Simulation and Optimization of Integrated Ground and Surface Water Resource Systems

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Introduction

Physics-Based Management Optimization (PBMO)
- Water Resources Support (WRS) Simulation / Optimization Tool Kit

Optimization Formulation
- General formulation
- Lipschitz Global Optimizer (LGO) solver suite for nonlinear optimization

Site Examples:
- Large-scale physics-based water resource simulations
- Water resources simulation / optimization

Optimization using HydroGeoSphere (HGS) and LGO: current status
Why Physics-based Water Resource Optimization?

- Competing water allocation needs: agriculture, reservoirs, recreation, etc.

- Future IPCC planning scenarios involving climate change
  - Scenarios outside historical observations

- Decision making under resource constraints is a key paradigm in strategic planning, design, and operations

Optimization: an act, process, or methodology of making something (as a design, system, or decision) as fully perfect, functional, or effective as possible; specifically: the mathematical procedures (as finding the maximum of a function) involved in this. Source: Merriam-Webster Online Dictionary
Why Physics-based Water Resource Optimization?

- Increased reliability of proposed resource management solutions
  - Conserves mass
- Increased stakeholder interaction
- Better understanding of the challenges and viability of decisions
- Increased confidence in solution process
- Reduced system performance risk
PBMO Medallion™ Coupling Concept

Global Optimizer (1st Half of the Medallion)

Graphical User Interface

A

Physics-Based Calibrated/Data Fused Model (2nd Half of the Medallion)

B

C

D

E

Stakeholders

Optimal Decision Strategy

Legend

A  Optimization
Specification Input

B  Modeling
Requirement Input

C  Scenario
Specification Input
System Performance
Prediction

D  Global Optimal Solution
Water Resource Optimization: Using HGS and LGO

Approach:

- Integrates optimization algorithms and physics-based models
  - Realistically captures important site physics and financial constraints
  - Uses state-of-the-art, robust optimization methods
  - Achieves coherent interpretation of disparate site data using all relevant information
  - Produces structured, credible solutions

Benefits:

- Optimal solutions honor site physics
- Transparent and reviewable
- Results updated in real-time
  - Estimates of system performance with quantified knowledge uncertainty
- Considers availability of resources and demands
- Optimal strategies: maximize benefits of resources
Global Optimization

Illustrative Objective Function (Response Surface) and Decision Variables. The feasible set is the 2-D rectangle formed by the range of the decision variables, the objective (cost) function $f(x)$ is the height of the response surface.

The objective of global optimization is to find the absolutely best solution, in the possible presence of a multitude of local sub-optimal solutions.
LGO Solver Suite for Nonlinear Optimization

▼ LGO is a suite of global and local nonlinear optimization methods in an integrated framework
▼ Global search methods (solver options):
  • Continuous branch-and-bound
  • Adaptive random search: single-start or multi-start
  • Exact penalty function applied in global search phase
  • Mixed integer nonlinear model: extension in progress
▼ Local optimization follows from:
  • Best global-search based point(s)
  • User-supplied initial point
  • Optimization by the generalized reduced gradient method

Lipschitz Global Optimization

General model formulation:

▼ Minimize the objective function $f(x)$

▼ Subject to the constraints $x \in D := \{x_l \leq x \leq x_u; g(x) \leq 0\}$

▼ Lipschitz continuity: $|f_j(x_1) - f_j(x_2)| \leq L_j \|x_1 - x_2\|$
  
  • In words, the slope (variability) of the function values is bounded with respect to the system input variables ($x$)

▼ Key generic feature of our optimization models and solvers:

  • For all “reasonable” model input arguments the model function values can be computed (using HGS)
  
  • LGO does not require higher-order model function information
Global Optimization Using LGO

An example: Complex response function successfully solved by LGO

LGO is able to analyze and to solve complex nonlinear models, under minimal analytical assumptions. Computable values of continuous or Lipschitz model functions are needed only, without requiring access to higher-order information handled by LGO.

Broad application scope meets the needs of real-world optimization

“Theorists interested in optimization have been too willing to accept the legacy of the great eighteenth and nineteenth century mathematicians who painted a clean world of [linear, or convex] quadratic objective functions, ideal constraints and ever present derivatives.

The real world of search is fraught with discontinuities, and vast multi-modal, noisy search spaces…”

D. E. Goldberg, genetic algorithms pioneer
Motivation for Integrated Simulation and Management Optimization Tools

- **Primary Challenges**
  - Interaction of surface and subsurface flow systems over a basin
  - Drought and land surface subsidence
  - Wetlands and ecosystem health
  - Water quality
Candidate Scenarios for Optimization of HGS-derived Simulations

- Quantify spatial/temporal distribution of subsurface recharge, surface-subsurface interactions in streams and wetlands
- Impacts of subsurface water extraction on surface water
- Effects of urbanization/land-use/climate change on water quantity & quality, health of aquatic ecosystems
- Restoration of adversely-impacted streams, wetlands, etc.
- Subsurface versus overland migration pathways of contaminants & pathogens
Water Resources Support (WRS) Tool-kit
Optimization Applicability

▼ Water supply systems
▼ Design of hydraulic structures
  • Reservoirs
  • Dams
  • Levees
  • Pump storage
▼ Selection of alternative water resource management options
  • Control of salt water intrusion in coastal aquifers
  • Watershed and groundwater source allocation, distribution and reuse
  • Well field design and operation
  • Design of water quality monitoring networks
  • Thermal distribution and impacts
▼ Renewable energy
  • Integrated hydropower energy generation and resource planning
  • Solar salt ponds
Large-Scale Simulation and Optimization

▼ Simulation
  • Large-scale simulation has been routinely used for design of water resource civil works projects for at least the past 30 years
  • Significant advancement in both algorithms and computer power has enabled use of larger and more complex (fully integrated) physics models.

▼ Optimization
  • Optimization of water resource projects routinely used for at least 30 years
  • Optimization algorithms have become more robust and smarter, requiring fewer function calls to provide a credible estimate of the globally best decision

▼ Hardware and software developments
  • Additional positive impact
Simulation Example 1: Manasquan, NJ Reservoir, River and Estuary System

- **Design of pump storage drinking water reservoir**

- **Issues:**
  - Maximize dependable yield
  - Water resource sustainability
  - Water quality of reservoir and estuary

- **Results:**
  - Reservoir built, operates as designed with excellent water quality

Relevance: reservoir, stream, estuary/delta, ocean water quantity and quality interactions (1984)
Simulation Example 2: Model Development for Evaluating Boston Sewage Outfall Impacts

Model development and simulations
- Boston Harbor
- Gulf of Maine
- Atlantic Ocean

Issue:
- Couple BOD & DOD calculations to predict water quality

Results:
- Model performed as designed (MIT-TEA_ELAL)
- Used by others for subsequent design studies

Relevance: oceanic (off-shore) water quality impact distribution and quantification (1985)
Simulation Example 3: Solar Salt Pond (R&D)

- Solar-powered electrical generation for deployment in the:
  - Qattara Depression
  - Southern California

- Issue:
  - Stability of the freshwater / saltwater interface due to wind shear

- Result:
  - Demonstrated solar salt ponds are a viable technology

Relevance: Coupled energy and environmental resource analysis: generates electricity but requires fresh water (1982)
Energy and the Environment
Integrated Simulation and Optimization

Power Grid Performance Optimization (2009)
Global Energy Transition Model (2010)

Relevance: simulation / optimization of integrated systems with transmission constraints, resource distance from point of use, and water, energy, agriculture and transportation synergies and competition
Additional Examples: Simulation-Optimization Using LGO and Physics-based Models

▼ Model Calibration
- Sediment-water interaction (shallow lakes)
- River flow, chemical and particulates transport
- Phosphorus release from sediments
- Aquifers
- Munitions and explosives of concern (MEC) Identification

▼ Management Options
- Industrial wastewater treatment optimization
- Multiple-source river pollution management
- Lake eutrophication management
- Risk management of accidental water pollution
- Aggregation of expert opinions

When Models are not Available: Derive Using Genetic Programming

**Inputs**

- Site-specific inputs include any aspect deemed important by the design team.
- Genetic programming (GP) is utilized to uncover the relationships necessary to understand the process.

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**Actual vs. GP Model Predictions**

- % Contaminant Response vs. Rank-ordered data

![Chart showing Actual vs. GP Model Predictions with Target and Model lines]

HGL HydroGeology, Inc.
Chemical Response Predictive Model Code

Complete Model Code (developed in Fortran):

Converting to mathematical equation for interpretation, acceptance, or refinement

```fortran
real function model(d)

  ! Parameters
  real, parameter :: G1C0 = 2.450073
  real, parameter :: G1C1 = -1.999177
  real, parameter :: G2C0 = 9.462036
  real, parameter :: G2C1 = 6.572907
  real, parameter :: G3C0 = -3.264129
  real, parameter :: G3C1 = -3.080017
  real, parameter :: G4C0 = -5.827912
  real, parameter :: G4C1 = -5.046691

  ! Variables
  real :: varTemp

  varTemp = 0.0
  varTemp = ((d(7)/d(14))-(log(d(16))-d(0)))
  varTemp = varTemp + (((d(13)+d(13))-
                       (((d(16)*G2C1)+(d(18)*G2C0))*d(17)))**(1.0/3.0))
  varTemp = varTemp + (G3C0/d(5))
  varTemp = varTemp + ((G4C0/d(14))-(d(2)-d(0)))

  model = varTemp

end function model(d)
```

Model Attributes & Value

- Developed using GP Procedure
  - Inductive algorithms design program structure and constants concurrently
  - Provides important inputs
  - Provides an understandable relationship for peer review and acceptability

- Predictive module can be used as stand-alone or incorporated into flow and transport model

- LGO is used to optimize the estimates of the model parameters, the system performance and decisions

GP derived relationship
Simulation and Optimization Tools for Optimal Design

▼ Primary Designs
• Spreadsheet models with plug-in optimizers
• Empirical relationships and/or machine learning for process approximation

▼ Full Designs
• Physics-based surface water and subsurface model (Flow and Transport)
  • HGS
• Global and local optimization algorithms
  • LGO

▼ Uncertainty Analysis
• Monte Carlo / Latin Hypercube / Experimental Design
• Geostatistical and weather relevant libraries and databases
• IPCC forecast scenarios

▼ Optimal State Estimation
• Kalman Filter Model Performance Optimizer (KF_MPO)
  • Reduces frequent need for model calibration updates

Goal: Build on previous simulation / optimization experience, customize for HGS and relevant BOR issues
Simulation and Optimization: Using HGS and LGO

- Successfully completed large-scale relevant projects
- Tools and approaches are problem-dependent
  - HGS and LGO selected for the applications discussed
  - Linkage of these tools is in progress
- Keys to success
  - Efficiency and effectiveness of both the simulation models and the optimization algorithm
  - Practical and prudent to approach a simplified problem initially; add details / complexity as needed
Thanks for your attention!

Questions and comments welcome. Please contact us for further information:
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