Remediation Optimization: The State of the Art

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June 15, 2004

Motivation

- There is growing interest in optimizing remedial actions to reduce costs, accelerate cleanup and improve performance
- Optimization means different things to different people
  - Professional assessment and improvement of operations
  - Trial and error searching for better solutions
  - Mathematical optimization, which is the focus of this talk

Mathematical Optimization

- Uses a computer to automatically search for the best solution to a problem that you specify
  - Finding the best well locations and pumping rates for a well-based remediation system
  - Finding the best monitoring locations
- Useful tool when many possible solutions exist and it's too time-consuming to examine all of them
- From this point forward, "optimization" refers to mathematical optimization

Optimization Applications

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- Optimization has been applied to find improved solutions at numerous field sites
  - Pump-and-treat design (containment or treatment)
  - Monitoring design
  - Calibrating simulation models
- Consistently found lower cost, more effective solutions
  - Often "out of the box" solutions
  - Savings over trial-and-error optimization in a recent ESTCP transport optimization project ranged from 5 to 50%, with a typical improvement of 20%

Mathematical Optimization Process

- Start with a real-life problem for which you are seeking the “best” or “optimal” solution
- Develop an “optimization formulation” that describes the essential elements of the real world problem *in mathematical terms*
- Select and apply an appropriate methodology to search the potential solution space for an “optimal” solution

Formulation for Optimizing a Groundwater P&T System

- Decision variables
  - Locations of extraction/injection wells
  - Rates at each extraction/injection well over time
- Objective functions could be
  - Minimize cost
  - Minimize cleanup time

Formulation for Optimizing a Groundwater P&T System

- Potential constraints
  - Limits on pumping rates at specific wells
  - Limits on total pumping rates
  - Limits on contaminant levels at target times
- Evaluating these constraints requires running a numerical model
  - If objectives and constraints only involve controlling flows, only need a flow model is needed
  - Otherwise need a transport model also

Formulation for Optimizing a Groundwater Monitoring System

- Decision variables
  - For each monitoring well in each period, whether or not to take a sample
- Objective functions could be
  - Minimize cost
  - Minimize error in the decisions made from the data

Formulation for Optimizing a Groundwater Monitoring System

- Potential constraints
  - Limits on allowable errors
  - Maximum sampling budgets
- Evaluating errors requires a model of how the data will be used
  - E.g., an interpolation model to estimate concentrations or heads with and without particular samples

Solving the Optimization Problem

- Numerous optimization methods exist to search for optimal solutions
- Which one is best depends upon the problem you've formulated
- Most field-scale applications have used heuristic approaches such as
  - Genetic algorithms (GAs)
  - Simulated annealing
  - Tabu search

What's Coming in Optimization?

- More field applications and demonstrations
- User-friendly software
  - MODMAN for flow control optimization with Modflow
  - SOMOS (Peralta) and MGO (Zheng) for transport optimization with Modflow and MT3DMS
- More training short courses
- New applications and improved approaches from the research community

New Applications

- Optimizing other remediation technologies
  - Bioremediation
  - Soil vapor extraction
  - Surfactant flushing
  - Thermal oxidation with pump and treat
- Selecting among multiple possible technologies

Improved Approaches

- Getting solutions faster and more effectively
- Handling multiple objectives
- Considering uncertainty
- Incorporating expert knowledge

Getting Solutions Faster and More Effectively

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- Optimizing remediation systems can sometimes be a challenging process
  - Formulating the problem appropriately
  - Figuring out what optimization approach to use and how to set its parameters
  - When simulation models are time consuming, optimization can take a long time
    - In the ESTCP transport optimization demonstration project,
      - Simulation models took 10 mins to 2 hrs for each simulation
      - Optimization requires 100’s to 1,000’s of simulation runs

Getting Solutions Faster and More Effectively, contd.

- Like numerical modeling, tackling these complexities requires training and expertise
- New approaches are being developed all the time
  - The solution you need may already exist in a research lab
  - Following are some highlights of recent findings from our lab
    - More details can be found at http://cee.uiuc.edu/emsa/research

Case Study: Umatilla Chemical Depot, Hermiston, Oregon

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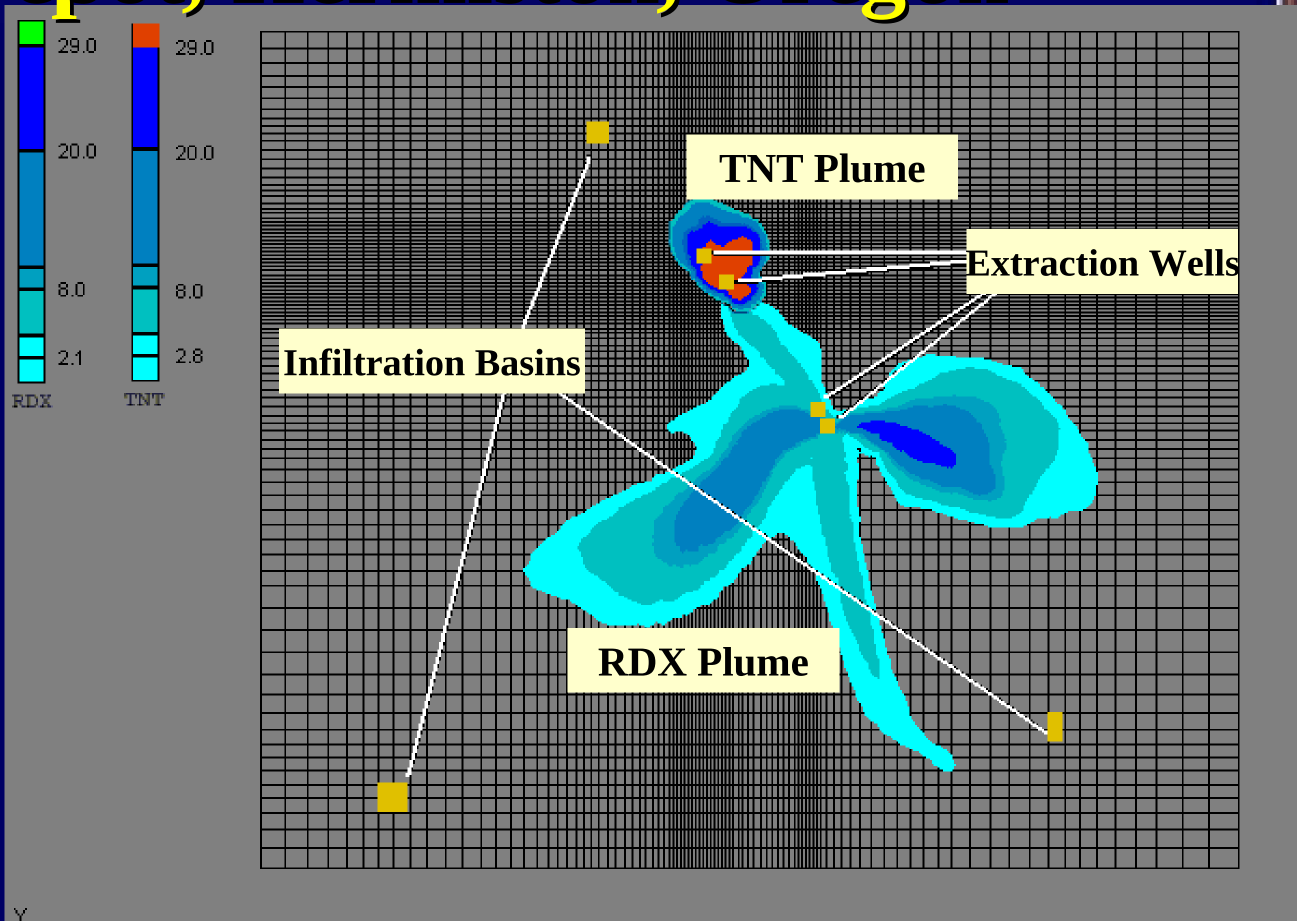
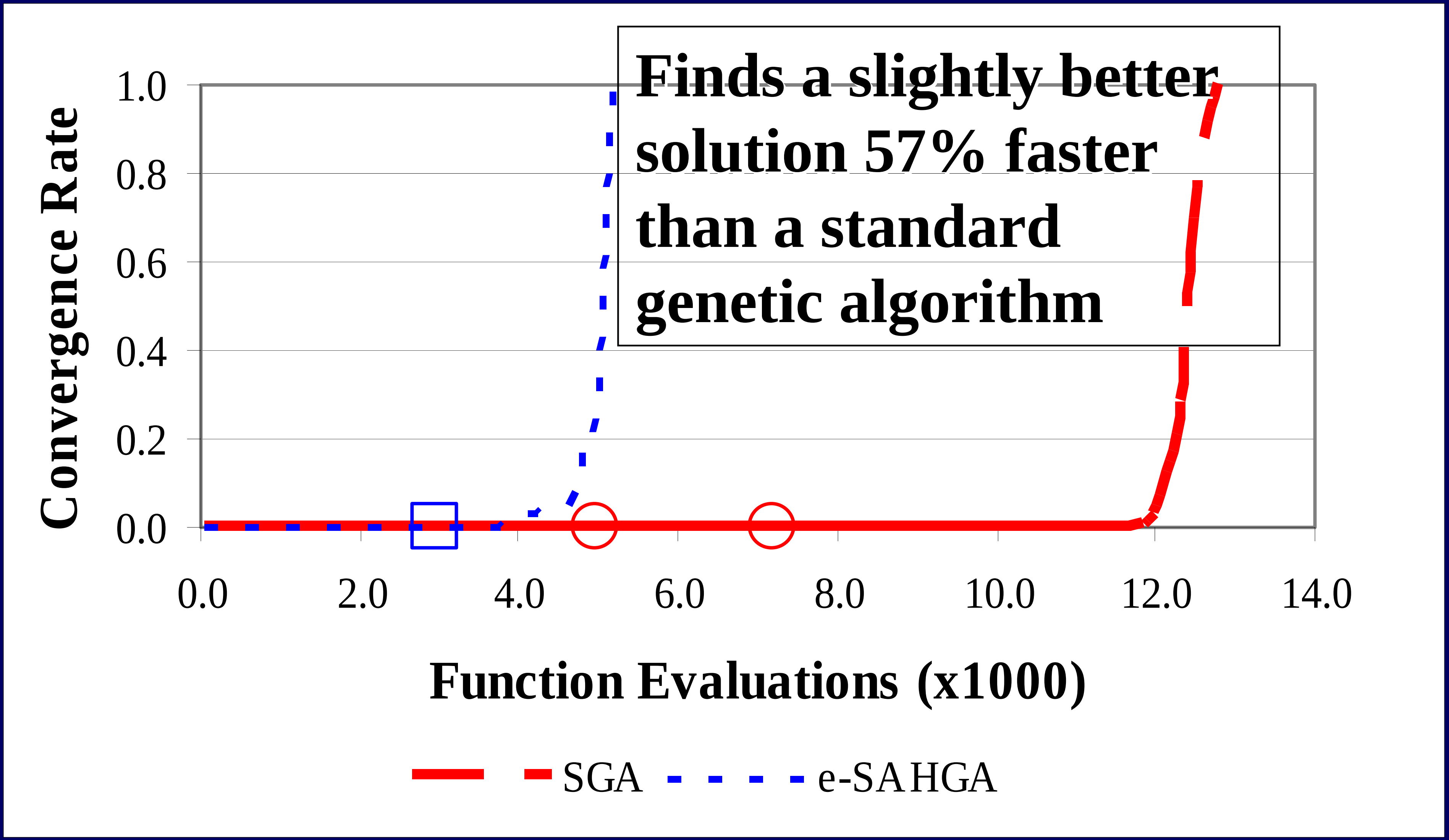
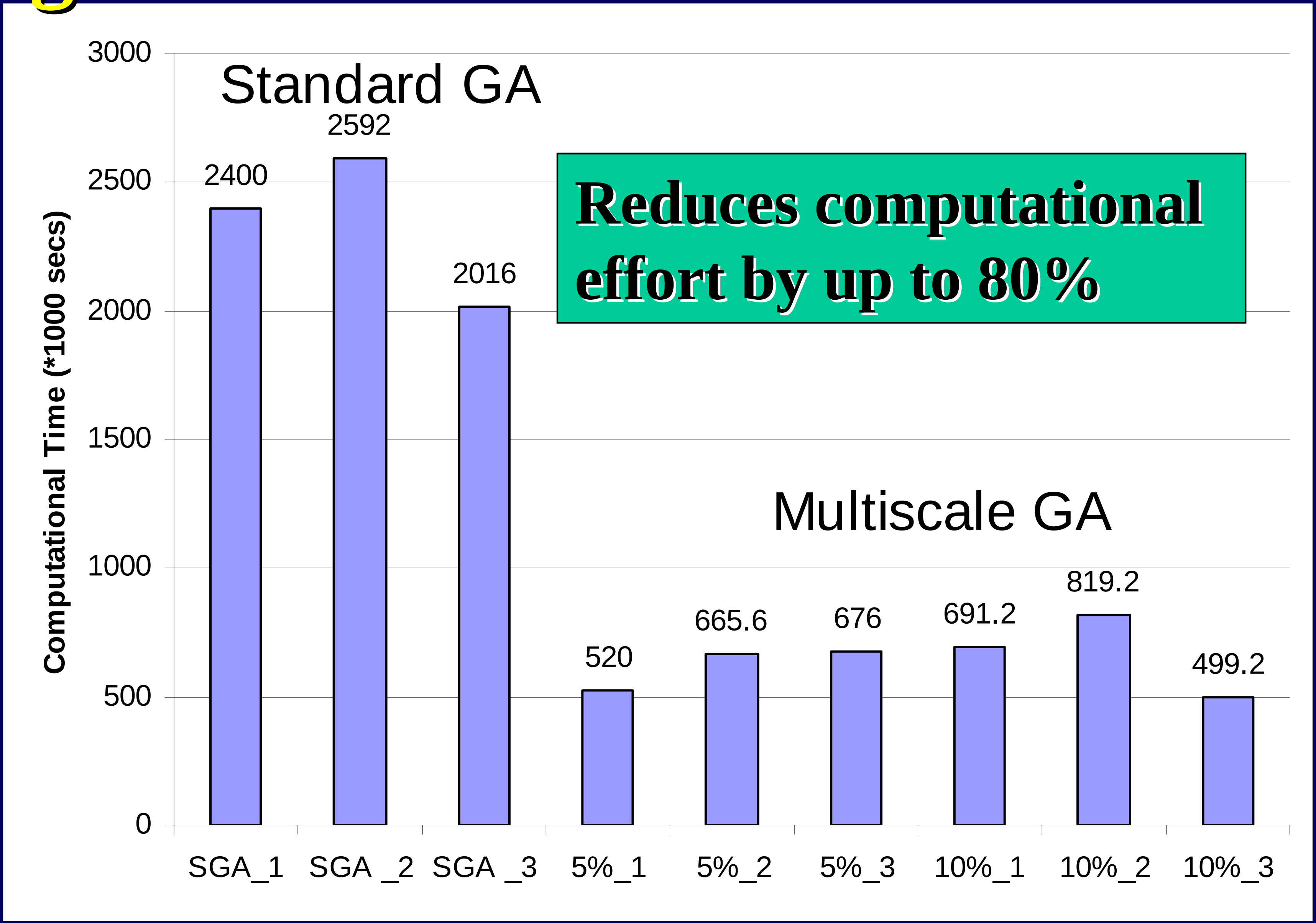


- Military reservation used for storage and handling of munitions 1960s
- Pump & treat system to treat RDX and TNT
- First site in the ESTCP transport optimization demo

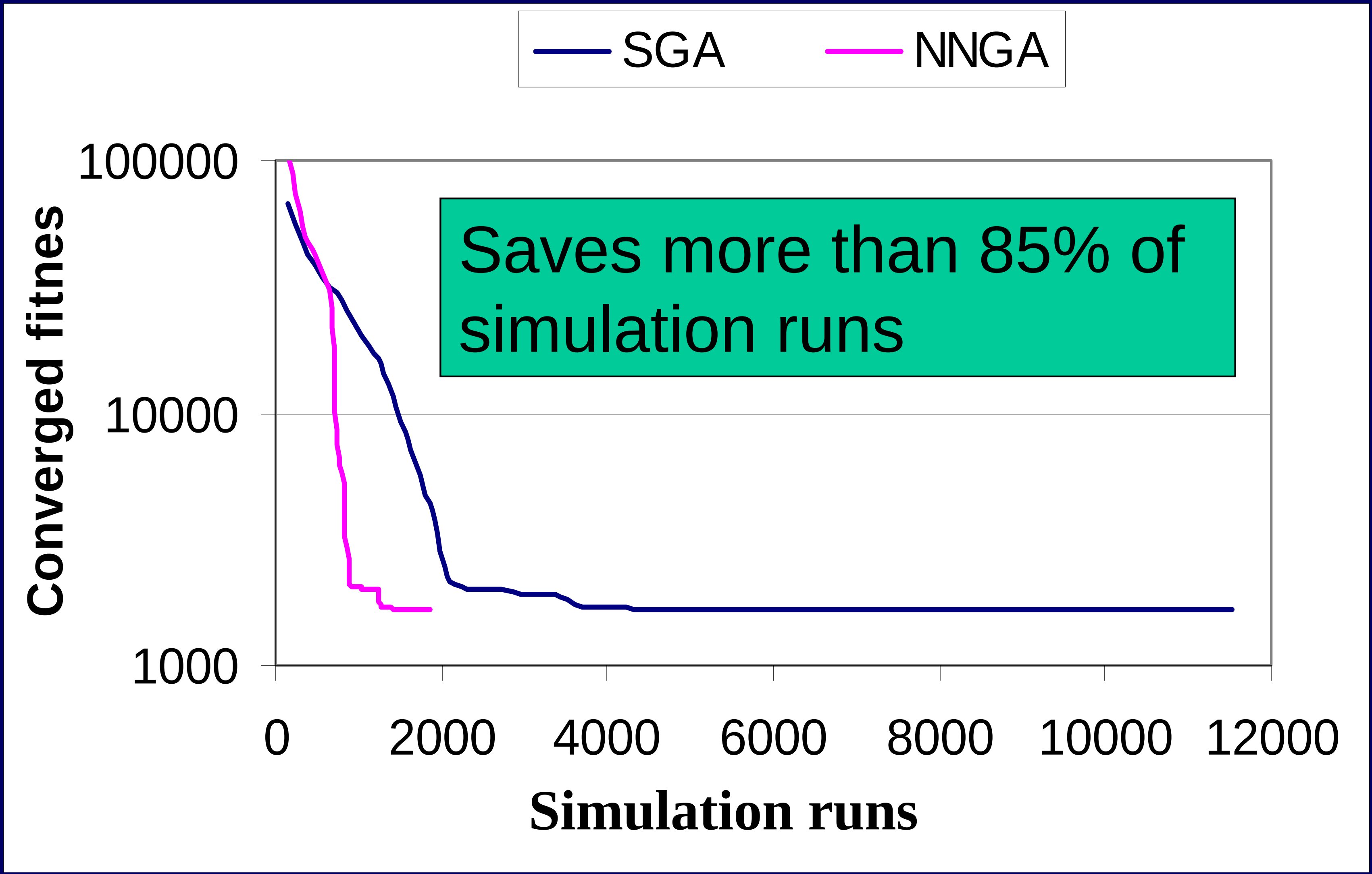
Hybrid Genetic Algorithm



Multiscale Genetic Algorithm



Adaptive Neural Network Genetic Algorithm



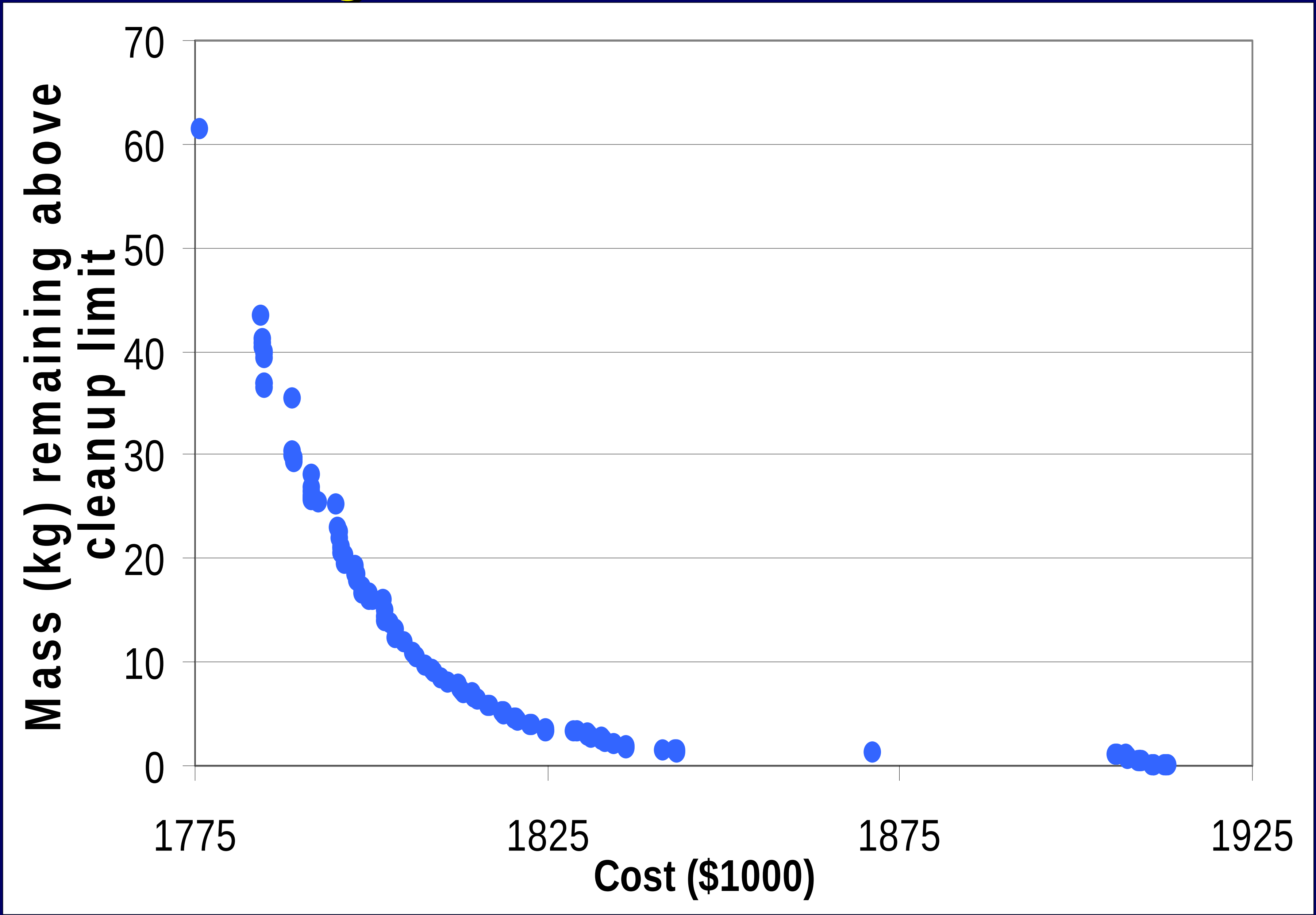
Guidance for Setting GA Parameters

- Setting optimization parameters appropriately can make the difference between success and failure of the optimization effort
- To help practitioners better set their parameter values, we developed guidance based on GA theory
  - See http://cee.uiuc.edu/research/emsa for details

Handling Multiple Objectives

- Many remediation problems have multiple objectives. For example, at Umatilla,
  - Two objectives are important:
    - Minimize cost
    - Maximize mass removal to cleanup levels
- New multi-objective genetic algorithms allow tradeoffs among multiple objectives to easily be considered

Optimal Tradeoffs Among Umatilla Objectives



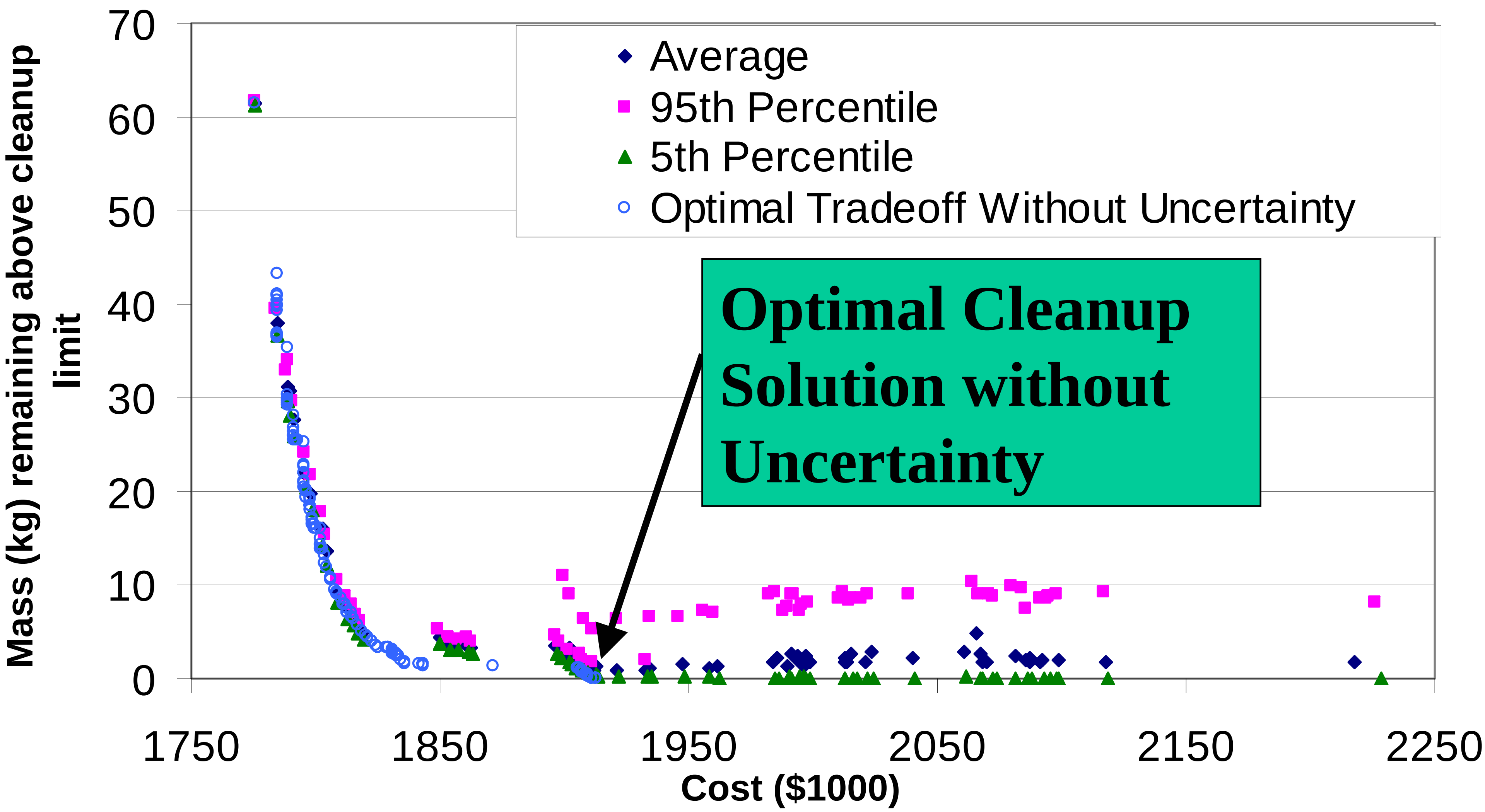
Considering Uncertainty

- Optimization efforts are usually based on models, which can have substantial uncertainty
  - Hydraulic conductivities
  - Locations of source areas
  - Preferential flow paths, such as root holes
- Many optimization approaches exist that can find solutions that will be more robust to uncertainty that can be quantified

Characterizing Uncertainty

- Finding optimal solutions that consider uncertainty requires that the uncertainty be characterized
- Can range from simple approaches to highly complex
  - Simple: Create multiple parameter values or models that represent the expert's best judgment
  - Complex: Full stochastic groundwater models, with conditional simulation

Multi-Objective Results Under Uncertainty



Incorporating Expert Knowledge

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- Many problems have objectives or constraints that cannot be put into mathematical form
  - Hydrogeologic insight
  - Social or political issues
- Emerging interactive approaches allow experts to guide the search to meet these and more traditional objectives
  - Rate initial solutions that optimizer finds
    - Optimizer learns what types of solutions meet objectives
  - Suggest alternative solutions to the optimizer

Incorporating Expert Knowledge, contd.

- We are in the early stages of exploring how these approaches can be used most effectively for remediation optimization
  - Applying to long-term monitoring optimization and model calibration
- Has been successfully used for many other applications:
  - Criminal face recognition
  - Hearing aid fitting
  - Jazz improvisation – hear a musician "trading eights" with the computer (8 measures)

Conclusions

- Mathematical optimization has been shown to provide substantial benefit for remediation design
- These approaches are meant to be another tool in the analyst's toolbox, but not to replace the analyst!
- New software and emerging methods will bring exciting opportunities for further improvements in the future
  - Want to know more? Come to the annual Environmental & Water Resources Institute World Water and Environmental Resources Congress (Salt Lake City 6/28-7/1/04, Anchorage 2005)

Acknowledgements

- Research funded by U.S. Army Research Office Grant No. DAAD19-001-1-0025, and U.S. Department of Energy Office of Science (BER) under Grant No. DE-FG07-02ER63502
- Major student contributors were Felipe Espinoza, Abhishek Singh, Shenquan Yan, Meghna Babbar
- Dr. David Goldberg and Dr. Hideyuki Takagi contributed ideas and advice on GAs
- For the Umatilla case,
  - Dr. Bruce Loftis and Shenquan Yan implemented the case on the pre-production Teragrid (funded by NSF grant no. ACI 0122296)
  - Andrejs Dimbirs and Richard Smith from US Army Corps of Engineers and Dr. Albert Valocchi helped with uncertainty analysis
  - Dr. Chunmiao Zheng helped with MODFLOW and MT3DMS