Simulation and Optimizing Groundwater Investigations, Conceptual Design Analysis, Model Calibration and Remedial Design Using Parallel Numerical Methods: Theory and Application - 16578

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ABSTRACT

Optimization of environmental restoration efforts at complex groundwater sites involves the development of a conceptual and often numerical flow and transport models. Typically, a limited number of simulations are done to assess the impact of parameter uncertainty, to evaluate remedial alternatives and develop a remedy, or to modify an existing remedy. A limited number of simulations are performed because each simulation can take upwards of several hours per simulation and until now the ability to conduct the 100s to 1000s of simulations needed to derive an optimal remedy was beyond the reach of the everyday practitioner. HGL has developed and implemented new parallel simulation and optimization methods in their software and has successfully deployed applications on high performance Cloud-based computing platforms. This advancement removes the impediment of burdensome and unpredictable runtime requirements these types of projects have typically exhibited using heuristic trial-and-error or even automated serial computation approaches. A parallel numerical solver has been added to the subsurface flow and transport simulator MODFLOW-SURFACT™ and has demonstrated reductions in solution time by as much as a factor of 9.8. This is accomplished by distributing the numerical computations of every time step over multiple processors. The integrated parallel simulation and optimization method uses the breadth and depth search approach; iteratively producing sets of tens or 100s of candidate solutions that are evaluated concurrently instead sequentially (i.e. one model evaluation at a time). Solutions within 80-100% of the globally optimal solution are regularly found expending only 5-10% of the usual computational effort using this new parallel optimization method (reducing computation effort by 10 to 20 times). Distributing optimal search runs across multiple processors additionally reduces calendar time to solutions. Practitioners evaluating multiple conceptual site models, model calibration by auto-calibration methods and remedial design by heuristics can enjoy significant reductions in model solution time by using the parallel numerical matrix solver in the physics-based simulator. Combining investigation and design analysis with breadth and

depth parallel optimization methods, projects at the fringe of practical optimization, along with projects that were beyond the reach of formal optimization methods are now wholly feasible and tractable optimization problems.

INTRODUCTION

This paper discusses and demonstrates fast computational simulation and optimization technologies used for optimally managing environmental remediation projects and programs. Those responsible for managing environmental restoration efforts at complex sites are looking for tools that will help them find acceptable, efficient and effective solutions to complex and multi-faceted planning challenges at efficient cost points (USEPA, 2012).

Environmental remediation has been ongoing in the Unites States for several decades and has produced some successes. However, the more complex sites remain challenging and resistant to efficient and effective remediation and remain as persistent fiscal and technological challenges. For example, the U.S. Army Corps of Engineers (USACE) has developed checklists to facilitate Remediation System Evaluations (RSEs). The checklists include typical site remediation performance challenges and problems. (USACE, 2016). The tools herein enable formal, physically consistent and robust analysis of optimal remedial designs for complex sites that overcome the computational challenges of achieving improved conceptual site models, investigation and remedial design uncertainty analysis, and high performance, robust optimal designs.

At the project planning stage, optimal design develops the best technical approach and promotes better estimates of pricing and project scheduling, which translates into increased project execution success. Developing an optimal program and project design requires consideration of cost, benefit, technological readiness, project interaction and dependencies, programmatic and project level constraints on available funding, uncertainty in both funding levels and the physical description of the subsurface environmental system. This paper demonstrates the technology and methods available that enable practitioners to simultaneously optimize a program while developing optimal solutions for individual projects with the transparency for stakeholders review and acceptance at both the planning and implementation stage.

DESCRIPTION

Optimal Remedial Design Focus

During the course of developing designs for remediation projects, the following set of questions were asked a decade ago, and remain relevant today illustrating the persistence of these challenges facing the environmental remediation industry (ITRC, 2007):

- How long will it take to remediate the site?
- What will it cost?
- When (and will) remediation be partially or fully complete (i.e., meet site remediation goals) everywhere?
- If only partial source (i.e. DNAPL) mass removal is achieved, what will be the benefits?
- What is the best approach for removing X% of the mass?
- What will the DNAPL and dissolved plumes look like over time?
- What are the best design and operations parameters (extraction and injection well locations, best biostimulation materials to add, microbes to add if any, rates, concentrations, frequency of injections, etc.)?
- How can the impact and remediation best be monitored?
- How certain are we that the remedy will perform as expected/designed?

Remedial Design Approach

The Physics-Based Management Optimization (PBMO™) project design involves selecting the appropriate combination of its fully comprehensive solution options, including full capability of mixing and matching various approaches.

- Select proper descriptive model or model set that adequately describes the system to be optimized (physics based model(s))
- Select optimization algorithm or set of proper optimization algorithms to best optimize the system while honoring all stakeholder requirements (management optimization).
- Select computer operation system, or a mixture of operating systems, to successfully execute the numerical analysis within project schedule constraints.

It is important to note that “optimization” refers not just to cost minimization but also to the effective and efficient balance of cost, performance, risk, management, and societal priorities along with uncertainty analysis. The PBMO™ process formally integrates all of these elements into a single decision framework, and provides not only the "optimal solution" but also "what-if" capability that includes management override control on remedial design analysis. It provides a consistent approach to designing optimal solutions that are transparent and defensible. The approach is modular and scalable. It can be applied either as individual components or in total. By developing the approach in a complex systems framework, the solution methodology represents a significant improvement over the non-optimal “trial and error” approach to environmental response(s). Table 1 depicts the applicability of the PBMO™ system (Deschaine, 2014, Appendix B). PBMO™ has also been configured to run in parallel and has been successfully deployed on high performance Cloud-based computing platforms (Fox, et. al, 2015).

Table 1. PBMO™ Solution Scope[1] and Analysis Results

Scope	Description	Affects	Analysis Results
Optimization of environmental *response program*	Optimal FS/CMS planning-level design considering all reasonably viable alternative remediation responses including waste isolation and monitoring.	Total response cost, multi-period fiscal budget planning and allocation strategies; calculations and contingencies	Optimal and balanced solution that best meets needs of site and stakeholders
Optimization of environmental *remedial design*	Optimal detailed design of FS/CMS selected response program	Total response cost, specific capital expenditures, annual costs, plant operations	Optimal design basis for site including constructability assessment and predicted performance
Optimization of *long-term monitoring*	Optimal design of monitoring well network and sampling program	Total response cost, annual costs, stakeholder confidence that the remedial design and installation are operating as intended.	Proactive management of stakeholder expectations, early warning detection if as-built and operated systems' performance begins to deviate from design intent.
Optimal *contingency plans*	Optimal and pro-active considerations for addressing remedial design *and observed* environmental system response	Total response cost, annual costs, stakeholder confidence that the remedial program and design are robust and amenable to refinement, if warranted.	Optimal and robust remedial system designs, installations and monitoring that incorporate feedback from the operation. Efficiently allow for modifications or inclusion of additional components or processes.

1. *Each scope element of PBMO™ is designed and implemented as a stand-alone module. The optimal solution is developed based upon the information collected to date; is easily revised as new data are collected; and methods employed here can identify best locations for new treatment technology trains and sample collection that will maximize confidence in optimal remedy performance.*

The solution from the PBMO^{TM} methodology has always exceeded the subjective engineering solution (see Table 2) when available for comparison (Deschaine, 2014).

Table 2. Representative Benchmarked Successes of PBMO^{TM} Solutions by Application Scope

Scope	Industry	Example	Contribution
Optimization of environmental *response program*	National Association of Manufacturers	Regulatory Analysis (Superfund Reform; HR2500)	Provided analysis of new regulations that supported environmental remediation decision making and strategy development (Deschaine *et al*., 1999). Analysis characterized cost savings of Superfund program at 35%.
Optimization of environmental *remedial design*	DoD-Umatilla Army Depot	Optimal Environmental Remedial Design	Optimal design of groundwater remediation systems saves both time and money, reduces greenhouse gas emissions. Demonstration of algorithm. Savings $2.2M over existing remedy in place. (Deschaine, *et. al.* 2013).
Optimization of *long-term monitoring*	DOE-Pantex and DoD-Anniston Army Depot (ANAD)	Optimal monitoring	Provided an optimal monitoring plan for tracking environmental contamination such that containment of plumes can be monitored effectively and safely and groundwater resource protected for less money (DoD ANAD savings to date $5.52M, DOE Pantex investigation savings $2M)) (Deschaine, et. al. 2010).
Optimal *contingency plans*	DOE-Pantex	Human Health Risk Assessment, Corrective Measures Study, and Groundwater resource protection	Provided input for an environmental monitoring, compliance and remediation program. The program concerned chemical releases to groundwater. The subsurface environment includes a sole-source drinking water aquifer. (BWXT & SAIC, 2002).

Commonly Solved Problems

Examples of the PBMO™ method for optimization of remedial designs involving routine application of groundwater pump-and-treat technology include:

- Groundwater flow control for construction or mine dewatering;
- Groundwater hydraulic plume containment using particle tracking;
- Groundwater plume remediation using remedy-in-place (RIP) infrastructure unmodified;
- Groundwater plume remediation of RIP with infrastructure augmentation, and;
- Groundwater plume remediation design from a blank slate.

PBMO™, as a universal optimizer, is not constrained to optimizing groundwater pump and treat systems, nor even to the environmental field, rather it is extensible to any form of problem which has a computable objective function and constraint evaluator (Deschaine, 2014).

Simulation Models

Emphasis is placed on modeling codes with mass conserved numerical techniques and robust and efficient solvers of systems described by linear or non-linear elliptic, parabolic and hyperbolic models. This includes many of the commonly used and accepted open access numerical models in the environmental industry such as single- and multi-phase subsurface flow, multi-component chemical and radionuclide transport, and integrated groundwater/surface water flow and contaminant transport models that use text files for input, and accessible output files (text or binary).

Objective Function and Constraints

The fundamental requirement of single and multi-objective optimization is the development of a quantitative statement that describes the design objective to be minimized or maximized: an expression of system cost or performance as a function of the design elements as well as the constraints (Deschaine, et. al, 2013).

Objective function: The objective function is a numerical formulation that includes one or more combination of fixed and variable costs that comprise the construction, operation, maintenance, monitoring, and exit validation demonstration costs (Deschaine, et. al, 2013). Optimization for groundwater remediation includes options for minimum cost, minimum remediation time, maximum removal and the like. The flexibility of the system allows the user to formulate the site specific objectives and constraints as if the solution was being accomplished by trial and error. Standard templates are used for the commonly used design options. For the more unusual design, the formulation is translated using the PBMO™ programming language. Hence, the design approach can be predetermined, and the operations optimized, or both the design and the operations analyzed simultaneously. For example, the user can optimize using a single remediation technology, or a complicated and integrated treatment train approach (e.g., initiate a site remedy with pump and treat including optimal flow rate determination during the clean-up and time to transistion - by incrementally reducing and then eleminating the pump and treat system - to a fully monitored natural attenuation solution). The optimization method executes the model and uses the results to quantify the value of the objective function.

Constraints: The optimizer also determines whether the candidate design is feasible or not. The feasibility of any design is defined by one or more constraints on the design or its performance. Constraint definition includes, but is not limited to (Deschaine, 2007):

- Design element activity (minimum, maximum flow rate of individual wells; when the well may be active; aggregate pumping rate for one or more wells; maximum number of wells; balance between total injection and extraction rates)

- Design element location (location of extraction wells and infiltration basins)

- Simulated remediation performance results (constraints at a location (point) or over a region (areas) regarding hydraulic head, hydraulic gradient, groundwater table drawdown, land surface subsidence, contaminant concentration; remediation timeframe, green house gas (GHG) emissions, and the like.

Each candidate solution is fully evaluated by the software, and each run's specification is stored for future use and inspection, as desired. Automating and record keeping assists in focusing review on a set of the optimal or near optimal solutions derived from 100s to 1000s of individual simulation results. If all constraints are satisfied, the design is considered feasible and the new cost is compared to the current “best” cost to see if the current design has improved the objective function value or not. Failure to satisfy one or more constraint yields an infeasible solution.

METHODS

Understanding optimization rationale and theory, methodological strength, applicability, and limitations, is critical for understanding why optimization is valuable and how to successfully deploy computational optimization analysis on projects. Project implementation experience has shown several predominant optimization methods are routinely successful when used. These methods are linear programming (LP), sequential linear approximation (SLA), and mixed integer non-linear programming (MINLP). These techniques are found applicable and valid for a broad range of environmental restoration problems under consideration. Problem configurations consist of single and multiple management periods.

Computational Approach

PBMO™ is a universal optimization tool. It is designed to be used with any process formulation of physics-based simulator, no matter how complicated the process or objective function calculation. In mathematical language, this includes optimizing physical processes that are described by linear or non-linear elliptic, parabolic and hyperbolic models and objective functions that are continuous, non-continuous and mixed integer. In other words, it handles the complete set of physical processes and project objective calculations that one will encounter in the environmental field. It is a tool system that helps users perform complex high-level tasks with amazing simplicity. Modes of operation include standard and expert modes, and it runs on computers with single and multiple CPUs, including local area grids and the Cloud. Because it is programmed as a set of modules using standard FORTRAN, it is platform independent. It has the capability for including applications with mixed operating systems and can deploy with multiple, independent or blended process models including subject matter expert (SME), data-driven (DD), Physics-based (PB) or integrated model (IM). Analysis can begin with the best result from a trial-and-error approach, or from a random starting point so efforts engaged to date by the design teams can be fully used. The optimal solution search relies on evaluations of candidate solutions, which can be completely physics-based or response function or minorant approximated solution search (Deschaine, 2014). When the response function approximation method is employed, the resultant objective and constraint functions are tested using blind examples (that is, examples not used in function development). This ensures the functions are adequately generalized and approximated and have not succumbed to the pitfall of "overfitting".

Optimization Algorithms

PBMO™ uses a breadth and depth search strategy. The breadth search identifies good solution(s) quickly, whereas the depth (Local Search) drills down to find the optimal value. The Local Search is evaluated by the Generalized Reduced Gradient or Adaptive Local Random Search methods. The optimization methods used include (cf. Pardalos and Romeijn, 2002; Neumaier, Shcherbina, Huyer, and Vinkó 2005; Locatelli and Schoen, 2013):

- Derivative-based global methods
    - Linear programming (LP)

    - Sequential linear approximation (SLA)
    - Sequential Quadratic Programming (SQP)
    - Generalized Reduced Gradient (GRG)

- Derivative-free global methods
    - Adaptive Design of Experiment (ADOE)
    - Adaptive Global Random Search (AGRS)
    - Adaptive Local Random Search (ALRS)
    - Branch and Bound (B&B)
    - Global Adaptive Random Search (GARS)

- Machine Learning for objective function approximation
    - Genetic programming
    - WEKA Machine Learning Toolbox

The PBMO™ tool is based in part on the Lipschitz Global Optimization LGO(c) method, which is commercially available optimization software that contains some of the methods listed above (Pintér, 2014). PBMO™ is a non-trivial, parallel, breadth and depth, optimal search technique which extends and augments the LGO(c) technique. The LGO(c) method was selected for integration into the PBMO™ tool as it was among the best performers in an independent test of 23 optimization techniques (Rios and Sahinidis, 2013). By integrating these two methods, results equal to or better than those independently demonstrated are achieved.

Optimization Results

PBMO™ provides the user with the capability to specify the maximum length of calendar time allowed to generate a reliable numerical estimate of the globally optimal solution, or to provide the best solution identified in the time and number of processers allocated for the optimization task. The standard user mode has upper limits as follows:

- Maximum of 100 binary (yes/no) decision variables
- Maximum of 5,000 continuous variables
- Maximum of 2,000 general constraints

The standard model automatically selects the optimization method for the user to facilitate the ease of use, while the expert model allows full control of method and parameter setting and is, for all practical purposes, unlimited in problem size and capability for this class of problems.

The optimization can proceed sequentially by producing one candidate solution at a time, which is applicable for fast executing simulation models with a low number of decision variable and constraints, or the parallel version can produce sets of candidate investigation solutions for simultaneous evaluation. These new methods produce solutions to within 80% to 100% of the global optimum using only 5-10% of the computational effort, and executing this search in parallel produces additional orders of magnitude reduction in solution calendar time. The user can decide the amount of time and project resources to allocate and when the solution is good enough for design purposes since the methods produce estimated and realized values of the optimal solution. For example, in remedial design projects a solution within 5-10 percent of the estimated optimal solution can be within acceptable design tolerances given uncertainties regarding the physical description of the system (i.e. hydraulic conductivity, biological reaction rates, sorption, desorption, dispersion, etc.). In applications where achieving a solution within 1% or less of the estimated optimal solution is desired, the parallelization allows the significant additional computational power be allocated without significantly increasing the calendar time to generate the solution.

A project example using the parallel optimization method (and the numerical simulator executing in serial mode) entailed determining the optimal location of new extraction wells within a multi-well groundwater extraction and treatment system RIP. There were 1221 candidate well locations. For each candidate well location, the new set of optimal pumping rates required for plume containment was computed. Even this apparently simple sounding problem is one with high dimensionality. PBMO™ produced an optimal solution which reduced pumping by 40%, reduced energy consumption by 8,000 KWh per month, which saves cost and reduces greenhouse gas emissions. By running the simulations in parallel, the optimal solution was obtained over 10 times faster than if the problem had been executed in serial mode. Importantly, the serial approach simply was not an option given project time constraints. The optimal solution was verified by performing an analysis on the same problem using the serial optimization technique.

Simulation Model Results

A primary numerical simulation model used by PBMO™ (MODFLOW-SURFACT™) can execute in serial or parallel mode. It uses new serial and parallel Preconditioned Conjugate Gradient (PCG) matrix solution techniques. The parallel version targets multi-CPU machines with Xeon chips, the common CPU deployed on the Cloud. When configured to run multiple scenarios in parallel, the simulation model efficiency is gained by OpenMP architecture allocation of OpenMP threads to distinct CPUs. The new parallel solver was tested using a groundwater problem with a size of 3.6 million cells and was benchmarked using both a serial PC and a High Performance Cluster (HPC) with Xeon CPUs. The test was conducted on the Cloud using 32 vCPUs, and the parallel computed solution was obtained 9.8 times faster (clock-time) for this steady-state flow problem. These significant reductions in model solution time are applicable whether using the flow and transport model in the simulation of conceptual designs, auto-calibration of models or to support design optimization.

CONCLUSIONS

The basic PBMO^{TM} methodology has been previously tested, verified, validated and documented on a wide range of industrial projects. Those results indicate that it meets or exceeds the best available solution either in use (i.e. as an RIP), proposed by the subject matter experts or developed by other optimization methods. These two new parallelization methods now allow for the optimization of remedial designs for the more complicated problems. These are precisely the environmental problems that remain in the environmental contamination site portfolio as persistent challenges. The earlier successes of the heuristic trial-and-error approach, which assisted in remediating the simpler sites, has reached it limit of applicability in these cases. By simultaneously combining project level optimization with optimal programmatic design, the optimal design and implementation for environmental challenge response is now computationally tractable, practical and viable.

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