DOE Site Remedial Management Optimization Utilizing on the Cloud Computing Systems – 15676

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ABSTRACT

Environmental cleanups at complex sites necessarily address many competing demands and answer questions such as:

"What is the best way and in a sustainable manner to minimize risk to human health and the environment during active restoration efforts and/or long term legacy management, while incorporating parameter uncertainty, management considerations, and stakeholder concerns into the process?"

Physics Based Management Optimization (PBMO™) provides a means to answer such questions. "Physics Based" indicates incorporation of numerically computed groundwater flow and transport processes into the analysis. This enables optimal remedy design based on comprehensive mass removal/destruction metrics and optimal monitoring strategies. "Management Optimization" indicates the ability to incorporate objective functions (e.g., management constraints, sustainability considerations) into the evaluation. PBMO™ components have been successfully implemented for optimal plume delineation (points of compliance) and monitoring, for optimal system design and to optimize existing active treatment systems in the US at multiple DOE, DOD and industrial sites since the mid 1990s.

PBMO™ has been recently extended and implemented on multi-core, multi-CPU grid computing systems including computational clusters, local area networks and the Cloud. This extension allows for increased flexibility and adaptation of computational resources which can now support optimal remedy design and long term management strategies for complex soil and groundwater sites. In the PBMO™ -Grid case study, we evaluate flow and transport for a typical optimization search for a realistic project against sequential optimization. PBMO™-Grid reduces the CPU time required to solve the optimization problem by more than a factor of 14X compared to sequential optimization.

PBMO™-Grid can be deployed for deterministic or stochastic optimization and formally computes design risk and predicted degree of remedial action success. The numerical models used can consist of a single "mega" model (aka a monolith), or a mixture of models and other

calculations or expert systems. PBMO™-Grid integrates the computational models in a seamless manner, and models run on the Cloud can be implemented in Windows or Linux platforms.

INTRODUCTION

Remediation Program Managers (RPM) need a simple yet reliable tool that easily incorporates the objectives and constraints of the remediation challenges on both the project and programmatic levels. Stakeholders need to be able to understand and inspect how the solution is generated. Such tools must be flexible, adaptable and extensible to accommodate the site and contaminant variety and parameter uncertainty, be user friendly, transparent, able to incorporate a variety of management priorities and stakeholder inputs, and produce viable solutions in reasonable time frames.

Background

The Department of Energy (DOE) Office of Environmental Management (EM) has projected over $300 billion dollars and at least 40 years to remediate contaminated DOE sites (NRC 2014, Volume 1, pg 13). Many complex soil and groundwater sites lack adequate characterization; others cannot be cleaned up to unrestricted use with available technologies (NRC 2013, pg. 7) and are transferred to long term stewardship (forecasted to continue past 2060 with costs of up to $209 billion dollars). Tightening federal budgets may prolong schedules and further increase environmental restoration costs. While the foundational technology to comprehensively optimize remediation projects and programs using integrated subject matter expertise (SME), physics-based models, observed data, and management constraints exists (Deschaine, 1985, 2001, 2003, 2013, 2014; ITRC, 2007; Karatzas and Pinder, 1993; Peralta, 2012), computational requirements of using comprehensive physically based numerical models - some of which can require days or weeks to solve - has placed an upper limit on the complexity of the problems that can be practically optimized. Often, computational burden is reduced through the use of approximate models. But, these simplifications can reduce the fidelity of the analysis and may lead to sub-optimal or in-accurate solutions. Furthermore, optimal solutions to complex problems benefit from the integration of many disciplines including SMEs, data observations along with the physically based numerical models (Deschaine, 2014) whilst many techniques rely solely on physically based models. Additionally, some decision support analysis tools are available as "software as a service" and not as distributed programs; a trend likely to continue. Migrating the optimization process to the Grid / Cloud computational environment provides the ability to utilize complete, unaltered, non-simplified models in the process. This capability both maximizes the ability for increased accuracy optimization analyses while mitigating the long and impractical calendar time required for sequential optimization techniques when run on a single desktop or workstation.

Overview of PBMO™:

Strategic planning of environmental responses requires optimal remedial design tools that not only embrace the complex constraints associated with these systems but that can support decision making within a framework of varying levels of uncertainty in all aspects of cradle to grave environmental response planning and execution. The aspect of PBMO™ discussed in this paper is focused on the optimal groundwater remediation design module. It uses physics-based models[1] with cost, certainty and management objective functions to provide estimates of remedial system design performance. Physics-based models are used because they are:

- Comprehensive: Physics-based models provide the best representation of subsurface flow and transport system and the processes affecting contaminant migration. And in doing so, becomes more defensible and better foundation for making predictive simulations.

- Efficient and Effective: Physics-based models are better at capturing the performance of candidate remediation solutions than are over-simplified, lumped parameter, or ad hoc models. This increased accuracy yields a solution that makes better use of scarce financial resources

- Flexible: Physics-based models readily incorporate planning scenarios that are outside historical observations. Models built on regression, interpolation, or extrapolation methods simply cannot capture these new conditions.

PBMO™ analysis includes examining uncertainty range for both the time and cost of remedial projects, and optimization algorithms are deployed to minimize the uncertainty[2] in the remediation project performance, resulting in the optimal design. Cost and schedule uncertainty is captured from the subject matter experts. Geologic uncertainty is captured by tools such as GSLIB[3] and SmartGEO[4]. PBMO™ provides functionality to manually explore remedial alternatives (technologies and designs), or conversely automatically optimizes a single or comprehensive set of remedial alternatives using single or multiple management periods. It includes a manual/automated mode in which the user is allowed to force certain alternatives or configurations to be mandated (or precluded). The automatic optimizers solve for the best solution while honoring these requirements. Manually exploring alternatives offers the user full control over the solution and facilitates learning system behavior. In the automated mode, the tool selects the best arrangement of alternatives. These alternatives are assembled and assessed following standard EPA protocols and using specific models that provide optimal knowledge of the source

[1] Such as MODFLOW/MT3DMS, MODFLOW-Surfact, HEC-RAS.
[2] For optimal decision making under uncertain conditions, cf Deschaine, et. al, 2001.
[3] http://www.gslib.com/
[4] SmartGeo performs the generation of heterogeneous random fields conditioned to measurements, in particular hydraulic measurements, by the inversion of such measurements in a Bayesian framework.

location, its strength, the resultant plumes and changes over time in response to natural attenuation or active remediation. The optimally selected remedy represents the solution that meets all the project criteria, including uncertainty, at the least cost (Deschaine, 2003).

METHODS

HGL's Physics-Based Modelling and Optimization™ or "PBMO™ Medallion" Tool Box integrates physics-based models with a customized and extended implementation of the Lipschitz Global Optimization (LGO(c)) Solver Suite of global and nonlinear optimization methods to provide decision support for environmental remediation (Pinter, 2002). Because PBMO™ 's design is modular, it facilitates linking the appropriate physics-based simulator with the best global optimization algorithm(s) for each individual problem while allowing for parallel processing in Grid/Cloud deployment environments. This configuration of the PBMO™ architecture develops a credible optimal strategy using the appropriate modelling and optimization tools whilst solving industrial grade problems in practical time frames.

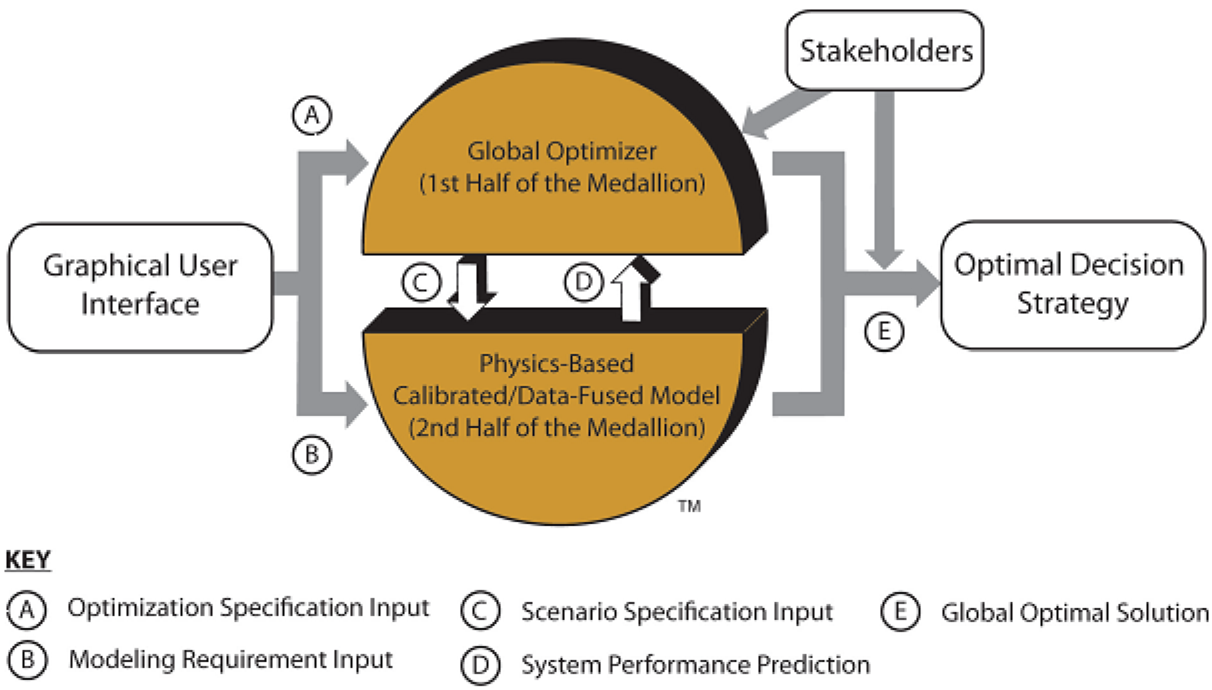

Figure 1: PBMO™ : Optimization Process Flow Diagram

Figure 1 shows how PBMO™ Medallion's modular design permits the linkage of the best global optimization algorithms with the most appropriate physics-based simulators to develop an optimal strategy in a sequential, iterative process. Optimizers available in the top half of the PBMO™ Medallion include LGO, HGL Opt™, Outer Approximation (Deschaine and Pintér, 2003), Kalman Filtering (Deschaine, 2003), linear and sequential linear programming, and various heuristic methodologies including genetic algorithms, Tabu Search, and Simulated Annealing (Deschaine, 2014). These optimizers are then linked with physics-based, calibrated/data fused models for fate and transport — MODFLOW-SURFACT™, MODHMS®, and the HEC family of codes — as well as machine learning (e.g., response function and equation writers). In the serial version of PBMO™, the arrows C and D represent information flows for a single candidate solution. In the parallel version, the arrows C and D represent asynchronous flows of multiple candidate solutions (C) and associated performances (D). The number of candidate solutions in a set is a function of the number of processing nodes[5] activated in the Grid / Cloud computing environment (Sterling, 1999).

Optimization Approaches and Tools

The general process of applying PBMO™ to a site problem involves defining a scope of work and deliverable(s), setting up the project objectives and constraints, selecting a suitable model to predict future scenarios, solving and interpreting results, and achieving stakeholder acceptance. Because the core physical equations and numerical models of PBMO™ are applicable in the water resources, mining and environmental remediation fields, a generalized approach to solving each challenge is possible, with only some customization required to adapt per field of interest.

Once a team-acceptable model is developed, the objective and constraints are defined. Then some level of the feasibility (or infeasibility) is assessed, and a candidate solution is developed. The assessment of developing an optimal solution is discussed in the literature (Deschaine, et. al, 2013). An optimal solution (or a set of such solutions) is generated by linking the model(s) with an optimization algorithm(s). Optimization algorithms can be either deterministic or stochastic, can solve for single- or multi-objective functions and the model equations and constraints can be linear, mildly nonlinear, or highly nonlinear. Furthermore, the characteristic of the model state equations can transition between linear and nonlinear, which can complicate the optimization process. Solving these situations is discussed and demonstrated in (Deschaine, *et. al*, 2013, Deschaine, 2014).

In industrial decision making, the objective is to determine how to allocate limited resources optimally, in order to achieve a certain objective under the constraints. Such decision problems can be formally modeled by corresponding constrained optimization (mathematical programming [MP]) models.

[5] A Cloud deployment can activate 100's or 1000's of computational nodes.

While the decision model formulation is evidently always problem specific, for discussion purposes we provide an overview of the constrained optimization problem. The objective is to minimize the total cost of an environmental or industrial management program expressed by the net present value of all related (construction, treatment and/or operational) cost components. The decision is subject to the following requirements: the solution has to meet all considered physical, engineering, environmental, and stakeholder constraints.

The goal of this section is to summarize the state-of-the art of algorithms for solving global optimization problems and selecting a set of algorithms to use to support making optimized decisions. Reflecting the realities of industrial applications, the present exposition will be focused on global nonlinear optimization.

The general MP model is defined by the following ingredients:

- x decision vector, an element of the real n-space $\boldsymbol{R}^n$;
- $f(x)$ continuous objective function, f: $\boldsymbol{R}^n \quad \boldsymbol{R}$, ($\boldsymbol{R}=\boldsymbol{R}^1$);
- D non-empty set of admissible decisions, a subset of $\boldsymbol{R}^n$.

More specifically, the set D is defined by:

- l, u explicit, finite n-vector bounds of x (a “box”) in $\boldsymbol{R}^n$;
- $g(x)$ m-vector of additional continuous constraint functions, g: $\boldsymbol{R}^n \ \boldsymbol{R}^m$

Applying these notations, the (continuous) MP model is stated as follows: we want to minimize the objective function $f(x)$ under the assumption that x belongs to the feasible set D. Applying standard notation, this is concisely expressed as

$$\min f(x)\ x \in D,\ D: = \{l \le x \le u,\ g(x) \le 0\} \subset \boldsymbol{R}^n. \qquad (1)$$

In the definition of set D, all vector inequalities are interpreted component-wise (since l, x, and u, $l < u$ are n-vectors), and the zero in the relation $g(x) \le 0$ denotes an m-vector. The components of x are denoted by $x_1, x_2,\dots,x_n$; the components of the vector function g are functions $g_1, g_2,\dots,g_m$.

The model formulation is generalized as follows:

- Maximization problems can be deduced to the general form by using $-f$ as the objective function.
- Similarly, = and ≥ constraint relations and/or explicit lower and upper bounds regarding the constraint function values can be simply deduced to the model form (1).
- If the set of additional constraint functions g is empty (m=0), the formulation is a box-constrained optimization model.

Also, combinatorial optimization problems with discrete variables and thus mixed integer-continuous optimization problems can be, at least in a formal sense, directly transformed into continuous GO models (Pintér, 2002).

Next, we introduce the key concepts of *local vs. global* optimality. The point $x_l^* \in D$ is a local solution of (1) if $f(x_l^*) \leq f(x)$ holds for all points $x \in D$ located within a certain "neighborhood" of x_l^*. In the real n-vector space, the concept of a neighborhood can be defined by some norm function. (For concreteness, we can think of the standard Euclidean norm.) The point $x^* \in D$ is a global solution of (1) if $f(x^*) \leq f(x)$ holds for all points $x \in D$. The entire set of global solutions will be denoted by X^*. The basic analytical assumptions stated above guarantee that the optimal solution set X^* of the MP model is non-empty. [6]

The above technical remarks imply that (1) covers a general class of optimization models and useful for general industrial optimization problems discussed in this paper. Consequently, this class includes as provided in the examples, difficult model instances for which traditional (local) optimization methods will typically fail. Local scope search methods, as a rule, find only local solutions depending on the starting point ("initial solution guess") of the search algorithm. A significant class of nonlinear models for which local scope optimization suffices is the minimization of a convex function over a convex set. For completeness, we include definitions of convexity. The set $D \subset \boldsymbol{R}^n$ is convex if for each pair of points from D, the entire line segment connecting these points also belongs to D. A function f is convex over D if its level sets $D_c := \{x \in D: f(x) \leq c\}$ are convex, for all real values of c. If the decision model does not meet (essentially) these convexity requirements, then in general solving the model calls for global scope algorithms.

HGL_Opt™ is the core optimization solver for both the serial and Grid/Cloud deployment. It is a suite of global and local nonlinear optimization methods within an integrating framework. The core solvers are based on a non-trivially extended implementation of LGO(C), Linear and Sequential Programming (LP/SLP) and the outer approximation algorithms. These tools work synergistically to provide a reliable numerical estimate of globally optimal or best solution that can be found in the time allocated to optimization. The solvers can handle at least up to 100 binary (yes/no) decision variables, 5,000 continuous variables, and 2,000 general constraints. Built-in solvers handle arbitrary optimization problems including linear/nonlinear and convex/nonconvex objective function and the constraint sets, and mixed continuous / discrete decision variables. The core global optimizer employs a mild assumption of Lipschitz continuity, which allows for an efficient and robust search for a global optimal value through a systematic partitioning and

[6] This key result directly follows by the classical theorem of Weierstrass that establishes the existence of the minimizing point set of a continuous function over a non-empty, closed and bounded set.

exploration of the entire constraint set using the branch-and-bound approach or an extended implementation of our globally adaptive [depth and breadth] iterative search.[7]

PBMO™ currently includes the following specific objective functions {*f(x)*} PBMO™ for optimizing pump and treat systems:

- Minimize remediation cost
- Minimize remediation timeframe
- Maximize contaminant mass removal
- Minimize Green House Gas (GHG) emissions
- User defined (custom objective function; max or min)

Representative constraints { *l, u, g(x)* } for pump and treat remedies include:

- Cleanup Constraint
- Cleanup Time Constraint
- Maximum Number of New Wells Constraint
- Total Pumping Rate Constraint
- Individual Pumping Rate Constraint
- Contaminant Extent Constraint
- Concentration Constraint by Location
- Head Constraint by Location
- Head Constraint by Area Constraint
- Gradient Constraint by Location
- Pumping-Recharge Balance Constraint
- Well Group Pumping Rate Constraint
- Particle Containment Zone Constraint
- Objective Function Value Constraint
- Maximum Annual Funding Constraint
- Minimum Annual Funding Constraint
- Maximum Total Funding Constraint
- Minimum Total Funding Constraint
- Minimum Annual Mass Removal Constraint
- Maximum Annual Mass Removal Constraint
- Minimum Annual GHG Generation Constraint
- Maximum Annual GHG Generation Constraint

[7] The partitioning allows the algorithm be evaluated using parallel code structures.

One can readily see how the above formulation is directly applicable and extensible to a wide variety of issues encountered in environmental restoration challenges where optimal design is desired.

DISCUSSION

HGL_Opt™ and its precursors have been deployed at some of the most challenging sites from the USDOE, USDOD, USEPA as well as private industry that have ever been analyzed. It has received numerous awards (including a U.S. Vice Presidential Hammer Award) for the application at the USDOE- Savannah River Site where documented cost savings exceeded $20M (Coffield, *et. al*, 1998). A representative example of the tool's applicability and acceptability is the work conducted at the DOE-Pantex Plant, which is described below.

Optimization Application DOE-Pantex Plant

The DOE Pantex Plant in Amarillo, TX provides an example of how comprehensive optimization strategies have been embraced by a program team and have delivered both good will among stakeholders and invaluable overall program savings.

Site Description:

The Pantex Plant, located near Amarillo, TX, USA, is a nuclear material plant covering 9,100 acres. The Plant was established in 1942 to build conventional munitions and high-explosives compounds in support of WWII. It is currently used for the development, testing, and fabrication of high explosive components; nuclear weapons assembly and disassembly; interim storage of plutonium and weapon components; and component surveillance. Historical waste practices at the facility have resulted in 140 known SWMUs containing metals; radionuclides, inorganics (e.g., perchlorate), various explosives such as RDX, VOCs, and semi-volatile compounds. Plant discharges have created a large mound (16BG) of impacted perched groundwater at a depth of 250-300 feet. The impacted groundwater lies about 150 feet above Ogallala aquifer, which is the principal source of groundwater for the City of Amarillo and agriculture in the region.

Work Objectives:

The work objectives were defined as follows: (1) Develop a stakeholder-acceptable project approach; (2) Find and define the TCE and RDX plumes and design a risk-acceptable remedial action; (3) Optimize long-term monitoring to provide stakeholders assurances that impacts are monitored properly; and (4) Develop a contingent remedial design should conditions change (e.g., potential migration of contaminants from the perched to the regional aquifer) to quickly mitigate impacts to the Ogallala Aquifer from future impacts, should they occur. Significant numerical computation challenges were experienced during this effort. The regional transient, multi-phase subsurface flow and transport models of the vadose and saturated zone required up to 23 days per simulation.

Pantex Stakeholder Involvement

Although PBMO™'s integrated modeling and modeling technology for environmental restoration is highly sophisticated, transparency is built into every stage of an analysis/response action to ensure interested parties are kept apprised of site investigation processes and progress, and therefore, are fully prepared to critically review and implement the best, all-round remedies. At the Pantex Plant, this approach helped transform an adversarial situation into a highly productive partnership between stakeholders and the government.

In 1999, a Pantex Plant Technical Advisory Group (TAG) was convened comprised of plant personnel; representatives from universities, national laboratories, government centers of excellence, and state and federal regulatory authorities; industrial experts (including Dr. Deschaine); and community stakeholders. As the TAG team conducted its analysis of the situation, it requested field tests and obtained guidance from leading SMEs on the physics-based simulation and optimization tools available to simulate the subsurface processes operating within Plant's complex geological, hydrological, biological, and chemical subsurface environmental systems. Pantex stakeholders were kept fully apprised of what the TAG had learned, what models and tools were being recommended for selection, and why. Stakeholder involvement was facilitated through regular technical meetings and training courses, so once the work progressed to developing simulation models and optimization systems, Pantex stakeholders understood − and therefore trusted − the analysis and the visualizations (and 3-D physical model) used to translate the complex models and physics data into physical processes and alternative, simulated solutions. Most importantly, the Pantex TAG was prepared to reach an informed decision about the path forward and unanimously endorsed the simulation/optimization system. The TAG proposed to resolve the challenges at the Plant and to continue to stay involved to review the work as it was implemented over a 10-year period (USEPA, 2010). A 24-node (50GHz) grid on a local area network was constructed to conduct the analysis.

RESULTS

The key value of these analyses was that they reduced uncertainty and gained unanimous stakeholder acceptance without conducting unnecessary work. This meant that plans could be, and have been, implemented efficiently and effectively (USEPA, 2010). This effort, though very successful, provided a clear recognition of the need for a more computationally flexible platform to promote use at other complex DOE locations.

Limitations of Computational Approach at Pantex Plant

While the successful application of the simulation/optimization approach on a computational grid at the DOE-Pantex Plant was recognized with a DOE Scientific Award, several factors were identified in the implementation that limited system performance.

- The scalability of the computational network was limited to locally available resources (24 nodes), limiting the amount of computation performed per calendar day.
- Node availability varied from competing (internal and external) computing resource demands, limiting the rate of daily computation performed, resulting in uncertainties when jobs would be completed.
- Significant project-specific coding was required by specialized personal, resulting in high software legacy and maintenance costs, this reduced the portability of the approach making it more difficult and costly to apply the successful solution methodology at other sites.

Migration of PBMO™ to Cloud Computing

Optimization algorithms, including PBMO™, have been designed to produce the most efficient sequence of candidate solutions. In Figure 1, PBMO™ generates a candidate solution (top half), evaluates the solution in the numerical model (lower half), computes the objective function value and evaluates compliance of the constraints. This approach is very practicable on a single computer for moderately complex problems (Deschaine, 2013) with short model execution times or few decision variables, calendar times required to compute and solve an optimization problem can be on the order of months when model run times exceed several hours or decision variables and constraints are in the 100s or 1000s; this is an unacceptable duration for many practical applications. Additionally, many of the numerical flow and transport model codes that are candidates for use in optimization analysis do not employ parallel solvers, so reducing run-times of these models through parallelization often is not a viable option. Hence, it is more feasible, practical and viable to parallelize the PBMO™ optimization algorithm than it is to write parallel solvers for each numerical model. Cloud computing provides the platform that addresses the items needing improvement:

- **System Scalability**: The number of CPU's available has no practical limit. The Cloud platform is fast, flexible and agile providing on demand, extensible performance. [8]
- **Node Availability**: Computational resources, once allocated, are dedicated for the process.
- **Generality**: Cloud vendors and independent researchers have developed and openly share 1000s of tools and techniques to facilitate migration of applications to Cloud computing environments.

In addition, migration of PBMO™ to the Cloud[9] offers the following benefits:

- **Multiple Operating System Option:** Available operating systems include various versions of both Microsoft Windows and Linux. This allows seamless use for calculation of a wide variety of different models - written for different platforms - to be used in the optimization –no portage required.
- **Security:** Multiple levels of security are available, allowing protection of proprietary models and data.
- **Global Database Availability:** Onboard database availability, combined with global internet access and specified levels of security allows collaborative optimization to occur with multiple partners, and multiple data streams (Deschaine, et. al 2000). Utilizing the database allows participant's to provide just the analysis results - as opposed to the entire decision support tool - thereby protecting intellectual property.
- **Hybrid Implementation**: PBMO™ is implemented as a hybrid Cloud system. This hybrid Cloud system promotes an effective blend of usability and practicality.
- **Parallel Implementation**: PBMO™ now generates 100s or 1000s of candidate solution for potential evaluation in contrast to one at a time. Distributing batches of candidate solutions for evaluation makes it easier to explore unsearched regions and exploit searches near promising solutions (Barto, 1998). Participants can also submit candidate solution using various optimization methods, such as SME, observed operational data or even from other optimization algorithms, for inclusion (Deschaine, 2014).

[8] For example, one has the freedom to start with one or several CPU's, then spin up 1000s as needed to compress the calendar time needed to generate an optimal solution. A 1,000 node system (assuming 2Ghz CPUs has 2,000 Ghz capability, 40 times the power of the computational grid used in the Pantex application.

[9] Refers to the Amazon Cloud system EC2 (http://aws.amazon.com/ec2/)

PBMO™ Grid/Cloud Computing Test Case

PBMO™ was applied on a test example optimizing an existing pump and treat system. The optimization problem consisted of 180 decision variables (e.g. extraction rates and pumping periods), hundreds of constraints (e.g., maximum pumping rates, maximal plume geometry extent). The numerical model required 30 minutes per candidate solution evaluation. PBMO™ was implemented using 14 nodes, and produced a solution better than the previously reported solution in less than one week of calendar time[10]. A serial implementation is expected to take months before producing a similar result rendering the serial approach as non-viable.

CONCLUSIONS

A formal comprehensive environmental remedial design optimization system that is Grid and Cloud enabled has been developed and tested. It is important to note that this new capability is radically transformative, and industry can now enjoy the benefits of applying formal optimization to large and complex problems heretofore unviable by current means. Also, in this implementation, “optimization” does not singularly refer to cost minimization but rather to the effective and efficient balance of cost, performance, risk, management — as well as societal priorities and uncertainty. The tool integrates all of these elements into a single-decision framework and provides a consistent approach for designing optimal systems that are tractable, traceable, and defensible. Because the system is modular and scalable, it can be applied either as individual components or in total. Modular deployments of PBMO™ ’s components have already produced savings in excess of $20M at DOE-Savannah River Site (Aiken, SC USA)RS where project duration has been reduced to half of what was originally expected without sacrifice of safety, human health, or environmental standards. The methods used in the tool have been accepted by state and federal agencies (U.S. DOE, U.S. DOD and USEPA) beginning as early as 1985. Now in its 30th year of development and deployment with recent enhancements leveraging Cloud computing, the optimization tool is increasingly being applied to an ever-wider range of highly complex environmental challenges; those complex site challenges that require strategic and expert integration of subject matter expertise, value engineering, simulation, information fusion, and optimization technologies. PBMO™ implemented on the cloud, enables better representation of complex sites during optimization efforts, permitting targeted data acquisition where new data can reduce system/decision uncertainty the most; provide a better foundation for adaptive site management at complex soil and groundwater sites. The comprehensive scope of the PBMO™ formulation includes green remediation and sustainability considerations (triple bottom line of environment, economics and social) aspects of complex site restoration. The fact that management

[10] Greater acceleration of optimal solution generation is enabled by activating additional Cloud computation nodes.

and stakeholder considerations or formally incorporated provides assurance that solutions generated have a high level of acceptability.

REFERENCES

1. Barto, A. G. (1998). Reinforcement learning: An introduction. MIT press.

2. Coffield T and Guy G (1998). “Pollution Prevention through Contaminated Area Rollbacks – Deploying Technologies and Industry Best Practices to Reduce Waste”. DOE-Savannah River Site, WSRC FY98, PBI#8 Status review, Westinghouse Savannah River Company, Slide 9, September 29.

3. Deschaine LM and Singarella PN (1985). “Priority Ranking of 114 Salt Storage and Maintenance Facilities with a Lotus Spreadsheet Model,” Prepared for the Connecticut Department of Transportation in concert with a Department-wide environmental assessment and remediation program. Presented at the MIT Microcomputer Short Course, Cambridge, MA, June.

4. Deschaine LM, Brice RS, and Nodine MH (2000). Use of InfoSleuth to Coordinate Information Acquisition and Analysis in Complex Applications. Society for Computer Simulation’s Advanced Simulation Technology Conference, Washington, DC, USA April 2000. ISBN 1-56555-199-0, pp. 13-18, 2000.

5. Deschaine LM, Rawls P, Manfredo L, and Patel JJ (2001). The DOE NETL Program and Project Source Selection, Risk Quantifier, Management Support and Optimization Tool-Kit The Society for Modeling and Simulation International: Advanced Simulation Technology Conference, Seattle, WA, USA, April. ISBN: 1-56555-238-5, pages 165-174.

6. Deschaine, L. M., Simulation and Optimization of Large Scale Subsurface Environmental Impacts; Investigations, Remedial Design and Long Term Monitoring (2003). Journal of "Mathematical Machines and Systems", National Academy of Sciences of Ukraine, Kiev. No 3, 4. 2003. Pages 201-218.

7. Deschaine, LM, and Pintér, JD (2003) A Comparison of the Outer Approximation Method and Lipschitz Global Optimization on Optimal Groundwater Quality Management, Presented at the INFORMS Annual Meeting Conference, October 19-22, Atlanta, Georgia.

8. Deschaine, Larry M., Theodore P. Lillys, and János D. Pintér (2013). "Groundwater remediation design using physics-based flow, transport, and optimization technologies." Environmental Systems Research 2, no. 1: 6.

9. Deschaine, Larry M (2014) Decision support for complex planning challenges - Combining expert systems, engineering-oriented modeling, machine learning, information

theory, and optimization technology. PhD Dissertation, Chalmers University of Technology, Gothenburg, Sweden.

10. Interstate Technology and Regulatory Council (ITRC) (2007). Simulation and Optimization of Subsurface Environmental Impacts; Investigations, Remedial Design and Long Term Monitoring of BioNAPL Remediation Systems. Chapter 9, in In-Situ Bioremediation of Chlorinated Ethene DNAPL Source Zones: Case Studies, Prepared by The (ITRC), Bioremediation of Dense Non-Aqueous Phase Liquids (Bio DNAPL) Team.

11. Karatzas GP and Pinder GF (1993). "Groundwater Management Using Numerical Simulation and the Outer Approximation Method for Global Optimization." Water Resources Research 29, No. 10, October: 3371–3378, 1993.

12. NRC (2014). Best Practices for Risk-Informed Decision Making Regarding Contaminated Sites: Summary of a Workshop Series. Washington, DC: The National Academies Press. Available at http://www.nap.edu/catalog.php?record_id=18747

13. NRC (2013) Alternatives for Managing the Nation's Complex Contaminated Groundwater Sites. Washington, DC: The National Academies Press. Available at http://www.nap.edu/download.php?record_id=14668.

14. Pintér JD (2002). Global optimization: software, test problems, and applications. In Pardalos, P. M. and Romeijn, H. E., eds. Handbook of Global Optimization, Volume 2, pp. 515-569. Kluwer Academic Publishers, Dordrecht.

15. Peralta, R. C. (2012). Groundwater optimization handbook: flow, contaminant transport, and conjunctive management. CRC Press.

16. Sterling, T. L. (1999). How to build a Beowulf: A Guide to the Implementation and Application of PC Clusters. MIT press.

17. USEPA, 2010. PANTEX PLANT (USDOE) in Carson County, Texas Site Status Summary, USEPA Region 6, October, 6p. http://www.epa.gov/region6/6sf/pdffiles/0604060.pdf