

Optimizing management of nonlinear flow and transport in groundwater and surface water systems

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Abstract Software for formally optimizing groundwater and conjunctive water management has improved dramatically in recent years. Demonstrated integrated capabilities include a range of classical and heuristic optimizers, and of simulator and surrogate simulator (response matrix, surface, neural network) techniques. Different combinations of optimizers and simulators are best for different optimization problems—surface water and groundwater quantity and quality management, and for problems of varying degrees of nonlinearity. Recently developed hybrid and robust algorithmic approaches are useful for optimizing management of the more nonlinear systems. These include: deterministic and stochastic flow and contaminant transport in groundwater; and in linked reservoir-river-aquifer systems.

Key words management; groundwater; optimization; simulation/optimization; S/O; SOMOS; conjunctive; remediation; planning; heuristic; evolutionary; stochastic

INTRODUCTION

Simulation/optimization (S/O) models can develop optimal water management strategies for posed optimization problems. A S/O model links a simulation module (that predicts system responses), with an optimization module (that computes the best strategy for the problem, scenario, or formulation).

A pumping (groundwater management) strategy is a set of spatially and possibly temporally distributed groundwater extraction rates. An optimal strategy is mathematically the best that can be developed for a posed problem.

Modellers must input management strategies into simulation models (here termed S models, and all data needed to adequately describe the physical system within the S model. S models (such as MODFLOW and MT3DMS) predict how the modelled physical system will respond to a strategy input by the user.

A S/O model user must input data to describe the physical system and the management problem, but does not need to provide the management strategy—that is what they output. S/O models must incorporate S models or surrogates.

The ease with which optimal strategies are exactly applied in the field depends on how easily decision variables are actually controlled by management. Sample decision variables include groundwater extraction and injection, surface water diversion and return flow, irrigation application, and reservoir release. The more controllable the decision variables, the more likely the optimal strategy is to be implemented directly. Peralta (2001) and Peralta *et al.* (2003) list examples applying optimization in complicated groundwater contamination remediation pump and treat (PAT) system design and operation. They report that all constructed systems have operated successfully.

S/O modelling can also be useful for situations in which decision variables are not directly controllable by managers in the field. For example, regional plans and policy decisions can be significantly affected by S/O modelling results (Das *et al.*, 2004; Peralta, 2004). At the least, in such cases an S/O model can predict the most favorable result of implementing a particular policy.

This paper describes S/O applications to nonlinear systems that use single or multi-objective heuristic optimization (HO) to increase likelihood of achieving globally optimal solutions. To reduce computer processing time, some employ artificial neural networks (ANNs) as surrogate simulators, or are hybrids.

APPLICATIONS

Case I. HO with S model and ANN simulator for contamination remediation

Peralta *et al.* (2003, 2004) describe optimal design of PAT systems for three formulations for remediating a 7 mile long plume of trichloroethylene (TCE) and associated trinitrotoluene (TNT) at the Blaine Naval Ammunition Depot (NAD), in Hastings, Nebraska. The simulation model had over 66912 cells and required 1.5 hours for one MODFLOW and MT3DMS simulation. Optimization problem formulations required simultaneously determining optimal pumping strategies for six five-year periods and 12 to 25 wells. They used S model and ANN simulators, and genetic algorithm (GA), simulated annealing (SA), and tabu search (TS) optimizers. SOMOS advanced features speed convergence to optimality and can reduce the number of needed simulations by almost 50 percent.

Our team had three months to develop optimal strategies for all three formulations using Simulation/Optimization Modelling System, SOMOS, (SSOL, 2001; Peralta, 2003). Simultaneously, an experienced consultant team used the same MODFLOW and MT3DMS simulation models and the normal S model trial-and-error approach to design strategies for the same optimization problems. Both teams used the same post-processor to evaluate the results and compute the objective function value for each formulation.

SOMOS-developed strategies were 20-33 percent better for the three formulations than the designs developed by trial-and-error. This is representative--for eight sites at which our S/O-developed strategies were compared with others developed by trial-and-error, generally our S/O strategies are 20-40 percent better.

Case II. HO with ANN simulator for multi-objective conjunctive use

Fayad & Peralta (2004) report using multi-objective GA with ANNs for optimizing conjunctive use in a hydraulically connected reservoir-stream-aquifer system. This approach reduces computer processing time and provides trade-off curves and surfaces for hydropower, water cost, and water delivery goals.

Case III. HO for maximizing yield with salt water intrusion constraint

An advanced SOMOS version can use any simulation model, not merely MODFLOW and MT3DMS. Coupling with SEAWAT, a density dependent flow simulator, allows one to maximize groundwater extraction near a salt water interface, subject to constraints on concentration of water being extracted.

Case IV. Stochastic HO maximizing robustness & minimizing cleanup cost

Peralta & Kalwij (2004) demonstrate simultaneous multiple-realization optimization to increase the robustness of min-cost optimal strategies. For Umatilla Army Ammunition Depot in Oregon, deterministic methods found hundreds of well locations yielding the

same \$1.66M least-cost to remediate Royal Demolition Explosive (RDX) and TNT. However, strategies were only robust for a small change in global hydraulic conductivity values. Their new robust optimization greatly increased strategy robustness without increasing cost.

SUMMARY

Nonlinear optimization problems exist for a wide range of water management issues. These include the relatively easily-addressed nonlinearity of unconfined aquifers and flows addressed via piecewise-linear functions. Much more nonlinear are state-variable based response surfaces derived for multiple-realization problems.

Often, optimization difficulty increases as nonlinearity increases. Increased difficulty translates into more simulations being required, longer optimization run times, and less certainty in achieving near-global optimality.

Nonlinear optimization efficiency is improved by methods that reduce the number of simulations, or search the solution space more effectively. Example hybrids combining GA, SA, TS, and/or ANN can significantly speed nonlinear optimization. Such hybrid HOs are effective for nonlinear contamination remediation, conjunctive use, stochastic, and salt water intrusion management.

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