requirement).

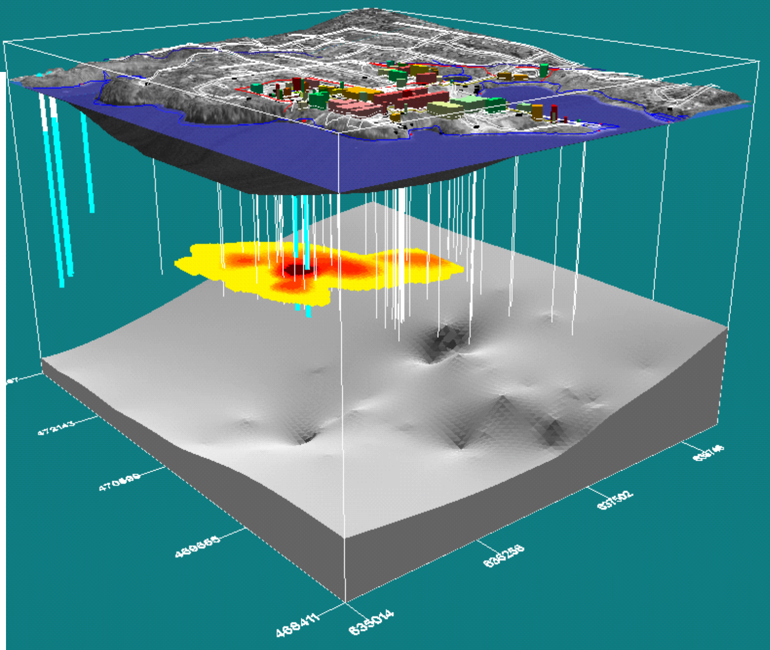
[d] MCL is for either a single isomer or the sum of the ortho, meta, and para isomers.

[e] National Interim Primary Drinking Water Regulation for total chromium is 50 ppb.

[f] National Primary Drinking Water Regulation Enforceable Action Level (Federal Register, volume 56, number 110, June 7, 1991, p. 26460).

[g] Thorpe *et al.* (1990) show that ground water in the one well that currently exceeds the tritium MCL will be naturally remediated *long before it migrates offsite*.

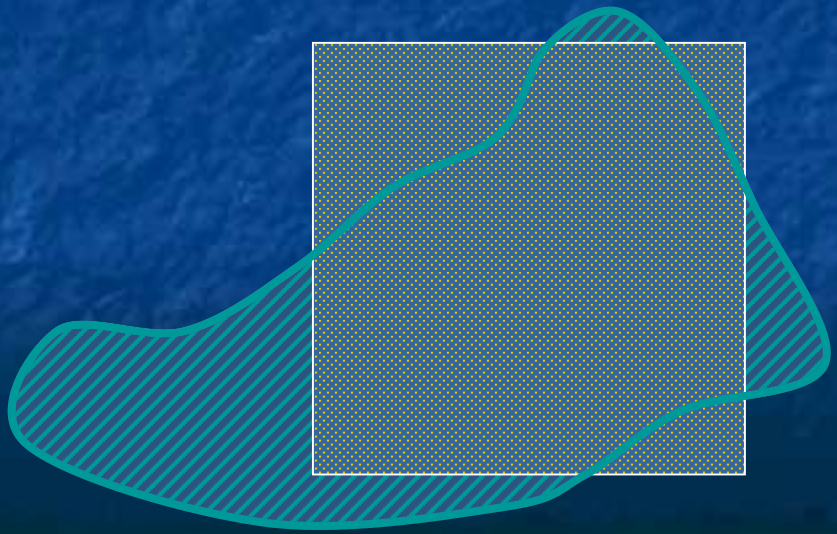
[h] There is currently no NPDES discharge limit for tritium. LLNL will use the MCL for tritium as the discharge limit.



Types of Contamination

Problem Description

- Reduce solute concentration, C(i), everywhere (onsite Ω_o and offsite Ω_{p-o}) to below MCL (C_{mcl} = 5ppb) over 30 years while minimizing costs.

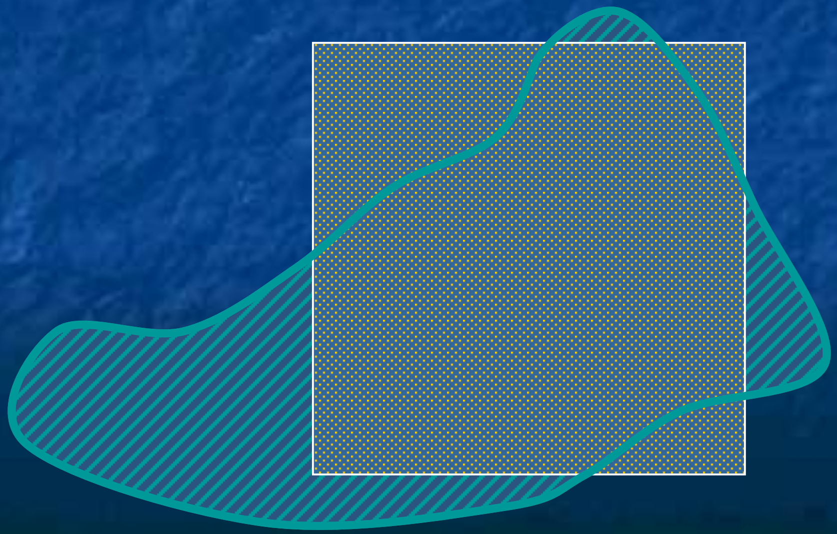


Problem Description

- Reduce solute concentration, C(i), everywhere (onsite Ω_o and offsite Ω_{p-o}) to below MCL (C_{mcl} = 5ppb) over 30 years while minimizing costs.

Constraint:

- Maximum number of distinct wells installed over the total 30-yr simulation is fixed at 28.



Problem Description

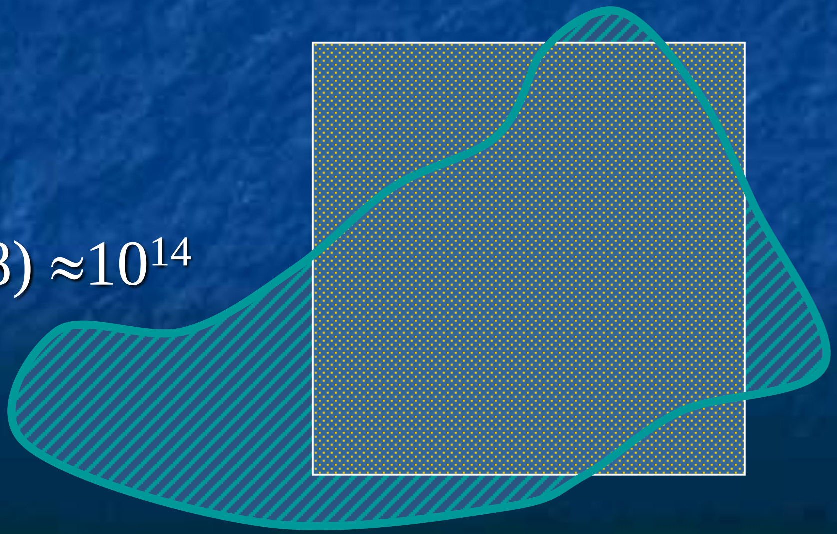
- Reduce solute concentration, C(i), everywhere (onsite Ω_o and offsite Ω_{p-o}) to below MCL (C_{mcl} = 5ppb) over 30 years while minimizing costs.

Constraint:

- Maximum number of distinct wells allowed to pump over the total 30-yr simulation is fixed at 28.

- Ex.

L = 50 N = 28 $C(50,28) \approx 10^{14}$



Problem Description

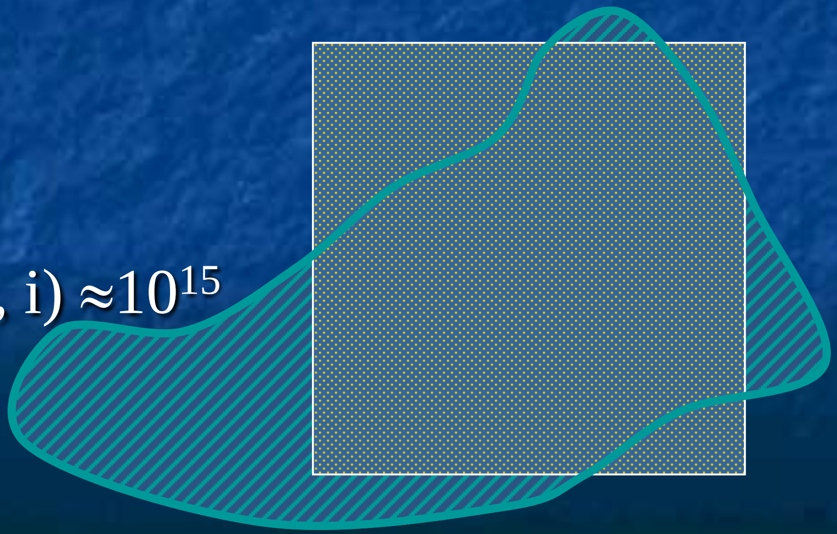
- Reduce solute concentration, C(i), everywhere (onsite Ω_o and offsite $\Omega_{p\text{-}o}$) to below MCL (C_{mcl} = 5ppb) over 30 years while minimizing costs.

Constraint:

- Maximum number of distinct wells allowed to pump over the total 30-yr simulation is fixed at 28.

- Ex.

L = 50   N = up to 28 $\sum^{28} C(50, i) \approx 10^{15}$

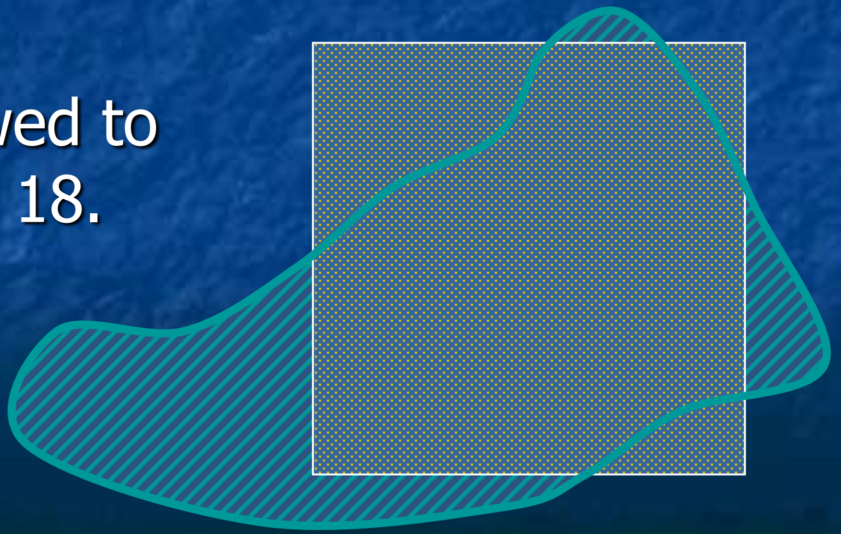


Problem Description

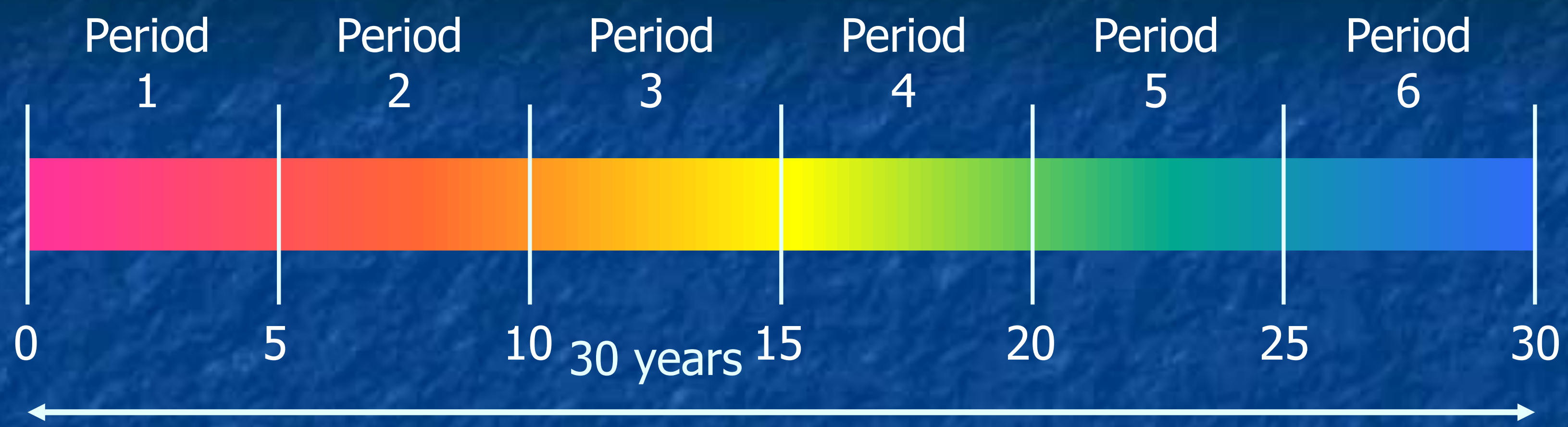
- Reduce solute concentration, C(i), everywhere (onsite Ω_o and offsite Ω_{p-o}) to below MCL (C_{mcl} = 5ppb) over 30 years while minimizing costs.

Constraints:

- Maximum number of distinct wells allowed to pump over the total 30-yr simulation is fixed at 28.
- Maximum number of wells allowed to pump simultaneously is fixed at 18.



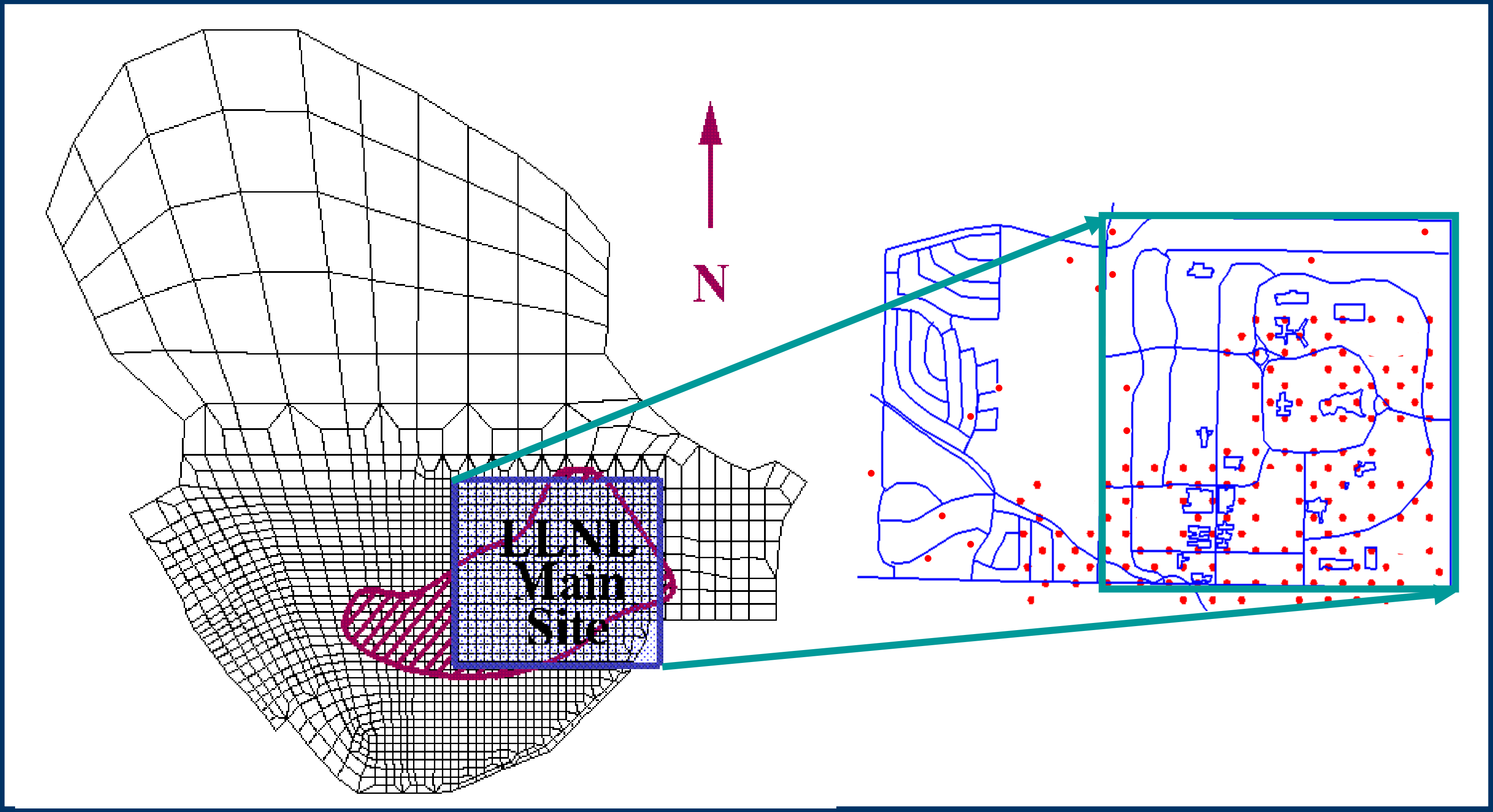
Multiple Management Periods



A management period = time interval over which the design variable (e.g., location of wells) and the corresponding intensity of its application (e.g. pumping rate) remain fixed.

- Allows for time-varying management goals and priorities

Additional (practical) constraints:



Challenges Arise:

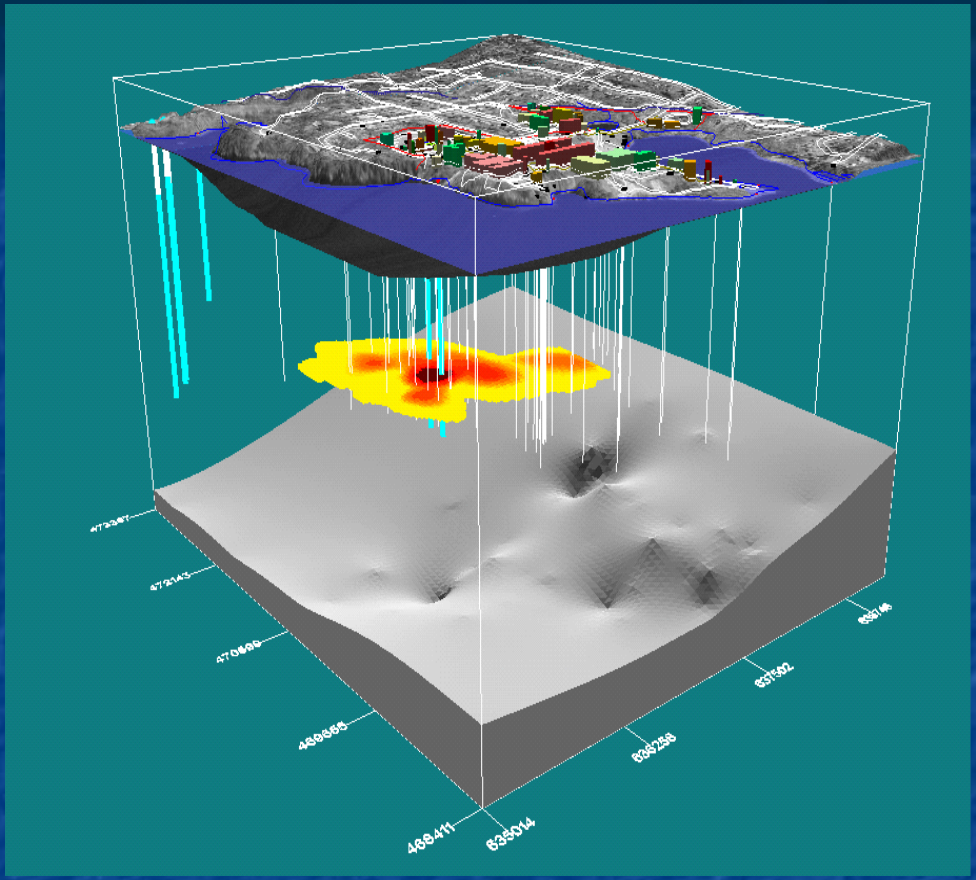
- Computational resources needed to accommodate large number of decision variables and constraints

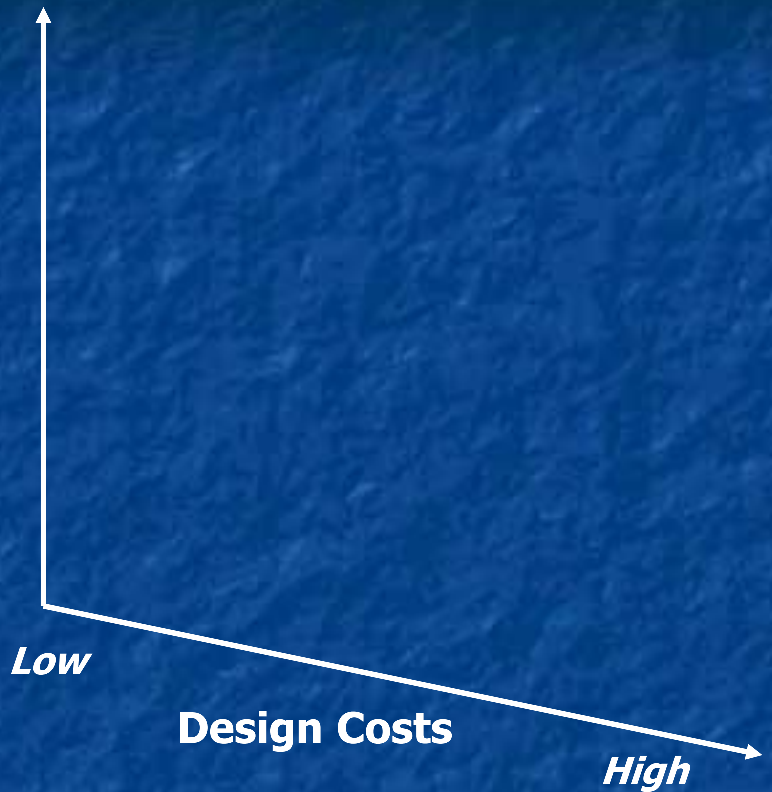
- Ex.

$L = 50$ $N = 28$ $P = 18$ and $m = 6$

Possible Configurations $\approx 10^{61}$

Multi-Objective Optimization

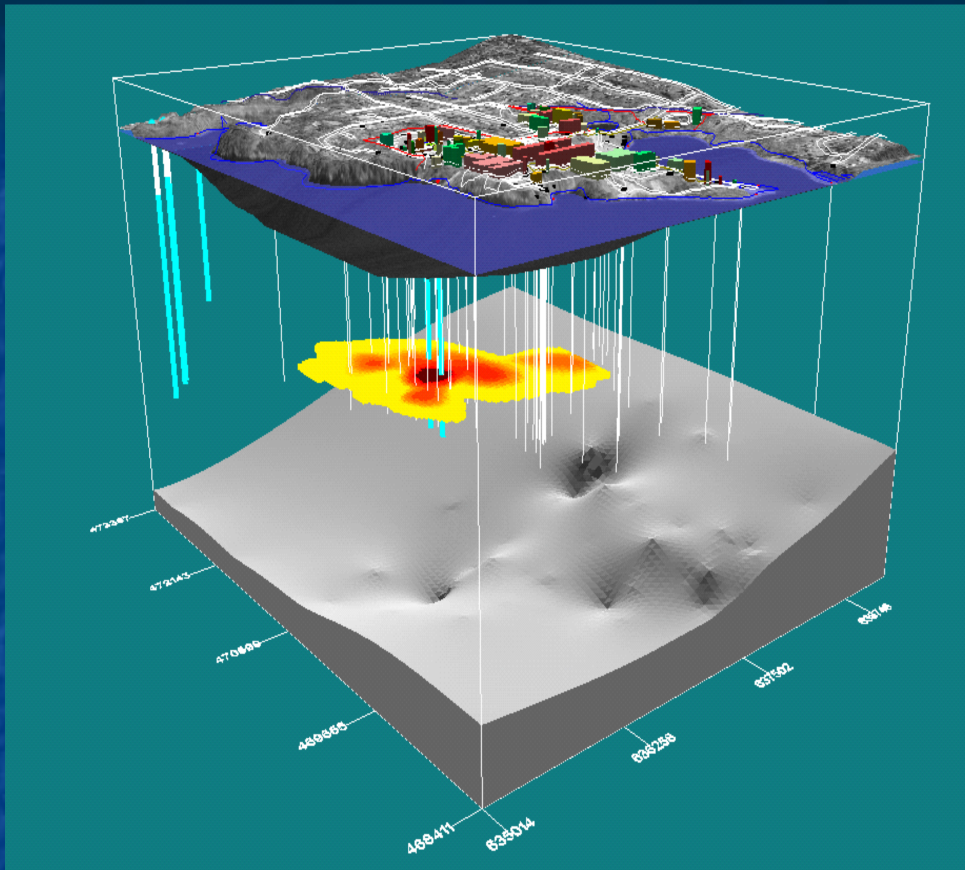


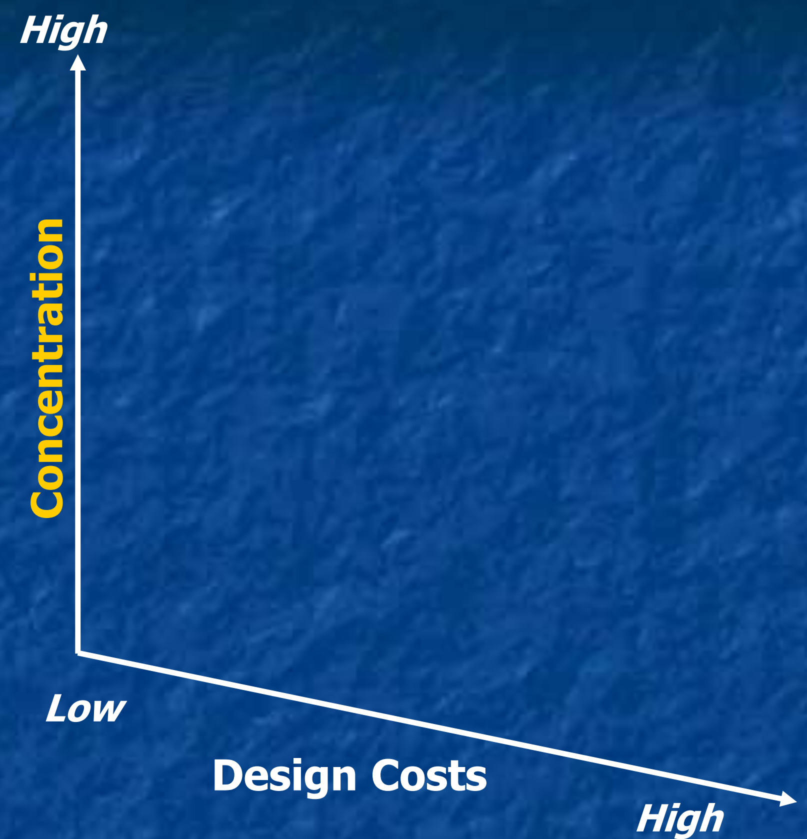


Minimize:

= Design Costs $

Multi-Objective Optimization

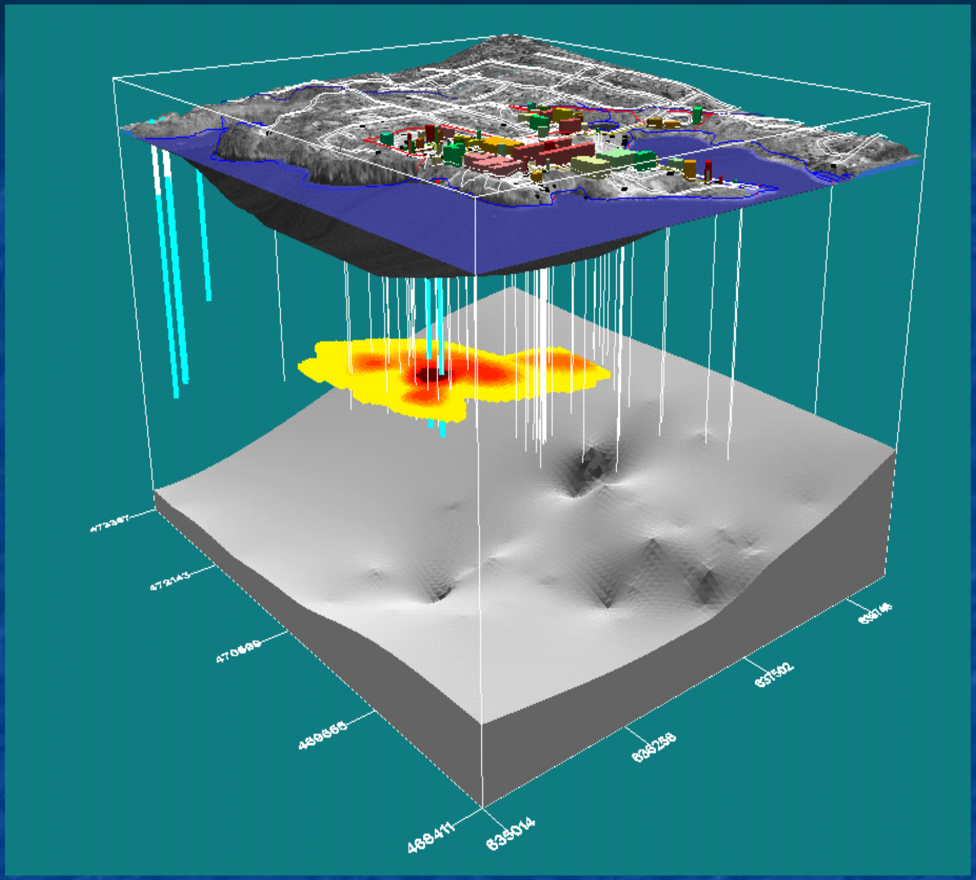


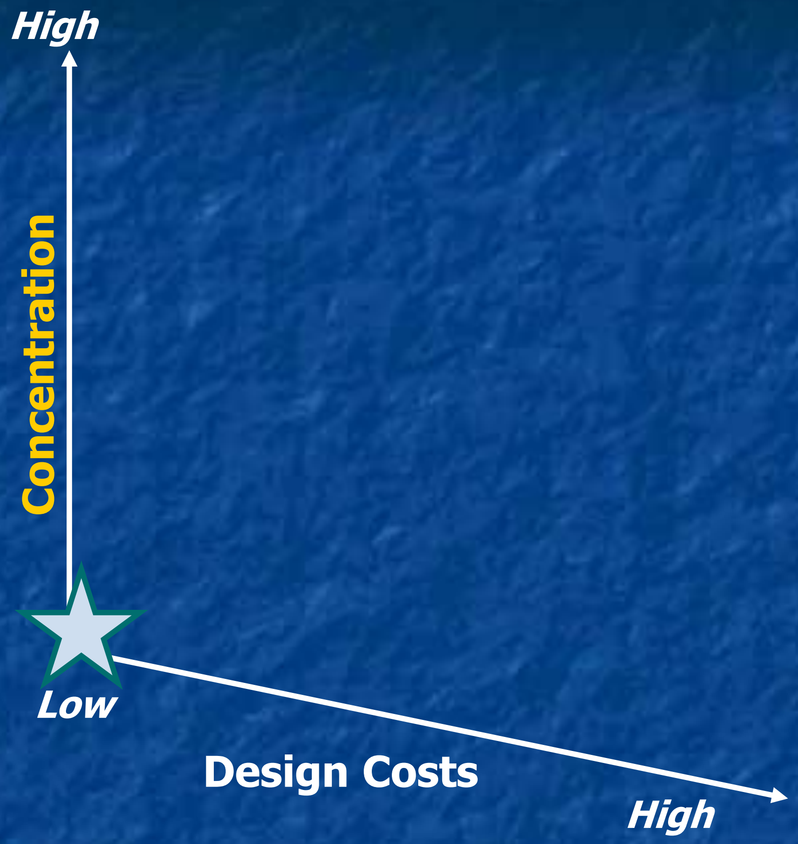


Minimize:

= Design Costs \$ + λ_1*(Water Quality)

Multi-Objective Optimization





Minimize:

= Design Costs \$ + λ_1*(Water Quality)

Constrained Optimization Function

Minimize: Treatment/O&M Installation

Real Costs = $N_{yrs}\sum_{i=1}^{N_w} q_i F_{treat}$ + $F_{cap}\sum_{i=1}^{N_w}(1-e^{-bq_i})$

Constrained Optimization Function

Minimize: Treatment/O&M Installation

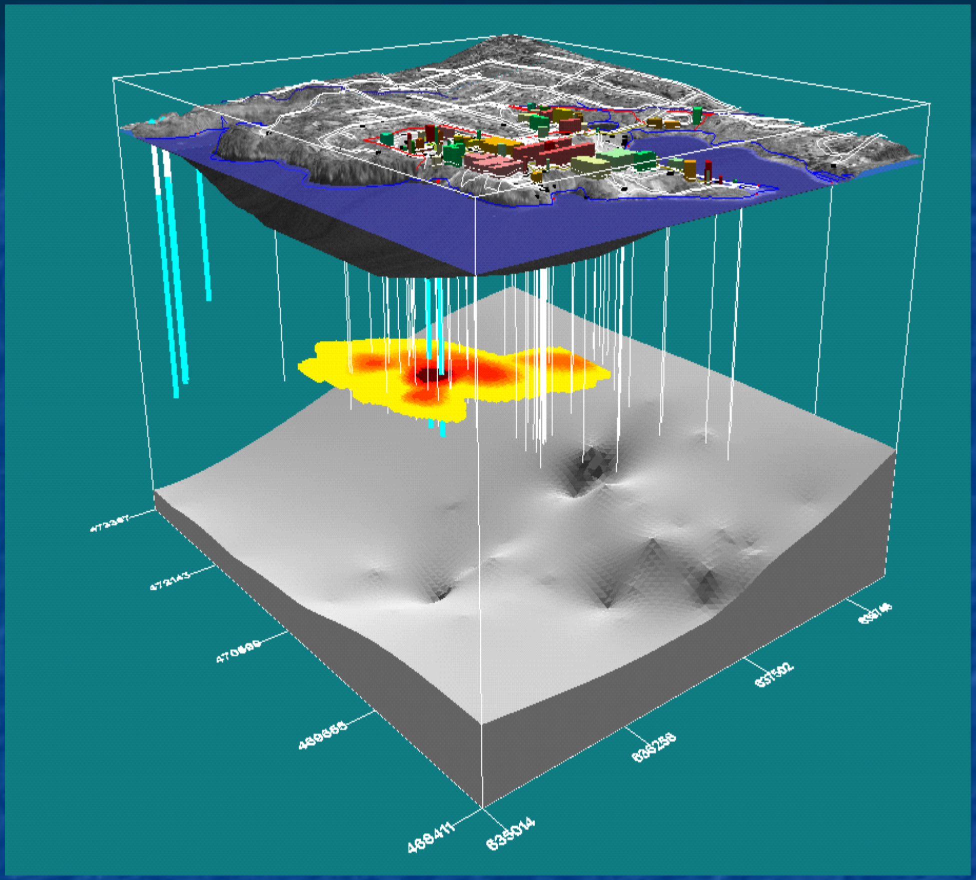
$$\textbf{Real Costs} = N_{yrs}\sum_{i=1}^{N_w} q_i F_{treat} + F_{cap}\sum_{i=1}^{N_w}(1-e^{-bq_i})$$

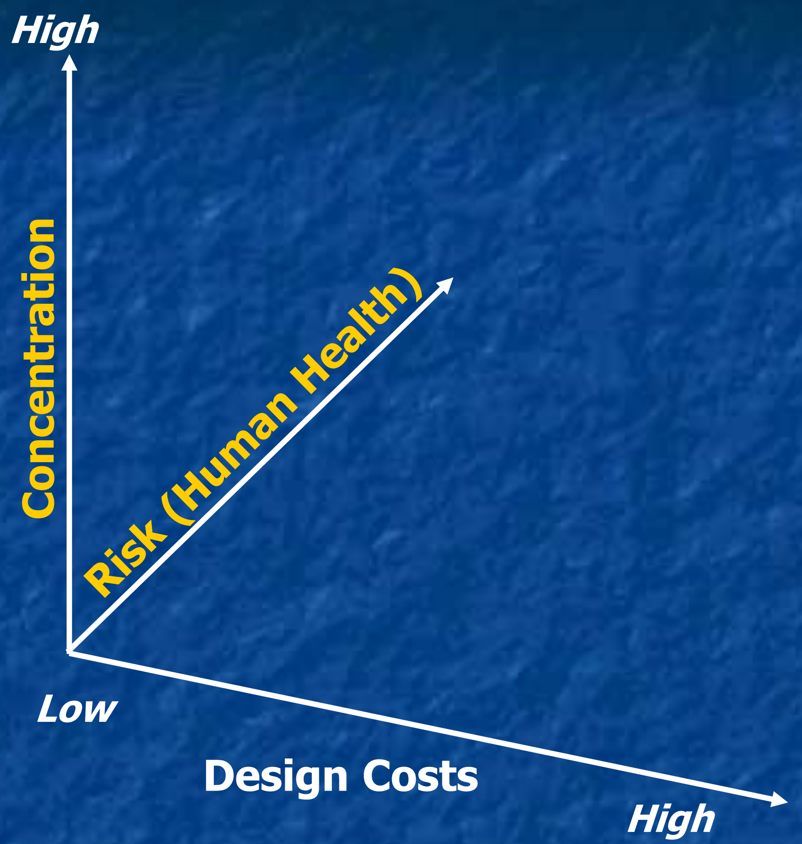
Subject to:

$$C(x_j) \le C^* \qquad j \in J$$

$$q_i^1 \le q_i \le q_i^u \qquad i \in I$$

Unconstrained Multi-Objective Optimization

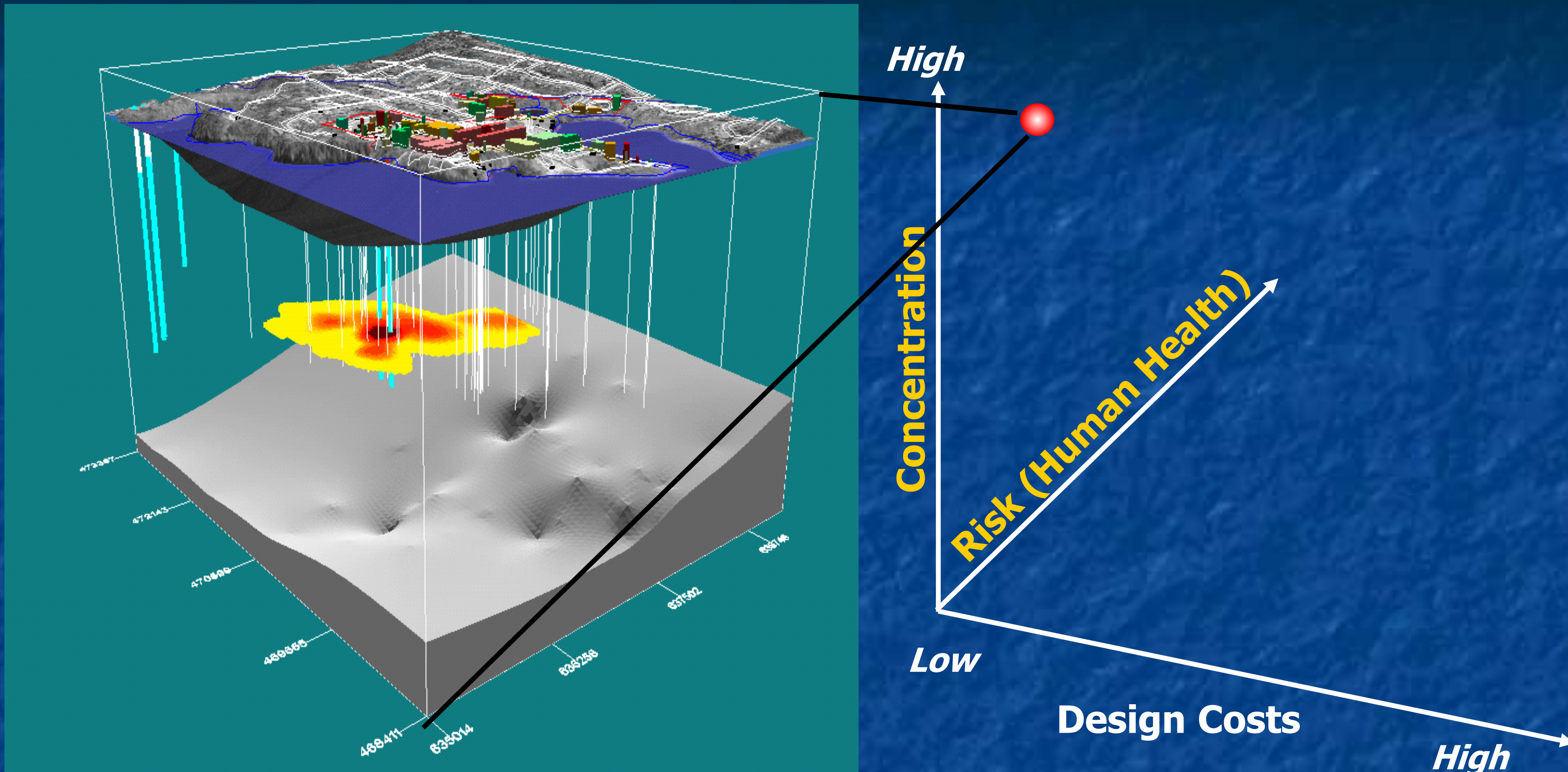




Minimize:

= Design Costs \$ + λ_1*(Water Quality) + λ_2*(Impacts to Environment/Human Health)

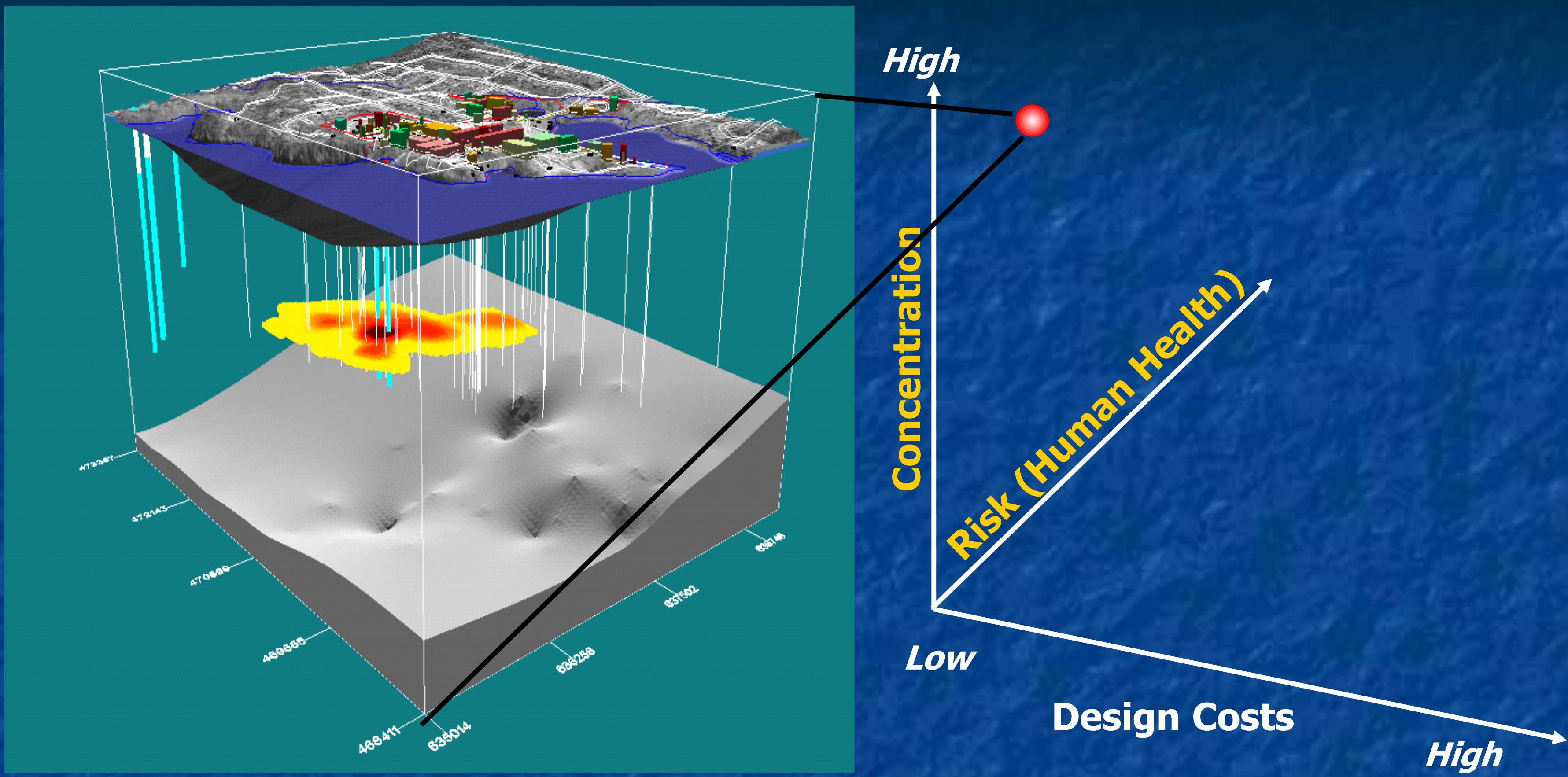
Multi-Objective Optimization



Minimize:

= Design Costs \$ + λ_1*(Water Quality) + λ_2*(Impacts to Environment/Human Health)

Multi-Objective Optimization

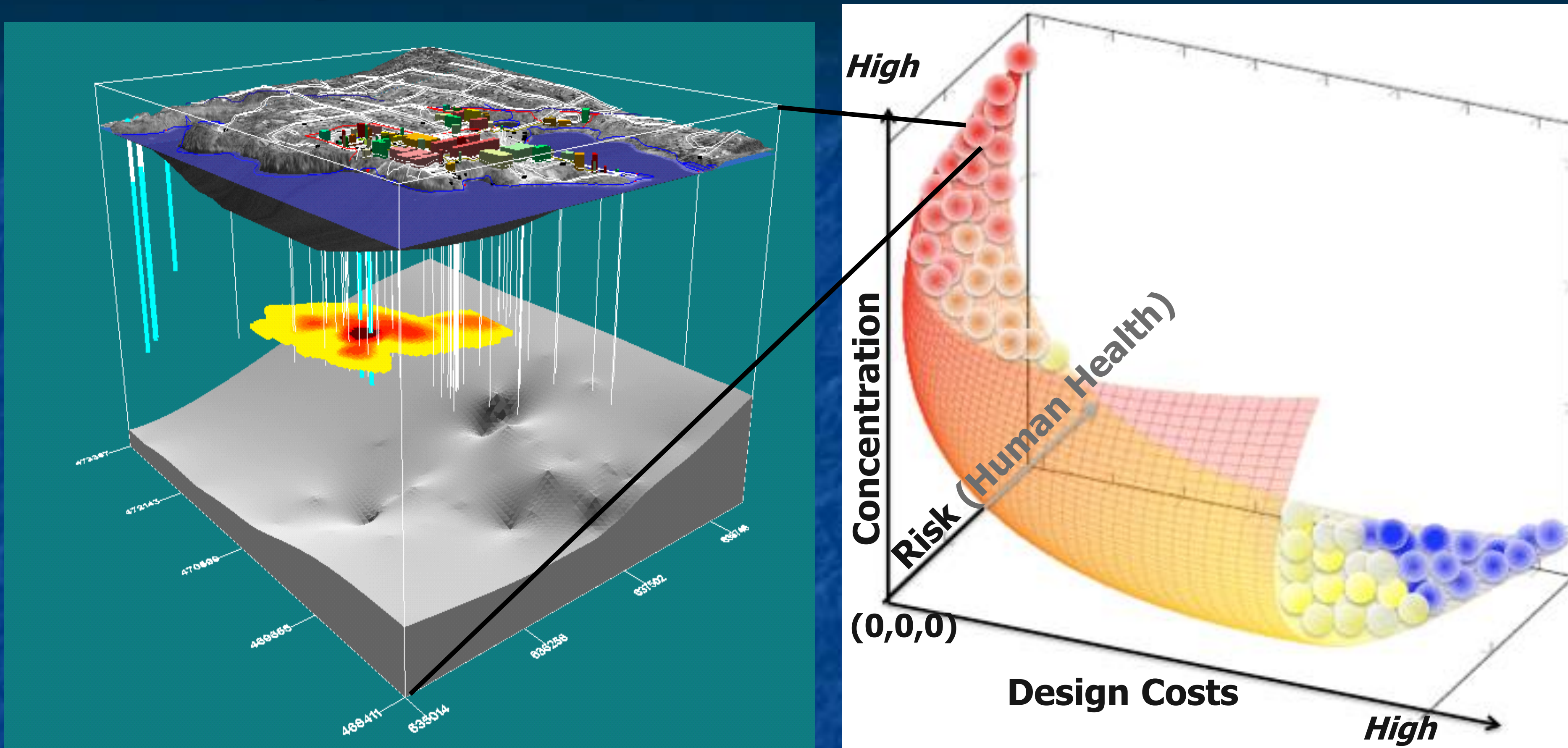


Minimize:

Treatment/O&M   Installation   Clean Water   Location

$$= \sum_{k=1}^{N_p} \sum_{i=1}^{N_w} q_i F_{treat} + N_w F_{cap} + \lambda f(C, C_{MCL}) + \lambda f(\Omega, T)$$

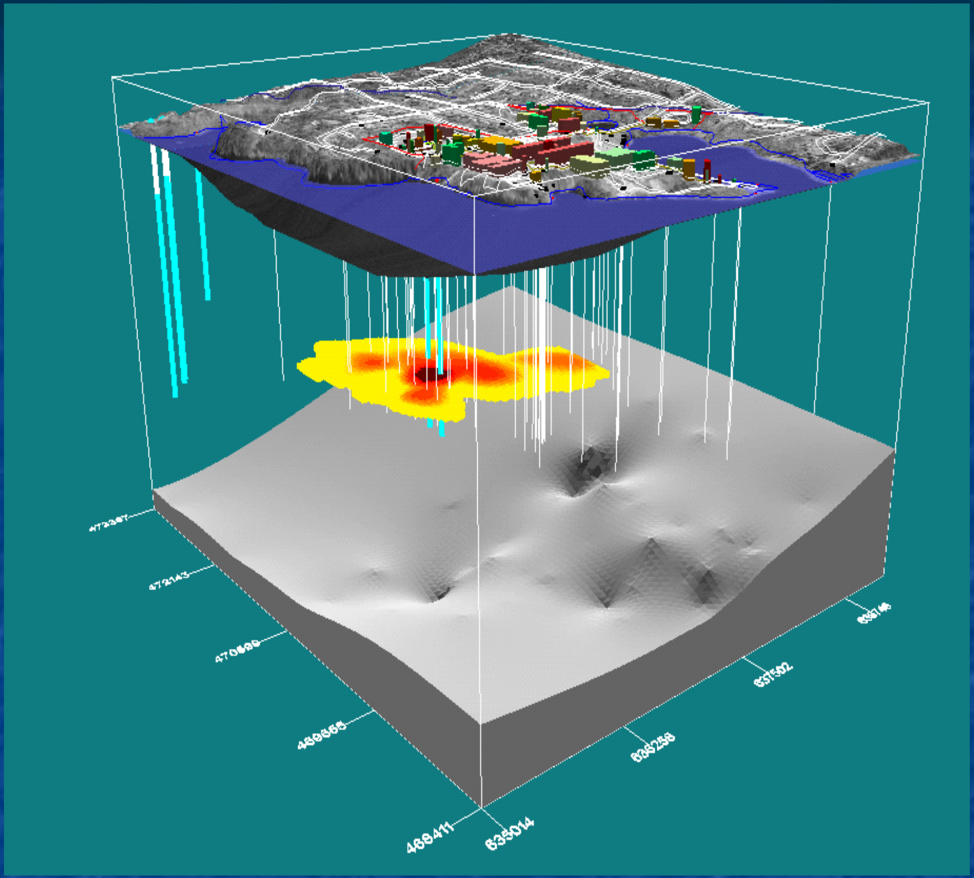
Multi-Objective Optimization

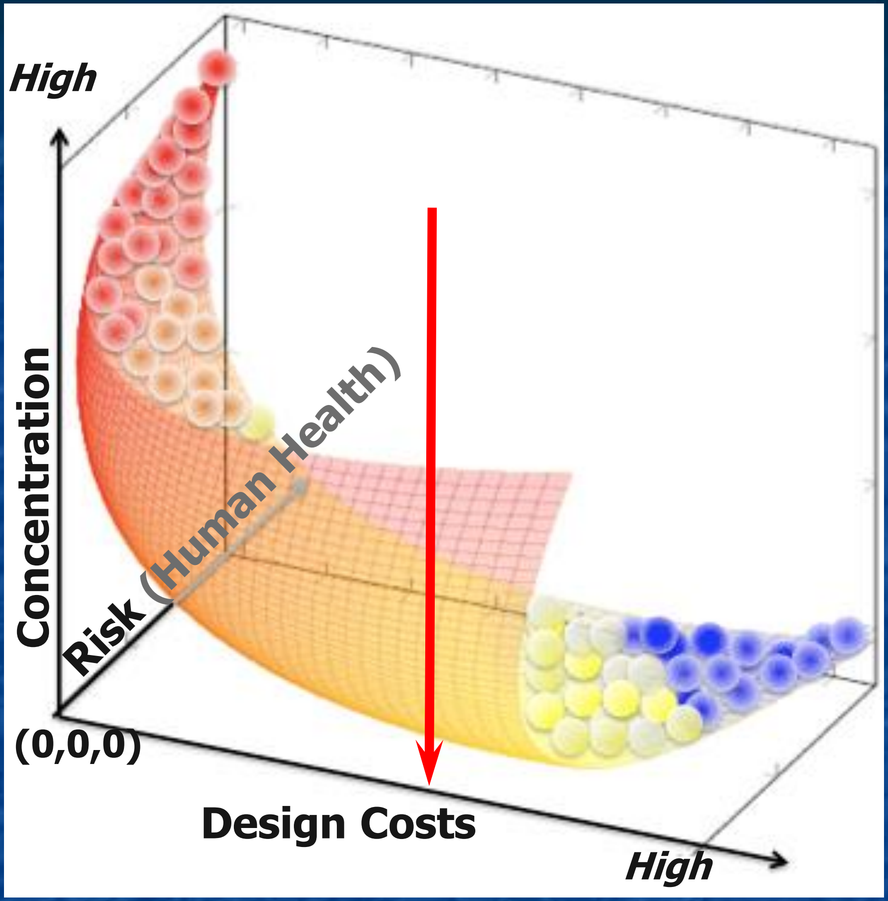


Minimize:

= Design Costs \$ + λ_1*(Water Quality) + λ_2*(Impacts to Environment/Human Health)

Multi-Objective Optimization

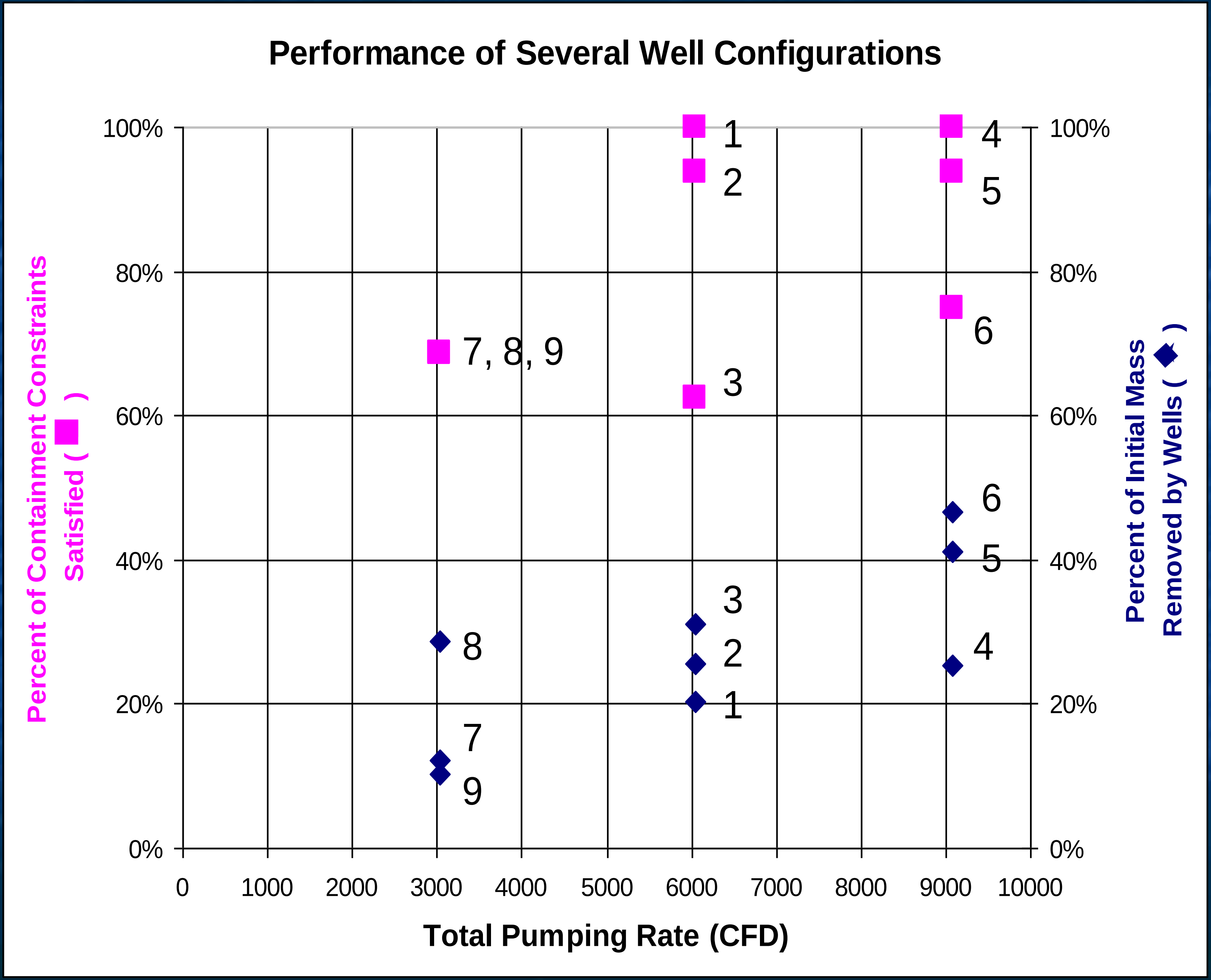




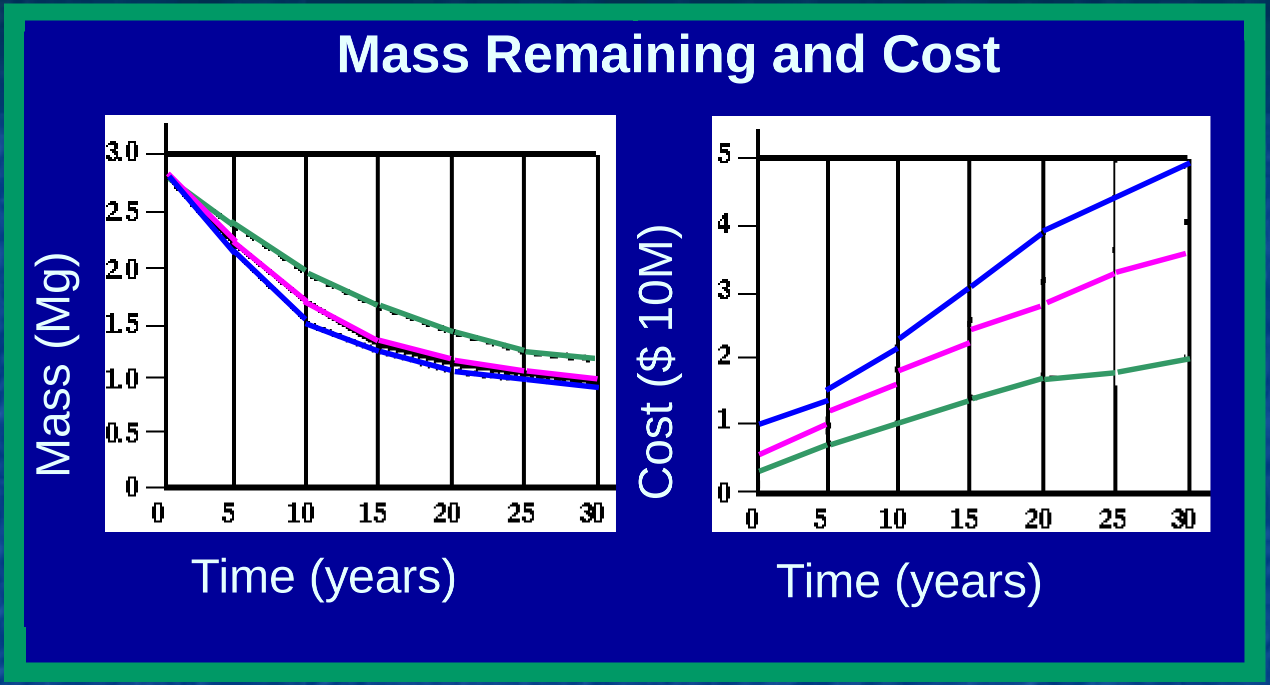
Minimize:

= Design Costs $ + λ_1*(Water Quality) + λ_2*(Impacts to Environment/Human Health)

How to represent Solutions/Results?



Multiple Stakeholder Goals



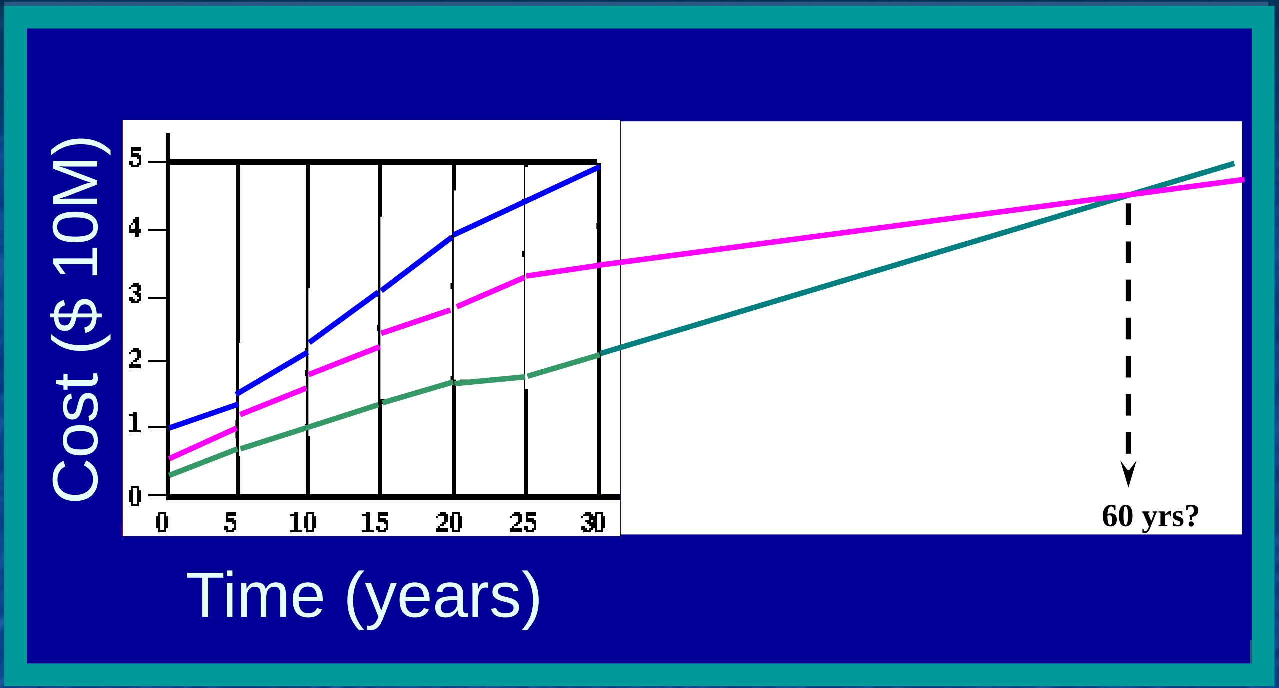
Rizzo and Dougherty, *Water Resources Research*, 30 (2), pp. 483-497, 1994.

$\lambda = 1$ (9 wells)

$\lambda = 5$ (18 wells)

$\lambda = 10$ (28 wells)

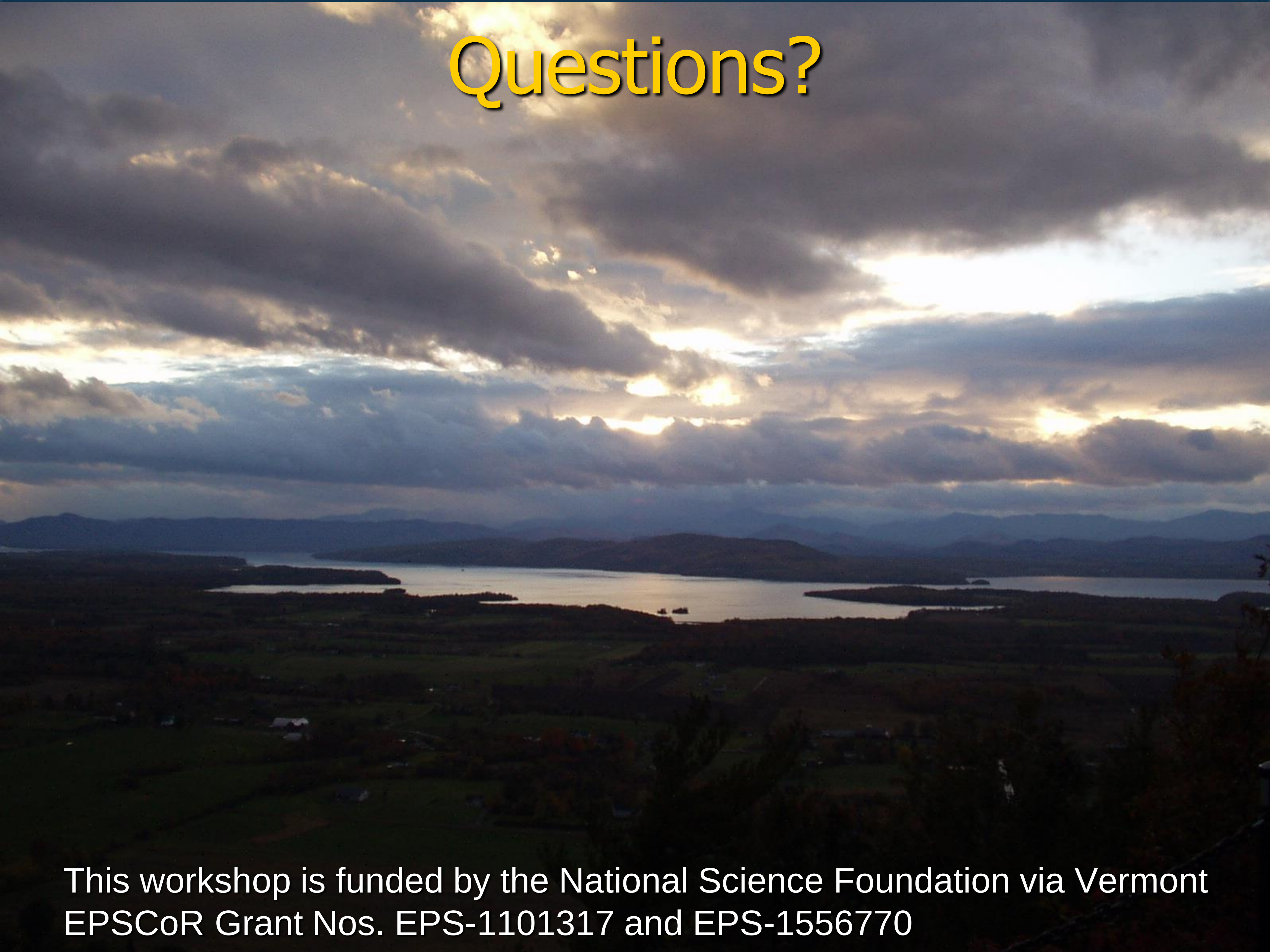
Multi-objective Optimization



Rizzo and Dougherty, *Water Resources Research*, 30 (2), pp. 483-497, 1994.

- Which scheme is “optimal” ?
  - How long do we *really* have to operate?
  - How long do we *really* have to monitor?
  - How much residual risk are we willing to accept?
  - Will a new technology or public policy shift become available?

Questions?



This workshop is funded by the National Science Foundation via Vermont EPSCoR Grant Nos. EPS-1101317 and EPS-1556770

Performance Cost ‘Ratio’

18 wells Multiple Management Periods
(44 ppb; 3,856 Million gals)

18 wells Single Management Period
(45 ppb; 5,635 Million gals)

Table 1. Preliminary Comparison of the Number of Gallons Pumped During Each Management Period Between Multiple and Single Management Periods

Period	Simulation, Years	Number of Wells	Billions of Gallons, per Period	Maximum Concentration, ppb
		Multiple Management Periods		
Initial	0	0	0.000	814
1	5	10	0.585	288
2	10	13	0.729	189
3	15	15	0.808	129
4	20	12	0.657	93
5	25	10	0.578	63
6	30	8	0.499	44
Summary			3.856	
		Single Management Period		
Best 18 wells	30	18	5.635	45

One gallon equals 0.003785 m^3.

Challenges Arise:

- Computational resources needed to accommodate large number of decision variables and constraints

- Formulation of certain physical and operational objectives and constraints into “continuous and differentiable” functions

- Complexities of real decision making and fixed or integer-related costs, non-convex behavior of complicated physical processes