APPROACHING THE GROUNDWATER REMEDIATION PROBLEM USING MULTIFIDELITY OPTIMIZATION

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Abstract

We consider two optimization formulations of the hydraulic capture (HC) problem. One is more exact but computationally expensive. The other requires fewer computational resources but entails difficult calibrations to ensure correctness. In an effort to extort the positive aspects of each model, we apply a multifidelity optimization (MFO) algorithm. This approach takes advantage of the interactions between multifidelity models and results in a dynamic and computational time saving optimization algorithm. We present the HC problem, two models of differing fidelity, and the MFO method. We describe how the algorithm was applied to the HC problem and give some preliminary numerical results.

1. INTRODUCTION AND MOTIVATION

The objective of the hydraulic capture (HC) method for optimal groundwater remediation design is containment of a contaminant plume at minimal cost. To reach this goal, barrier wells are placed such that the direction of groundwater flow is reversed. Additionally, the wells are installed and operated as cheaply as possible. Finding a solution to the HC problem involves applying optimization algorithms in conjunction with simulators for groundwater flow and possibly for contaminant transport. The formulation of the objective function and its corresponding constraints dictate which optimization algorithms are appropriate for finding the optimal well field design. Computational efficiency and accuracy further influence the choice of solution method.

Many models of the HC problem have been proposed. Some are more exact but require extensive computational resources to simulate. Others are less computational intensive but may not capture the contaminant plume correctly. In this study, we consider two such models and examine the applicability of a method of multifidelity optimization (MFO). The MFO algorithm was designed to improve computational speed and efficiency of the optimization by taking advantage of the interactions between multifidelity models.

The problem studied here is motivated by a HC application proposed as part of a suite of benchmarking test problems in [14]. In Section 2, we state two formulations of the problem. Section 3 includes a general description of the MFO algorithm. The particulars of how this algorithm is applied specifically to the HC problem are given in Section 4. Finally, in Section 5, we present and discuss some numerical results.

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2. TWO MODELS OF HYDRAULIC CAPTURE

In this study, the two models of hydraulic capture considered are: transport-based concentration control (TBCC) and flow-based hydraulic control (FBHC). For both models, the optimization problem is

$$\min_{\mathbf{u}\in\Omega} J(\mathbf{u}) \tag{1}$$

where $\mathbf{u}$ is a vector of decision variables and Ω is the feasible region of $\mathbf{u}$ and is represented by a set of constraint equations that we describe later. For this work, the decision variables are the number of wells, $n \leq N$, the pumping rates, $\{Q_i\}_{i=1}^{n}(m^3/s)$, and the well locations, $\{(x_i, y_i)\}_{i=1}^{n}(m)$. Here, N is the maximum possible number of wells in the final design.

The objective function J is the sum of the capital (or installation) cost J^c and the operational cost J^o and can be stated as follows [14, 13]:

$$J = \underbrace{\sum_{i=1}^{n} c_0 d_i^{b_0} + \sum_{Q_i<0.0} c_1 |Q_i^m|^{b_1} (z_{gs} - h^{min})^{b_2}}_{J^c} + \underbrace{\int_0^{t_f} \left(\sum_{i,Q_i<0.0} c_2 Q_i (h_i - z_{gs}) + \sum_{i,Q_i>0.0} c_3 Q_i \right) dt}_{J^o}. \tag{2}$$

In J^c, the first term accounts for drilling and installing each well, and the second term represents the additional cost for pumps for extraction wells. In J^o, the term pertaining to the extraction wells includes the lift cost associated with raising the water to the surface. Note that a negative pumping rate means a well is extracting and a positive pumping rates means a well is injecting. Injection wells are assumed to operate under gravity feed conditions. More specifically, in (2) c_j and b_j are cost coefficients and exponents, respectively, $d_i = z_{gs}$ is the depth of well i, Q_i^m is the design pumping rate, and h^{min} is the minimum allowable head.

The hydraulic heads, $h_i(m)$ for well i, vary with the decision variables, and obtaining their values at each iteration requires a solution to equations that model saturated flow. This model is given by

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{K} \cdot \nabla h) + \bar{S}, \tag{3}$$

where $S_s(1/m)$ is the specific storage coefficient, $h(m)$ is the hydraulic head, $\mathbf{K}(m/s)$ is the hydraulic conductivity tensor, and $\bar{S}(m^3/s)$ is a fluid source term that incorporates the decision variables into the state equation for the HC problem. Numerically, the simulator MODFLOW2000 [16] is used to find a solution to (3).

In HC models, constraints on the decision variables typically include bounds on the well capacities and the hydraulic head at each well location. For example, we incorporate the inequalities

$$Q^{emax} \leq Q_i \leq Q^{imax}(m^3/s), i = 1, ..., n \tag{4}$$

$$h^{max} \geq h_i \geq h^{min}(m), i = 1, ..., n \tag{5}$$

where, Q^{emax} is the maximum extraction rate at any well, Q^{imax} is the maximum injection rate at any well, h^{max} and h^{min} are the maximum and minimum allowable head, respectively. Note that assessing whether or not (5) holds requires a solution to (3). In addition to (4) and (5), the HC problem constrains the net pumping rate using the inequality

$$Q_T = \sum_{i=1}^{n} Q_i \geq Q_T^{max}, \tag{6}$$

where $Q_T^{max}(m^3/s)$ is the maximum allowable total extraction rate. This constraint is enforced to avoid dewatering of the aquifer.

This is a challenging optimization problem in that it is a black-box, mixed integer problem. Evaluation of the objective function and constraints requires a groundwater flow simulation, and there are both integer and real-valued decision variables. Inclusion of the installation term, J^c allows the removal of a well from the design. Although this can lead to a large decrease in cost, it also makes objective function discontinuous. We apply optimization algorithms that are equipped to handle discontinuities, but we include an added constraint to avoid explicitly using the integer variable for the number of wells. Specifically, if, in the course of the optimization, a well rate satisfies the inequality $|Q_i| \leq 10^{-6}(m^3/s)$, that well is removed from the design space and excluded from all other calculations. Furthermore, we assume that all wells have a fixed depth, but that their location can vary in the $x-y$ plane. These well locations, $\{(x_i, y_i)\}_{i=1}^n$ are also decision variables, but do not explicitly appear in the objective function.

2.1. **Flow-based Hydraulic Control (FBHC).** Flow-based hydraulic control is a technique for plume containment that enforces head gradient constraints around the perimeter of the plume. In the particular model we consider, a head gradient constraint is formulated as a constraint on the difference in hydraulic head values at specified locations. Consider

$$h_1^k - h_2^k \geq d(m), k = 1 \ldots M \tag{7}$$

where M is the number of head gradient constraints imposed around the boundary, h_1, h_2 are hydraulic head values at specified, adjacent nodes for each constraint k, and d is the bound on the difference. This set of constraints can be used to enforce head gradients vertically or horizontally. For example, in the simple case where h_1 are h_2 are aligned at a distance of distance Δx apart, then dividing (7) by Δx yields

$$\left(\frac{h_1^k - h_2^k}{\Delta x}\right) \geq \frac{d}{\Delta x}(m/s). \tag{8}$$

The FBHC approach to the HC problem is minimizing the objective function J subject to (4), (5), (6) and (7). Use of this method is attractive because it is relatively inexpensive. However, it requires (7) to be calibrated to ensure that the contaminant plume is properly captured and to avoid excessive pumping [15].

2.2. **Transport Based Concentration Control (TBCC).** A direct approach for plume containment is to impose constraints on the concentration at specified locations. This constraint can be expressed as

$$C_j \leq C_j^{max}(kg/m^3) \tag{9}$$

where C_j is the concentration at some observation node j, and C_j^{max} is the maximum allowable concentration. Evaluation of this constraint requires a solution to the contaminant transport equation

$$\frac{\partial(\theta^\alpha C^\iota)}{\partial t} = \nabla \cdot (\theta^\alpha \mathbf{D}^\iota \cdot \nabla C^\iota) - \nabla \cdot (\mathbf{q} C^\iota) + I^\iota + R^\iota + S^\iota, \tag{10}$$

where $C^\iota(kg/m^3)$ is the concentration of species ι in the aqueous phase, θ^α is the volume fraction of the aqueous phase, $\mathbf{D}$ is a hydrodynamic dispersion tensor, $\mathbf{v}(m/s)$ is the mean pore velocity, $\mathbf{q}(m/s)$ is the Darcy velocity, and $I^\iota, R^\iota, S^\iota$ represent interphase mass transfer, biogeochemical reactions, and source of mass respectively. Numerically, the simulator MT3DMS [17] is used to obtain a solution to the transport equation.

Solving the HC problem using the TBCC model is minimizing the cost function J with respect to (4), (5), (6), and (9). Therefore, the TBCC approach requires a solution to both (10) and (3) making it computationally expensive. Moreover, objective functions and constraints involving concentrations are nonconvex in some situations [4, 2], making the minimization problem more difficult.

3. MULTIFIDELTIY OPTIMIZATION (MFO)

The MFO scheme used in this study is based on a direct search optimization algorithm and space mapping techniques. It is applicable to a wide range of problems [5].

3.1. **Asynchronous Parallel Pattern Search (APPS).**

The derivative-free optimization used by the MFO method is called Asynchronous Parallel Pattern Search (APPS)[10, 11]. Direct search methods, such as APPS, are appropriate for problems in which the derivative of the objective function is unavailable and approximations are unreliable. Pattern searches use a predetermined pattern of points to sample a given function domain. It has been shown that if certain requirements on the form of the points in this pattern are followed and if the objective function is suitably smooth, convergence to a stationary point is guaranteed [6].

A detailed procedural version of APPS is given in [9], and a complete mathematical description and analysis is available in [11]. Omitting the implementation details, the basic APPS algorithm can be simply outlined as follows:

(1) Generate a set of trial points **T** to be evaluated.
(2) Send the set **T** to the *conveyor* for evaluation, and collect a set of evaluated points, **E**, from the conveyor. (The conveyor is a mechanism for shuttling trial points through the process of being evaluated.)
(3) Process the set **E** and see if it contains a new *best point.* If **E** contains such a point, then the iteration is successful; otherwise, it is unsuccessful.
(4) If the iteration is successful, replace the current best point with the new best point (from **E**). Optionally, regenerate the set of search directions and delete any pending trial points in the conveyor.
(5) If the iteration is unsuccessful, reduce certain step lengths as appropriate. In addition, check for convergence based on the step lengths.

APPSPACK version 4.0 is [9] an open source software implementation of this algorithm. It can be executed in serial or parallel. For this work, we consider the parallel version.

3.2. **Space Mapping.**

Space mapping [3] is a numerical technique that allows linking design spaces of models with similar functionality but varying fidelities. In this paper, we refer to the model that is more exact but more computationally expensive as the high fidelity model. The low fidelity model is less exact but requires less computational resources. The relationship between the models can be defined by a mapping P from the high fidelity model design space, $\vec{x_H}$, to the low fidelity design space, $\vec{x_L}$, such that

$$f_L\left(P\left(\vec{x_H}\right)\right) \approx f_H\left(\vec{x_H}\right), \tag{11}$$

where f_H and f_L are the high and low fidelity model responses respectively. Equation (11) can be restated the minimization problem

$$min \left\{ \sum_{i=1}^{N} \|f_L\left(P(x_i)\right) - f_H(x_i)\|^2 \right\} \tag{12}$$

where N is the number of high fidelity design points x_i. The appropriate formulation for P is highly problem dependent. One option is

$$P(x_H) = \alpha x_H^{\beta} + \gamma \tag{13}$$

where α, β, and γ are determined by solving (12).

Note that $\vec{x_H}$ and $\vec{x_L}$ need not be equivalent in size or type. This is an important feature of space mapping since it is often the case that a low fidelity model has fewer design parameters to characterize than a corresponding higher fidelity model. This MFO scheme uses eliminates the requirement of a one-to-one correspondence between the design space of models by incorporating space mapping.

3.3. **The APPS/Space Mapping Scheme.** The APPS/Space Mapping approach to MFO can be described in terms of two loops– an outer loop and an inner loop. The main purpose of the outer loop is the application of the APPS algorithm to the high fidelity model. However, it also has the added task of maintaining a set of trial points and their corresponding response values. These are used by the inner loop to map the high fidelity space to the low fidelity space. The inner loop then uses this space mapping to optimize the low fidelity model. The complete MFO procedure is:

(1) Start the outer loop.
   - Optimize the high fidelity model f_H using the APPS algorithm.
   - While optimizing, collect a set of N pairs $(x_i, f_H(x_i))$

(2) Start the inner loop
   - Using the N high fidelity response pairs collected by the outer loop, obtain the space mapping parameters. In other words, find α, β, and γ such that

$$\sum_{i=1}^{N} \left\| f_L(\alpha(x_i)^{\beta} + \gamma) - f_H(x_i) \right\|^2 . \tag{14}$$

     is minimized.
   - Optimize the low fidelity model within the space mapped high fidelity space by minimizing $f_L(\alpha x^{\beta} + \gamma)$ with respect to x; obtain x^*.

(3) Return x^* to the APPS algorithm and determine if it is a new best point.

The implementation of this algorithm is described in detail in [5].

The inner loop acts as an *oracle* or predictor of points at which a decrease in the objective function might be observed. In optimization, oracles are free to choose points by any finite process. (See [12] and references therein.) Moreover, the selection of additional candidate points does not adversely affect an algorithm's convergence properties. Therefore, this MFO approach is provably convergent under the same mild conditions, stated in [11], required for convergence of the APPS algorithm.

4. SOLVING THE HC PROBLEM USING MFO

To apply the MFO approach to the HC problem, we use the FBHC model as the low fidelity model and the TBCC model as the corresponding high fidelity model. In order to test the effectiveness of the MFO approach, we compare results for the HC problem included in [14]. For the simple domain of this problem, the FBHC formulation has been shown to be sufficient [8]. However, other approaches are needed for more realistic domains [1].

In the HC problem used here, the physical domain is a $1000 \times 1000 \times 30(m)$ unconfined aquifer. Since the aquifer is unconfined, the head constraint (5), depends nonlinearly on the pumping rates. For the hydraulic conductivity field, we use the simple homogeneous case with $K = 5.01 \times 10^{-5}(m/s)$. Paired with the saturated flow equation (3), we use the following boundary and initial conditions:

$$\left.\frac{\partial h}{\partial x}\right|_{x=0} = \left.\frac{\partial h}{\partial y}\right|_{y=0} = \left.\frac{\partial h}{\partial z}\right|_{z=0} = 0, \quad t > 0$$

$$q_z(x, y, z = h, t > 0) = -1.903\text{x}10^{-8}(m/s), \text{ where } q_z = -K\frac{\partial h}{\partial z},$$

$$h(1000, y, z, t > 0) = 20 - 0.001y(m); \;\; h(x, 1000, z, t > 0) = 20 - 0.001x(m).$$

Here q_z is the Darcy flux out of the domain, representing recharge into the aquifer that could result from rainfall. The steady state solution to the flow problem without wells is $h(x, y, z, 0) = h_s(m)$, and $S_s = 2.0 \times 10^{-1}(1/m)$ is the specific yield of the unconfined aquifer. The ground surface elevation is $z_{gs} = 30(m)$. In (2), we use $h^{min} = 10(m)$, $Q_i^m = \pm 0.0064(m^3/s)$, and $d_i = 30(m)$ for each pump i. The simulation time is $t_f = 5$ years. Other pertinent cost data is given in [13].

A plume development was simulated using (10) from a finite source for five years with a constant concentration of $1kg/m^3$ located in the region bounded by

$$[(200, 225); (475, 525), (h, h - 2)](m).$$

We chose the $5 \times 10^{-5}(kg/m^3)$ contour line as the plume boundary and set $C_j^{max} = 5 \times 10^{-5}(kg/m^3)$ in (9). The MT3DMS [17] was used to generate this initial contaminant plume, as described in [13].

For the FBHC approach, we use five head difference constraints (7) with $d = 10^{-4}$. Five concentration constraints (9) are used for the TBCC approach, enforced in the same locations as (7) in the FBHC approach. The starting point includes two extraction and two injection wells for a total of $N = 4$ candidate wells and initial pumping rates of $\pm Q_i = 0.0064(m^3/s)$.

5. NUMERICAL RESULTS AND DISCUSSION

The financial cost of the groundwater remediation at the initial iterate is $J(u_0) = \$78,587$. Table 1 shows the minimum financial cost found and the %-decrease for each of the approaches– FBHC, TBCC, and MFO. Both the FBHC and TBCC models were solved using APPSPACK 4.0, the same software customized for the APPS/Space Mapping approach to MFO. Note that all three methods produce solutions with similar remediation costs and overall percentage decreases.

Model	Cost	% Decrease	mf2k calls	mt3d calls
FBHC	\$24,175	69.2%	117	0
TBCC	\$20,362	74.1%	188	160
MFO	\$22,428	71.5%	152	86

Table 1. Comparison of results from solving a groundwater remediation problem using three different models. The first column gives the model used, and the remaining four columns give performance information.

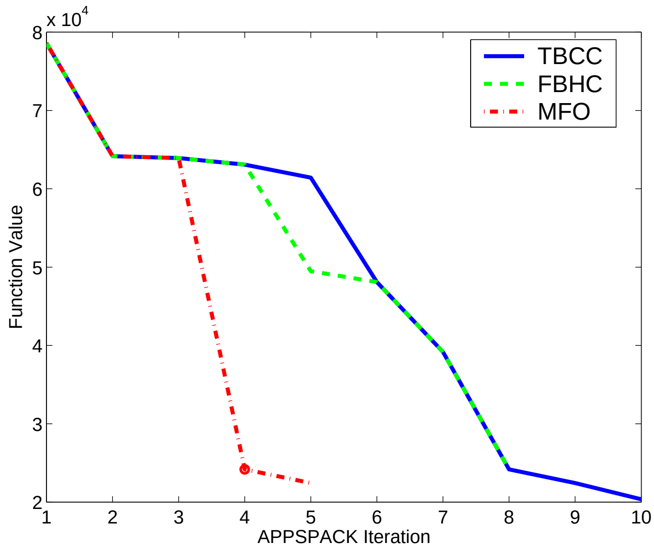

Figure 1. Graph of the reduction in the remediation cost function per APPSPACK iteration. The solid blue and green dashed lines correspond to the TBCC and the FBHC models, respectively, as solved with APPSPACK 4.0. The red dot-dash line corresponds to the MFO approach, and the red dot is the result of an inner loop calculation.

One way to view the computational performance of the algorithms is to consider the number of function evaluations needed to reach the optimal point. As with most simulation-based optimization problems, the majority of this computational cost is the calls to the MODFLOW2000 and/or MT3DMS simulators. Note that if (6) is not satisfied, a flow simulation is not performed in any approach and likewise if (5) is not satisfied, then no transport simulation is performed for the TBCC or MFO approaches. The fourth and fifth columns in Table 1 show the number of times that MODFLOW2000 (mf2k) and MT3DMS (mt3d) were called for each approach. For this problem, a MODFLOW2000 simulation takes approximately 2 seconds wall clock time, and a MT3DMS simulation takes anywhere from 40 to 50 seconds wall clock time.

Figure 1 highlights the differences in the three approaches by illustrating their performances over the course of the algorithm's execution. All three approaches start off the same. However, once the MFO approach receives the results of an inner loop calculation, it is able to make a significant decrease in the overall cost more quickly.

In [14], the lack of representative problems available for the testing and comparison of methods for the optimal design of saturated flow and transport problem is discussed, and a set of test problems is suggested. Although these test problems were developed with considerable thought and are indicative of real world situations, their domains are relatively simple. In this work, we consider one such simple, homogeneous case for which the FBHC model has been shown to be sufficient and computationally cost-effective [7]. However, the introduction of heterogeneities or other complexities will likely require the TBCC or other models in which the plume boundary is precisely defined. Since such models may not be viable with respect to computational cost, we offer the MFO approach. In this paper, we have shown the MFO approach to be comparable and hypothesize that it may be a reasonable method for the solution of more complicated groundwater remediation problems. To further investigate, we plan to extend our study to consider more representative physical models and simulators and to incorporate real-site data.

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