Time Stepping Classes for Optimization

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ABSTRACT

This report introduces the “Time Stepping Package for Optimization”, or TS0pt, which is an interface for time-stepping simulation written in C++. It packages a simulator together with its derivatives (“sensitivities”) and adjoint derivatives with respect to simulation parameters in a single object called a Jet, which can be used in conjunction with an optimization algorithm to solve a simulation-driven optimization problem. Further, TS0pt interfaces with the Rice Vector Library (RVL), allowing Jet objects to define a Operator subclass.

INTRODUCTION

We are interested in solving optimization problems of the form

\[
\min_c \quad J(c) = G(u(c, \cdot))
\]

(1)

where the state \( u(t) \) and the control \( c(t) \) solve the state equation

\[
\bar{H} \left( \frac{du}{dt}, u, c \right) = 0.
\]

(2)

Though many types of control and inverse problems fit the mathematical framework above, we note that the procedure of solving such problems numerically oft involve the same procedures (e.g., formation of derivatives). To exploit these commonalities, hence, we created TS0pt, or the “Time-Stepping for Optimization” package. TS0pt is a “middleware” package written in C++, designed to act as an “interface for time-stepping simulation”, providing a way for simulation software to inter-operate with optimization software. TS0pt is capable of encapsulating the reference, linearized and adjoint simulators in a single object, and properly arrange their execution. TS0pt also aids in providing necessary data structures for the optimization algorithm (e.g., the gradient, formed via the adjoint-state method).

This report is organized as follows: the first section introduces RVL and section two discusses the Alg framework developed by Tony Padula. RVL and the Alg framework provides the foundation for TS0pt. The most notable features of TS0pt include its modular code structure, due to use of the Alg framework from the Rice Vector Library (RVL), and also accommodation of a generic data structure type through templating. The specifics of the structure of TS0pt and its features will be discussed in more detail in section three.
The final section of this report presents the “Optimal Well-Rate Allocation” (OWRA) problem, which is a reservoir engineering inverse problem. We conclude this report by presenting numerical results for OWRA, obtained via TSOpt in conjunction with a reservoir simulation package and an external optimization package.

THE RICE VECTOR LIBRARY (RVL)

The Rice Vector Library is a software framework consisting of C++ abstractions of Hilbert space components, making it an appropriate foundation for Newton-based optimization algorithms (Padula et al., 2009). RVL was designed to enable expression and implementation of “coordinate-free” linear algebra and optimization algorithms. Further, RVL promotes creation of reusable algorithms, to accommodate “different application, data storage models and execution strategies” (Padula et al., 2009). RVL’s components can be grouped into two categories: the calculus classes and data management classes. The calculus classes include abstractions of “a vector space, a vector, a vector-valued function and a Linear Operator.” The data management classes include “Data Containers and encapsulated functions”.

One of the fundamental software frameworks that stem from RVL is called the Alg framework, which provides a computational abstraction of all algorithms. The Alg framework, for example, is the base for a suite of linear algebra and optimization solvers in RVL. The Alg framework will also be the foundation for the TSOpt framework; it is imperative, hence, that we discuss the Alg framework in more detail.

RVL AND THE ALG FRAMEWORK

Padula et al. explored what it means for a program to be an algorithm in (Padula et al., 2009). The answer was simple: an algorithm is a program that runs in a finite amount of time (i.e., it stops). Ideally, it should also be able to relay information if its execution was successful or not. This definition easily lends itself to the following C++ implementation of a base class:

```cpp
class Algorithm {
public:
    virtual bool run() = 0;
};
```

The class Algorithm became the foundation of the Alg framework. Using the base class Algorithm, a variety of subclasses can be defined as well – allowing us to abstract the functionality of different types of numerical algorithms, such as optimization and simulation algorithms (Padula et al., 2009). This led to the insight that, since all time-stepping
schemes are algorithms, TSOpt’s components can be implemented from Algorithm objects. In fact, three subclasses of Algorithm serve as the foundation of TSOpt. These subclasses are called the StateAlg, the LoopAlg and the ListAlg classes. The UML diagram in figure 1 show these subclasses, along with their methods. Since it is crucial that we understand their functionality, they are discussed in detail below.

**The StateAlg Class**

A StateAlg is an Algorithm that has an explicit state variable. This abstraction is useful in a variety of mathematical algorithms, such as a Newton method where the internal state is the current value of the optimization variable. A StateAlg must provide methods to assign and retrieve values from its state. The following is the implementation for the StateAlg base class:

```cpp
template<class T>
class StateAlg: public Algorithm {
public:
    virtual void setState(const T & x) = 0;
    virtual const T & getState() const = 0;
    virtual T & getState() = 0;
};
```

Also note that the state type is templated, meaning that this concrete subclasses of StateAlg can use other objects as its internal state.

**The LoopAlg and terminator Classes**

The Alg Framework also has a class capable of abstracting looping algorithms, such as GMRES. This class, which derives from Algorithm is called LoopAlg. A LoopAlg object’s
job is to repeat execution of an Algorithm object (through the run() method) until some criteria is met. This criteria is encapsulated in something called a Terminator object. The Terminator base class is implemented the following way:

class Terminator {
public:
    virtual ~Terminator() {} 
    virtual bool query() = 0;
};

All subclasses of Terminator must provide a query() method that either returns true or false. The LoopAlg object will then use this query() function to determine whether to stop the loop or not. Given the Algorithm inside and the Terminator term, we implement LoopAlg class’ run method as:

virtual bool run() {
    bool t1 = true;
    while( (!term.query()) && t1 )
        t1 = inside.run();

    return t1;
}

Note that the LoopAlg also needs to ensure that its Algorithm object completed it’s job successfully (i.e., it returned true).

The ListAlg Class

The ListAlg class is just an Algorithm that is composed of two other Algorithms. This particular Algorithm’s run() command executes the two Algorithms in order, one after another. Given two Algorithm objects one and two, we implement ListAlg class’ run method as:

virtual bool run() {
    bool t1 = true, t2 = true;
    t1 = one.run();
    if( islist )
        t2 = two.run();

    return (t1 && t2);
}
THE SOFTWARE FRAMEWORK OF TSOpt

After discussing RVL and the Alg framework, we can now discuss TSOpt. TSOpt is a software package that encapsulates reference, linearized and adjoint simulations in a single object. As mentioned in earlier sections, TSOpt uses RVL and the Alg package as the foundation of its framework. This section presents the main components of the TSOpt framework, which consist of the time, state, timestep, sim, terminator and jet classes.

The time Hierarchy

The time class is perhaps the most fundamental class in TSOpt. This base class Time is an abstraction of the simulation times. A time object only knows the current simulation time; it does not know extra information about the simulation, such as the final simulation time or the step length. All subclasses of time must provide methods for assignment of simulation time, as well as the comparison operators for “less than” (<) and “greater than” (>). There are two current concrete subclasses of time: the DiscreteTime object and the RealTime object.

The DiscreteTime object is used for simulations of fixed time steps; it uses a time index (in the form of an int) to keep track of the simulation time. Hence, by altering this time index, we can change the simulation time. The RealTime object, on the other hand, allows for variable time steps. It does not have an internal time index; it only holds a double to represent the current simulation time, which can be accessed and altered directly.

The State Class

The State class is not, strictly speaking, a part of TSOpt – though a couple of different concrete State classes have been implemented in TSOpt. Users of TSOpt can implement their own State class to act as an interface between their preferred simulator data structure and TSOpt. A State object is composed of two objects: a data structure to hold data (e.g., an array) and a time object, which holds the current simulation time associated with the data. This relationship can be seen in the UML diagram, figure (2). All State classes must implement methods to get and set the time object, and methods to access and alter its internal data structure. There are two examples of State subclasses that have been implemented in TSOpt, to accompany the two different time types: RnState and RealRnState. The RnState class contains a DiscreteTime object, and is used for fixed time step simulations. (The “Rn” refers to the vector space $\mathbb{R}^n$.) The RnState class internally contains an rn struct, defined with the following components:

```c
typedef struct {
    /** time index */
```
The class `RnState` then provides methods to access and initialize the components of the `rn` struct.

The `RealRnState`, in turn, contains a `RealTime` object and is used for adaptive time step simulations. Like `RnState`, `RealRnState` is a wrapper class for the `realrn` struct. There are two differences worth noting between the `RnState` and `RealRnState` classes, however. First, `RealRnState`'s internal data type is `double`, while `RnState`'s inner data type is `float`. Also, since it is not relevant in adaptive time stepping, the `realrn` struct does not contain a time index component.

The **TimeStep Class**

The `TimeStep` class is the base class for all time stepping methods in `TSOpt`. The `TimeStep` class is implemented as follows:
class TimeStep: public StateAlg<TimeState>, public Writeable {
public:
    virtual ~TimeStep() {};
    void setTime(Time const & t) { (this->getState()).setTime(t); }
    Time const & getTime() const { return (this->getState()).getTime(); }
    virtual Time const & getNextTime() const = 0;
};

Note that the TimeStep class derives from StateAlg. On top of StateAlg’s functionality, however, TimeStep adds the functions setTime() and getTime() for reading and changing the simulation time. Furthermore, TimeStep subclasses must provide a read-only method to get the next simulation time, which will be suitable for adaptive time-stepping schemes. TSOpt requires that the user define a single forward, linearized and adjoint step as (inherited) TimeStep objects.

The Sim Hierarchy

The Sim class, as its name implies, is a simulator class. It orchestrates a StateAlg object, a Terminator object and a Time object in order to perform the simulation. Concrete subclasses of Sim also implement different simulation/memory managing schemes for use in either the linearized or adjoint computations. The UML diagram 3 show the subclasses of the Sim class. These subclasses, the StdSim, RASim and CPSim classes, will be explained in more detail below.

The subclass StdSim is a “forgetful” simulator; to provide the appropriate reference state during the adjoint evolution, the StdSim will run the reference simulator from the
initial time until the desired time (which is taken to be the next time level in the adjoint computation). This Sim subclass does not require the storage of the simulation state history. Further, an Algorithm called initstep that is required for the construction of the StdSim object; this allows users to write custom initialization schemes for their simulator. One example use of the initstep class is to reset the simulation state to its initial values. Given a Timestep object step and a corresponding Terminator term, the StdSim’s run method is implemented in the following manner:

```cpp
void run() {
    try {
        LoopAlg a(this->step, this->term);
        ListAlg aa(this->initstep, a);
        aa.run();
    } catch (RVLEException & e) {... }
}
```

In contrast, the subclass RASim is a “remember-all” simulator. As it runs the reference simulation, it saves all the simulation states into a user-defined stack – eliminating the need to run the reference simulation more than once. The values in the stack are then appropriately accessed during the adjoint evolution.

In order to create a stack in TSOpt, users must implement a concrete subclass of the stackBase class, which is shown in the UML diagram 4 All Sim subclasses whose function-
Other Sim subclasses exist in TSOpt; of note is the CPSim class, which uses Griewank’s optimal checkpointing scheme (Griewank and Walther, 2000). Checkpointing is the “middle ground” between the two aforementioned strategies of a “forgetful” simulator and a “remember-all’ simulator. Two types of checkpointing exist in TSOpt: offline mode for fixed time step simulations, and online mode for adaptive simulations. I discuss the notion behind checkpointing in more detail below.

Checkpointing

Recall that using adjoint method to obtain the gradient of the objective function necessitates access to the values of the state vector in reverse. This, however, can be problematic because the state vector can be large. Repeatedly recalculating the state vector, as is done by the StdSim class, comes at a computational cost of \( N^2 \) (where \( N \) is the number of time-steps) and is generally prohibitive for large problems. Alternatively, storing the whole state vector like the RASim class can be costly in terms of memory. For example, for a typical 2D Reverse Time Migration problem, storing the full state vector requires \( O(10^6 \text{ Gigawords}) \) in space and \( O(10^4 \text{ Gigawords}) \) time steps. This could lead the program to use disk-swapped memory, which adversely affects the program execution time.

To avoid the steep computational and storage costs associated with the “forgetful” and “Remember-All” strategies, Griewank proposed an algorithm called checkpointing (Griewank and Walther, 2000). The idea behind checkpointing is actually an intelligent combination of the two previously mentioned strategies: save a few states in some buffer (called checkpoints), and then forward-simulate from the nearest saved state until the time of interest. As the backward traversal continues, the checkpoints are updated such that none have been passed (and rendered useless) by the traversal. Through this process, checkpointing eliminates the need to store the whole state vector while minimizing the recomputation of states. Given some assumptions of the costs of memory access and recomputation, Griewank also proved the optimality of his checkpointing algorithm in Griewank and Walther (2000); given \( N_B \) buffers and \( N_S \) states such that \( N_B \ll N_S \), his checkpointing scheme only adds logarithmic (i.e., \( O(\log(N_S)) \)) recomputation cost.

Griewank implemented his optimal checkpointing algorithm in a package called Revolve (Griewank and Walther, 2000). Revolve has two main phases in its execution. Given the number of time steps to be taken, the scheduling phase of Revolve determines the optimal checkpoint placement. Then, the backward traversal phase dictates what should be done to complete the backward traversal of states; this explicitly states if the saved checkpoints should be used, updated, or if a forward simulation (starting from a previously saved state) needs to be performed. Generally, Revolve is used such that the scheduling phase is immediately followed by the backward traversal phase. It was shown in (Enriquez, 2008), however, that separating execution of the scheduling phase and the backward traversal phase leads to a more efficient checkpointing algorithm. The implementation of CPSim in TSOpt follows the algorithm found in (Enriquez, 2008).
Adaptive Checkpointing

In ARevolve, adaptive checkpointing works like fixed-step checkpointing algorithms, with the exception of not requiring an input of the number of time-steps to be taken. In exchange, however, the user must set an algorithmic flag to denote that the forward evolution is finished, and the simulations are ready for the adjoint simulation. The biggest limitation of Hinze and Sternberg (2005)’s checkpointing algorithm, however, is that it does not cater to taking adaptive simulation in the adjoint field. ARevolve makes the assumption that the time levels in the adjoint and reference field align, implying that the adjoint time grid will be dictated by the reference simulation. This assumption is often incorrect, as the adjoint dynamics may have very little similarities with the reference dynamics (e.g., adaptive quadrature).

I hence create the adaptive checkpointing algorithm to cater to adaptive simulations in both the reference and adjoint fields. The idea is to use ARevolve to fill (and supply nodes to) an interpolation buffer, which moves along with the adjoint simulation. Ideally, the interpolation buffer should have size $n + 1$, where $n$ is the order of the time-stepping scheme. The extra algorithmic work then comes from managing the interpolation buffer, as well as managing the calls made to the ARevolve. Algorithm ?? in the Appendix shows though pseudo-code how this adaptive checkpointing algorithm was structured.

Similar to the checkpointing algorithm in (Enriquez, 2008), the adaptive checkpointing algorithm consists of a forward mode and a backward mode – ensuring that the full forward evolution runs only once before the adjoint evolution takes place. The key difference here is the incorporation of the interpolation buffer, which itself is a deque that is being managed by a class. (The deque is a good choice for such an algorithm since push and pop operations are supported at both ends of the buffer, for $O(1)$ computational complexity.) Every time we “update” the interpolation buffer, it simply means that one slot in the buffer is replaced with a new interpolation node, such that the interpolation nodes are in order (in time).

The Time Terminator Hierarchy

Recall that the Sim subclasses requires a Terminator class, which it queries when the simulation should stop. The main criterion for when the simulation should stop is when the simulation time has reached its intended target time. To this end, TSOpt has a Terminator subclass, TimeTerminator, that is aware of the the simulation time. Like all Terminator objects, it has a query() function; this particular base class just allows the query()’s output to rely on the simulation time.

The TimeTerminator class has a variety of useful subclasses: a FwdTimeTerminator (a time terminator for forward time-marching schemes), a BwdTimeTerminator (a time terminator for backward time marching schemes), an And Terminator and an Or Terminator. The And Terminator and Or Terminator have query() functions that output the result of the logical operation of two terminators’ query() function.
The jet Hierarchy

The term “jet”, in applied mathematics, refers to a collection of a function, its derivative and its adjoint. True to this definition, the jet class is meant to hold the reference, linearized and adjoint simulators, and is at the highest level of TSOpt hierarchy. The jet subclasses require a Sim object for the forward evolution, and two triples of timestep, stateAlg and timeTerminator objects for both the linearized and adjoint evolution. This class assumes that the collection of objects pertaining to the forward, linearized and adjoint evolution are related in the appropriate sense. The following figure is a UML diagram showing the relationship between the jet class and its components.

![Jet Hierarchy Diagram](image)

Figure 5: The jet class and its components.

The jet objects provide three very important functions that return the forward evolution Sim object or create a linearized and adjoint evolution Sim objects, respectively called getFwd(), getLin(), and getAdj(). It is worth noting how this simplifies coding at the top (user) level; in order to run the forward, linearized and adjoint simulations, one would only need to code the following lines in main():

```java
... // Construct various objects that jet needs
jet j(...); // Create jet object
j.getFwd().run(); // Run forward sim
j.getLin().run(); // Run lin. sim
j.getAdj().run(); // Run adj. sim
```
**TSOPT AND UMIN**

Recall that TSOpt provides various simulation operators whose output can be used in conjunction with optimization algorithms. If we are considering a purely unconstrained optimization problem, we can use RVL’s UMin ("unconstrained minimization") package. Similar to TSOpt, UMin was created by subclassing Alg components. Currently, the LBFGS and Conjugate-Gradient Trust-Region (CGTR) algorithms are available in UMin.

To use the UMin package, the user must create three RVL::FunctionObjects. In RVL, FunctionObjects act on RVL data containers, mimicking a (mathematical) operator acting on a variable. FunctionObjects are based on the “Acyclic Visitor” design pattern (Gamma et al., 1998), which “allows new functions to be added to existing class hierarchies without affecting those hierarchies, and without creating the dependency cycles.” In order to use the UMin package, a FunctionObject must be created to supply the following by using the Jet object: objective function evaluation, the gradient vector evaluation and the Hessian matrix evaluation.

The collection of FunctionObjects will be used to construct an RVL::Functional object, which is the interface for scalar-valued vector functions. Functional objects must provide first and second derivatives (gradient and Hessian), by using the FunctionObjects mentioned above. For example, the code below shows generic code that uses the Jet object to form a gradient FunctionObjects and Functionals.

```cpp
class GradFunctionObject{
private:
  jet j;

public:
  void operator()(LocalDataContainer<Scalar> & y,
                 LocalDataContainer<Scalar> const & x) {
    jet.setControl(x);     // set control for fwd/adj sim.
    jet.getAdj().run();     // run adjoint simulation
    jet.getAdj().getGrad(y); // get gradient via reference
  }
};

class ExampleFunctional {
protected:
  virtual void applyGradient(const Vector<Scalar> & x,
                              Vector<Scalar> & g) const {
```
TSOpt: Time-Stepping for Optimization Software

GradFunctionObject<Scalar> f(...); // make GradFunctionObject
g.eval(f,x); // eval uses overloaded ()
// operator defined in
// GradFunctionObject

}

The Functional object is used to make a FunctionalEvaluation object, which in turn, can then be passed to the UMin framework to perform the optimization. For a more thorough discussion of this process, and the associated classes, see (Padula et al., 2009).

**TSOpt AND EXTERNAL OPTIMIZATION PACKAGES**

Sometimes, it is necessary to consider explicit constraints for the optimal control problem. For example, my target application is an optimal control problem with (oil) reservoir simulation constraints. This problem features equality and bound constraints, representing physical limitations of a reservoir model and its wells. To deal with such problems, it is necessary to turn to external optimization packages that can handle explicit constraints. Fortunately, TSOpt’s modular design allows easy linkage with external optimization packages via the Jet object. Chapter 5 provides a specific example of how the Jet object links TSOpt to the optimization software IPOpt (“Interior-Point Optimizer”). IPOpt (Wachter, 2002) is open-source software designed to solve large-scale nonlinear optimization problems, and is capable of handling nonlinear equality and inequality constraints. IPOpt uses an interior-point method to generate search directions for the nonlinear optimization problem, then applies a filter linesearch globalization scheme.

**EXAMPLE: OPTIMAL WELL-RATE ALLOCATION**

The Optimal Well-Rate Allocation (OWRA) can be posed as the following problem: find the pumping and injecting rates for reservoir wells over a certain time window, as to maximize profit. Solving OWRA via optimal control theory is not a new topic; previous attempts have been made by Brouwer and Jansen (2004) and Sarma and Aziz (2005), for example. In this report, we solve the problem posed by Wiegand et al. (2008), that finds the optimal well rate that will maximize revenue from oil production, while penalizing water injection and production:

$$
\min_{q_i \in I \cup P} \quad J(q) = \int_0^T dt \left( \sum_{i \in P} \alpha (1 - s_a) q_i(t) + \sum_{i \in P} \frac{\beta}{2} s_q^2 q_i^2(t) + \sum_{i \in I} \gamma q_i(t) \right),
$$

(3)

where $q_i$ are the well rate at the $i$ is an index representation a location in the domain, $I$ is set of indices that correspond to injecting wells, $P$ is a set of indices that correspond to producing wells, $\alpha$, $\beta$ and $\gamma$ are scalar variables. By convention, we assume that the
producing well rates are represented as negative numbers, and injecting well rates are represented by positive numbers. The aqueous pressure \( p \) and aqueous saturation \( s_a \) solve the 2D, two-phase, incompressible Black-Oil equations:

\[
-\nabla (K(x)\lambda_{tot}(s_w(x,t))\nabla p(x,t)) = \sum_{i \in P} (1 - s_a)q_i(t)\delta(x - x_i) + \sum_{i \in P \cup I} s_aq_i(t)\delta(x - x_i)
\]

\[
\phi(x)\frac{\partial}{\partial t}s_a(x,t) - \nabla \cdot (K(x)\lambda_a(s_a(x,t))\nabla p(x,t)) = \sum_{i \in P \cup I} s_aq_i(t)\delta(x - x_i). \tag{6}
\]

In the equation above, \( K \) represents permeability, \( \lambda \) represents phase mobility and \( \phi \) represents rock porosity. The Black-Oil Equations stem from the phase continuity equations, which capture simultaneous, physical fluid flow behavior of up to three immiscible phases (namely: water, oil and gas). The Black-Oil Equations assumes that no mass transfer behavior between the water phase and the other phases occur, and is often used to model low-volatility oil systems (Peaceman, 1977).

Further, we incorporate explicit equality and inequality constraints on the well rates to model the physical limitation of the reservoir and the wells. We require that the sum of the well-rates add up to zero, which enforces a reservoir pressure condition. Also, we require that the well-rates satisfy bounds. Incorporating these explicit constraints, using a finite volume spatial discretization and a backward-Euler time-stepping scheme yields the following discretized optimal control problem:

\[
\min \ J_{\Delta t}(q) = \Delta t \sum_{k=1}^{N} l(t^k, s^k, q^k) \tag{7}
\]

\[ s.t. \quad e^T q^k = 0 \tag{8} \]

\[ q_{min} \leq q^k \leq q_{max}, \tag{9} \]

where \( s^{k+1} \) and \( p^{k+1} \) solve:

\[
\begin{bmatrix}
g(t^{k+1}, s_a^{k+1}, p^{k+1}, q^{k+1}) \\
f(t^{k+1}, s_a^{k+1}, p^{k+1}, q^{k+1})
\end{bmatrix}
:=
\begin{bmatrix}
q - Ap^{k+1} \\
D^{-1}(q_a - A\tilde{p}^{k+1})
\end{bmatrix}
= \begin{bmatrix}
0 \\
\frac{s_a^{k+1} - s_a}{\Delta t}
\end{bmatrix}, \tag{10}
\]

and the function \( l \) hides the objective function integrand:

\[
l(t^k, s_a^k, q^k) = \sum_{i \in P} \alpha(1 - s_a^k)q_i^k + \sum_{i \in P} \frac{\beta}{2}s_a^k(q_i^k)^2 + \sum_{i \in I} \gamma q_i^k. \tag{11}\]

The matrices \( D, A \) and \( \tilde{A} \) are defined in the following manner:

\[
A_{i,j} = -T_{i,j}\lambda_{t_{i,j}} \quad \hat{A}_{i,j} = \sum_j T_{i,j}\lambda_{a_{i,j}} \tag{12}
\]

\[
D_{i,i} = \phi_i \cdot |\Omega_i| \tag{13}
\]

\[
\hat{A}_{i,j} = -T_{i,j}\lambda_{a_{i,j}} \tag{14}
\]
The transmissibility between cell \( i \) and \( j \), \( T_{i,j} \) is defined as

\[
T_{i,j} = \frac{K_{i,j} A_{i,j}}{l_{i,j}},
\]

where the length between the barycenter of the cells \( i \) and \( j \) are denoted as \( l_{i,j} \) and the area of the face between two cells are denoted as \( A_{i,j} \).

Applying the optimality conditions to the fully discretized optimal control problem above yields the following adjoint evolution scheme. For \( k = N - 1, \ldots, 1 \), simultaneously solve for the adjoint variables \( \lambda_{s}^{k} \) and \( \lambda_{p}^{k} \) in the following equation:

\[
-\frac{\lambda_{s}^{k+1} - \lambda_{s}^{k}}{\Delta t} = D_{s} f(\ldots)^{T} \lambda_{s}^{k} - D_{s} g(\ldots)^{T} \lambda_{p}^{k} - \nabla_{s} l(\ldots) \tag{16}
\]

\[
0 = -D_{p} f(\ldots)^{T} \lambda_{s}^{k} + D_{p} g(\ldots)^{T} \lambda_{p}^{k}. \tag{17}
\]

After completing the adjoint evolution, the directional derivative of the objective function with respect to the wellrates \( q \) can be obtained from the following expression:

\[
\nabla J(q) \delta q = \sum_{k=1}^{N} \Delta t [\nabla_{q} l(\cdot)^{k} - D_{q} f(\cdot)^{k} \lambda_{s}^{k} + D_{q} g(\cdot)^{k} \lambda_{p}^{k}]^{T} \delta q^{k}. \tag{18}
\]

In order to use TSOpt to solve OWRA, we create a reference and an adjoint simulator, as well as a stack type that holds the primary variables \( p \) and \( s_{a} \). These simulators were then used to create an existing Jet class in TSOpt. The following show the algorithmic work behind the forward and the adjoint simulator.

- **BlackOil Forward Simulator** (solves discretized Black-Oil equations)

\[
\begin{bmatrix}
q - Ap^{k+1} \\
D^{-1}(q_{a} - \bar{A}p^{k+1})
\end{bmatrix}
= \begin{bmatrix}
0 \\
\frac{s_{a}^{k+1} - s_{a}^{k}}{\Delta t}
\end{bmatrix}
\]

Solution approach:

* solve for \( p^{k+1} \) and \( s^{k+1} \) simultaneously using Newton-Raphson
* linear system solves via UMFPACK

- **BlackOil Adjoint Simulator**

\[
\begin{bmatrix}
D_{s} f(\bar{q},p^{*},s^{*})^{T} \\
-D_{s} g(\bar{q},p^{*},s^{*})^{T}
\end{bmatrix}
\begin{bmatrix}
\lambda_{s}^{k+1} \\
\lambda_{p}^{k+1}
\end{bmatrix}
= \begin{bmatrix}
\frac{\lambda_{s}^{k} - \lambda_{s}^{k+1}}{\Delta t} + \nabla_{q} l(\bar{q},p^{*},s^{*}) \\
0
\end{bmatrix}
\]

Solution Approach:

* solve for \( \lambda_{p}^{k+1} \) and \( \lambda_{s}^{k+1} \) (linear system solve via UMFPACK)
* note: gradient accumulation is accomplished during the adjoint simulation
We now try to solve OWRA on a rectangular domain, composed of $220 \times 60$ cells, over a 200 day timespan. We set the initial guesses of the wellrates to 10 barrels per day, for all the injecting and producing wells. Further, we impose that wellrates must stay within the bound $[0, 20]$ barrels per day. We couple the BlackOil simulators with TSOpt and the optimization software IPOpt. Further, we use the data seen in figure 6 for porosity, permeability and well locations. Looking at the plot of producers and injectors we see that producing well 4 and injecting well 4 are deemed “too close” to one another. After some time, the water that placed into the reservoir by injector 4 will immediately be ejected by producer 4, implying a waste of resources. Hence, we expect to see the optimizer to throttle the rates for either producing well 4 or injecting well 4. As we can see from figure 8, the fourth producing well’s rate was indeed throttled by the optimizer. We note that the objective function (figure 7) significantly increased in value, over the initial guess for the wellrates.
Figure 7: Objective function for the fixed time-stepping approach to solving OWRA.

Figure 8: Progression of the control parameter for the first [l], third [m] and sixth [r] optimization iteration, taking fixed time steps. Note the well labels on the figure: “P” represents the producing wells and “I” represents the injecting wells.
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