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Aggregated surrogate simulator for groundwater-surface water management via simulation-optimization modeling: Theory, development and tests

Bassel Timani, Richard Peralta*

Civil and Environmental Engineering Department, Utah State University, Logan, UT, USA

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ABSTRACT

Computational requirements sometimes discourage using mathematical optimization for groundwater management. To dramatically reduce computation time, the presented hybrid response matrix method (RMM), Coefficient Generation and Use method 4 (CGU4), prepares surrogate simulators used during optimization. CGU4 reduces numerical model simulations needed to populate the surrogates (linearized convolution equations, LCEs). LCEs often represent flow and head constraints within groundwater flow optimization problems. CGU4 reduces computations for problems having: varying time period sizes; eras of sequential time periods of equal duration; and system (non)linearity. For a situation having: linear, piece-wise, and nonlinear groundwater flows; 20 periods of varying and sequentially constant durations; and optimization problems employing (non)linear objective functions and linear head and aquifer-surface seepage constraints, CGU4 requires 22–61% fewer simulations to compute optimal objective function values within 0.001–0.003% of the best alternative RMM. For hypothetical (non)linear dynamic stream-aquifer problems, CGU4 required the same or 63–89% less time than previous RMMs.

System availability

1.) Name of software or data set:
   a. Simulation module: MODFLOW
   b. Optimization module: GAMS
   c. Simulation-Optimization model: Simulation-Optimization Modeling System (SOMOS), SOMO1 module (Early version of SOMO1 was known as REMAX).
2.) Developer:
   a. SOMOS: Richard C. Peralta and contributors listed alphabetically: Alaa Aly, Yun Huang, Ineke M. Kalwij, Bassel Timani, and Shengjun Wu.
   b. Civil and Environmental Eng., 4110 Old Main Hill, Utah State Univ., Logan, Utah, USA (peralta.rc@gmail.com), (435) 797–2786; and Peralta and Associates, Inc. (435) 881-4947
3.) Software:
   a. Program language: C#
   b. Program size: 11MB excluding optimizer (GAMS)
   c. Available since 2015
   d. Hardware required: PC (not tested on MAC)
   e. Software required:
      i) Windows 7 (Various SOMOS versions have run under Windows NT, 95, 2000, XP, Vista, Windows 7, Windows 8, and Windows 10.)
      ii) SOMO1 module of SOMOS;
      iii) General Algebraic Modeling System (GAMS), available from GAMS.COM. The free demonstration GAMS version can solve manuscript System I and II problems. Solving manuscript System III problems requires professional GAMS license.
4.) Availability for download and cost: SOMOS free demonstration version or professional version (different arrangement) will be available from Richard Peralta, peralta.rc@gmail.com after user's manual is ready for release.
5.) Data:
   a. The simulation model data of the manuscript Systems III problem is available at http://www.waterrights.utah.gov/groundwater/gwmodelsview.asp#Cache.

* Corresponding author. Civil and Environmental Engineering Department, 4110 Old Main Hill, Utah State University, Logan, UT, USA.
E-mail address: peralta.rc@gmail.com (R. Peralta).

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List of acronyms

ACE	Aggregated Convolution Equation
CG	Coefficient Generation
CU	Coefficient Utilization
DV	Decision Variable
FCL	Flow Control Location
HCL	Head Control Location
IC	Influence Coefficient
MCIDV	Maximum Change In Decision Variable Rates (in any period between the last two cycles)
ME	Management Era
OFV	Objective Function Value
RMM	Response Matrix Method
SG	Scenario group
S-O	Simulation-Optimization
SP	Stress Period
SV	State Variable
T	last period of an ME
τ	1st period of an ME

b. Form of repository: Files
c. Size of archive: 1.93 GB (input and detailed output)

1. Introduction

Strategic planning and decision-making rely heavily on simulating the consequences of alternative scenarios (Greiner et al., 2014). Stakeholders should participate in evaluating scenarios or strategies and in developing natural resource and environmental management plans (Argent and Grayson, 2003; Martínez-Santos et al., 2010). Mathematical optimization is becoming increasingly desirable for developing alternative management strategies (Scholten et al., 2007; Maier et al., 2014). A management strategy refers to a spatially and perhaps temporally distributed set of groundwater pumping rates.

Mathematical optimization involves computing the optimal solution for a specified optimization problem. An optimization problem usually includes an objective function, decision variables (DVs), state variables (SVs), upper and lower bounds on these variables. The optimization problem must also include constraints linking DVs and SVs and defining criteria that must be satisfied. The optimizer computes the optimal set of DV values (a strategy) that produces the best objective function value. The optimal strategy also has to satisfy bounds (upper and lower limits) on variables and constrained values. Whether the objective is a maximum value or a minimum value depends upon the problem. Groundwater flow optimization problem objective functions have many forms. Examples include maximizing or minimizing pumping, economic benefit, cost, population, drawdown, or other descriptors. Common groundwater DVs, also termed 'instruments' (Katic and Grafton, 2011), are rates of extraction from or injection into aquifers. Sample groundwater flow model SVs include aquifer head, stream head, stream flow, stream-aquifer seepage, river-aquifer seepage, drain-aquifer seepage, and evapotranspiration. Numerical constraints employ DVs and SVs and represent physical laws, social, cultural, economic, and environmental concerns or aspects, and stakeholder preferences and discomforts.

A Simulation-Optimization (S-O) model couples one or more simulation models with optimization algorithms to provide management strategies that satisfy physical laws and management preferences. Simulation models predict the future system state in response to assumed management. To that capability, S-O models add the ability (Refsgaard and Henriksen, 2004; Scholten et al., 2004; Refsgaard et al., 2005; Henriksen et al., 2007) to design optimal strategies that consider and satisfy constraints (Peralta and Kowalski, 1988; Lemon, 1999; Parker et al., 2002; Oxley et al., 2004; McIntosh et al., 2007). S-O models can address many problems, including conjunctive and integrated water management (Jakeman and Letcher, 2003; Bromley et al., 2005). Properly and carefully formulated S-O models aid decision-making (Papathanasiou and Kenward, 2014; Hall et al., 2014), planning, and preparing for weather or climatic anomalies (Greiner et al., 2014). Engineers and scientists more readily use S-O models when the models can practicably handle large and complex management problems (El-Swaify and Yakowitz, 1998; Argent and Grayson, 2003; Argent et al., 2006; Housh et al., 2012). Yazdi and Salehi Neyshabouri (2014) state that the large computational effort required for groundwater pumping strategy optimization has impeded practical S-O modeling use.

Groundwater flow S-O models predominantly use response matrix methods (RMMs) to generate and use linear discretized convolution (superposition) equations. For linear and nonlinear aquifers, convolution equations are surrogate simulators when employed in lieu of full finite numerical models (Wang et al., 2014) to compute SV values resulting from DV values during the optimization process. Razavi et al. (2012a, 2012b), and Yazdi and Salehi Neyshabouri (2014) include such surrogate simulators under the umbrella of 'metamodeling'. The convolution equations employ the multiplicative and additive properties of linear systems theory (Maddock, 1974). These equations (Morel-Seytoux, 1975a; Illangasekare and Morel-Seytoux, 1982; Peralta et al., 1991, 1992, 2011) are also termed Algebraic Technological Functions (Maddock, 1972, 1974; Psilovikos, 2006). The convolution equations include summations of the products of selected pumping stimuli and linear influence coefficients (ICs). A matrix containing all the coefficients is termed a response matrix. A transient IC quantifies system response at a particular time to a 'unit' stimulus of specified magnitude occurring at a particular, possibly different time. To create and use these equations, RMM employment involves the separate phases of coefficient generation (abbreviated CG), and of subsequent coefficient use or utilization (abbreviated CU) during the optimization process.

For multi-period problems, S-O models that pair RMMs and classical optimizers require less computational effort than alternative S-O model types (Peralta and Kalwij, 2012). For simulation, the alternatives use embedded finite simulation models, embedded flow equations, or statistical learning machines (such as Relevant Vector Machines or Support Vector Machines). For optimization, the alternatives use classical algorithms (e.g. simplex, branch and bound, gradient search), or heuristic algorithms (such as genetic algorithms, simulated annealing and tabu search).

Previously employed compatible RMMs, Coefficient Generation and Utilization algorithms 1 and 2 (CGU1 and CGU2) are powerful, but neither is perfect for all situations. CGU1 and CGU2 use different: i) expressions to relate the time that a unit stimulus is exerted to the time at which system response is observed or computed, and ii) the form of the convolution equations. Software using CGU1 and CGU2 that we are aware of also differ in how they compute unit stimuli. CGU1 is attractive for situations in which the physical system response to pumping is linear or mildly nonlinear, but CGU1 requires that periods of pumping be of uniform duration. A stress period is a period of uniform pumping. We use period, time period, and stress period interchangeably in this manuscript. System Simulation and Optimization Laboratory (SSOL) (2004 and