

Letter of Transmittal

Subject. High Performance Computing in Natural Resources.

Purpose. This report focuses on Hatch project, and the challenges with managing data in the scientific research environment. The goal is to introduce new approaches to organizing data, and making it more searchable. The Hatch project creates a foundation for a tool that allows users to upload, search, format, and visualize their data in ways they didn't think of before. This report highlights some of the problems with computation and data management in the current research environment, and makes suggestions for new approaches. It talks about specific algorithms for searching data, and standards for formatting and storing it.

Background. The amount of data being stored in scientific databases today is growing exponentially. The amount of computational power in cpu's, however, is no longer growing exponentially. The consequence is an gap opening between data and results. Researchers are trying to build and rebuild their computational infrastructure, to try to get computational growth back to the pace of data growth. But in this report, we suggest a complimentary approach to computing research data. The Hatch project comes from the idea that a significant amount of research data is redundant or not wanted. But it is also vast and not managable. Researchers end up wasting computation time on data points and sets that they do not care about, at the expense of ones they do care about.

Preliminary Work. With the experience of the authors of this report, there is more than 8 years of work in computer science, bioinformatics, and natural resources. There is 2+ years of work in computing clusters for the University of Idaho Initiative for Bioinformatics and Evolutionary STudies (IBEST), as well as 1.5 years of research in wildlife management.

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Abstract

With today's exponential increase of data, the demand for processing is outpacing the supply. The way we processed data yesterday would take years to do today. Unfortunately, the lack of fluency with computing in today's research proposals results in processing a fraction of the data collected. This weakens research projects, and leads to a lot of unnecessary data collection.

Today's researchers need tools to become more efficient with processing data. Until computation can keep up again with exponential data growth, researchers will need to carefully select the data that they want to do research on, and throw away data that will not yield results. The users of such tools range anywhere from fish researchers in the Columbia Basin, to bioinformaticians, to economists, and more. Having more searchable, usable data applies to almost everyone, and the use cases and usefulness of a tool like Hatch are endless.

1 Project Summary

In today's scientific environment, there is a growing focus on data storage and processing. Some of the largest problems scientists face are related to the data deluge, and the inability to conceptualize problem and solutions from large tracts of data. The result is many attempts by scientific professionals to design software, leading to many bad software designs. Vast amounts of expensively collected data never get processed, because the software designs take so much maintenance. Data is often duplicated, often in different locations, lost, or never makes it from collection to analysis. The overall lack of system designs to handle the data further hinders analysis.

This proposal is for a project that helps solve these design problems for many scientists. The project is a data harvester and organizer tool. It is a local web interface that allows scientists to collect, query, organize, and share data with other researchers. Many of these scientists work with similar data sets, ask different questions, and need immediate search tools. The proposed tool would first allow users to visualize and filter data, and secondly prepare and ship the data off for analysis. It also helps users visualize data graphically, to help the conceptualize, organize, and refine data, before transporting and processing it. This project proposes using PTAG and other ecological data sets from the Columbia Basin to test design, but should be extendable to many different users with very different data sets.

The tool will not overlap with the functionality of existing tools like PTAGIS or DART. It will carefully handle data sharing, choosing opt-in, lock-down policies by default.

1.1 Background

In the Columbia Basin today, millions of federal dollars are spent on PTAG and other systems to collect environmental data. This data includes fish location, ecological community composition, and abiotic data. Yet, the project results from most research are far from concrete. Despite the lack of understandable results, important decisions that affect the local environment and economy have to be made. Decisions like whether or not to conduct major habitat restoration projects.

The Columbia Basin is just one small example. Bioinformatics is another data intensive study that generates more data than it can process. It is estimated that less than 10% of the data collected by bioinformatic researchers at the University of Idaho actually makes it through processing [?]. The rest has to be filtered as best as can be managed, and the low value data trimmed out. The problem with 10% data use, is that not just the fat, but the meat and bone has to be cut away. Either significantly more data must be analyzed, or significantly less should be collected. At the very least, storing the data in an easily readable format can show where the gaps are. So far, our experience and research shows similar shortfalls in data analysis in the Columbia Basin.

1.2 Problem Statement

One of the biggest problems researchers in the Columbia Basin have is getting their data somewhere meaningful. Central databases like PTAGIS offer a central storage and clients can push data there, but they don't offer useful tools for managing data. Once the data is pushed, it is hard to access

and manipulate. Researchers are often in remote locations, and have low bandwidth connections. Creating a robust tool will guarantee ease of use for the data, no matter the location.

Many researchers have significant data management tasks before even thinking about pushing data to the cloud. Once they are ready, they need seamless ways to synchronize data to and from the cloud. They also may want to query their data, and filter it into small subsets. Most researchers don't have time to learn new programming language or interfaces. They need a data management tool that has a user interface that is familiar to use cases they already understand. Once they have created a data subset, they will want to share it, save it, copy it, and compare it with other data sets. Getting the right data to the right place in the right amount of time is crucial.

1.3 Objectives

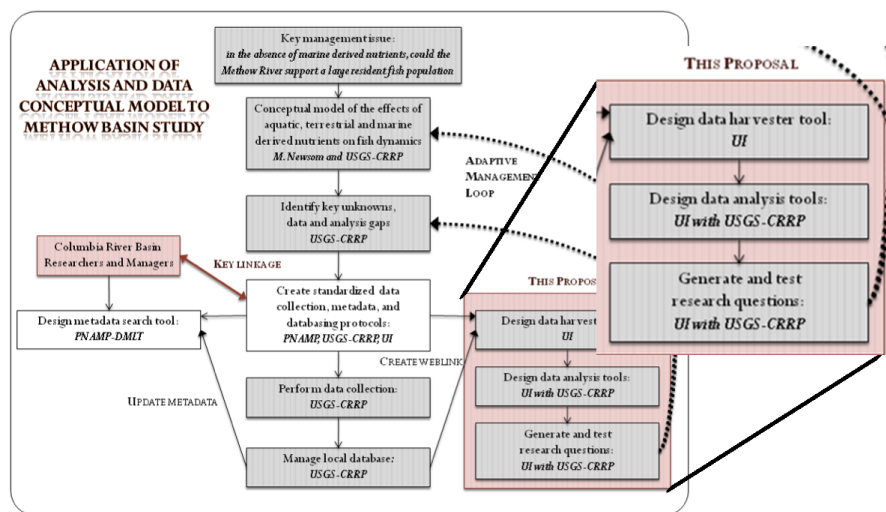


Figure 1: This proposal software's application domain in DE-CRRP

The proposed project will tackle the UI data harvester portion of the grant funded USGS-CRRP project (Figure 1), directed by Alex Fremier of the UI College of Natural Resources. The data management tool will be a web-like GUI that can be installed locally on the clients' computers. The tool will contain an expandable meta data server that can be connected to others, for a **decentralized** data storage cloud. The cloud will consist of the many instances of the tool, acting as a cloud of **decentralized databases**. It will contain an interface to an existing or custom **networking protocol** that will allow for many different data formats to be synchronized across the cloud. The project will also have graphic interfaces for **seamless data management**.

The decentralized cloud model allows some serious advantages to researchers. They can see exactly what their data looks like, before they submit it. They can filter out bad data before it consumes bandwidth, and can retract undesirable data from the cloud, even after synchronizing it. It also frees them from central storage service management and fees, and **encourages internode and inter-research communication**. The tool can be setup on multiple hosts, and can be used

for the benefits of the centralized cloud model. Each client can decide what topology suites them best.

The decentralized cloud model implements a distributed database model. Distributed databases increase availability and reliability. They are more easily expandable, and can better protect from data loss from local disasters or malicious attacks. Moving data to where it is in highest demand also increases query performance. Offloading archive data to remote site with more resources preserves local resources. Replicated datasets can guarantee better availability. By staging data locally and filtering it before allowing it to be exchanged, the autonomy of the organization is better preserved.

The network protocol will allow incremental synchronization of data from host to host, even in less reliable environments. The tool will create an **outreach** from researchers in high availability areas to those in low availability, low bandwidth areas, and back. The network protocol will have support for major data formats (i.e. SQL, CSV, more), and allow users to send incremental pieces of the data. In the case of very large data sets or low bandwidth, the receiver of the data can still use it. Whether the data takes more time to transfer, or never completes.

The seamless interface will allow users to sort their data needing only basic knowledge of computers. Users will be able their mouse to select datasets and apply filters to them. The tool will allow them to query local or remote data, or to dynamically join both. Queries will create data subsets that users can bring to a workspace. The tool will be able to sort data however the user likes, on the fly. It will then be able to graph the ranges in the subset in most ways the user could want to sort them.

Once the user has manipulated their data subset to their satisfaction, they will be able to save it in the meta data server's format, or in a set of major data formats. The tool will also have analysis modules that will allow them to run analysis on the local host. These modules will be extensible to running analysis jobs on other designated compute hosts, like workstations, clusters, or even Amazon's EC2. The tool will come only with basic functionality for local analysis modules, but will be extensible to the heavier compute options.

2 Database

2.1 Introduction

One of the biggest challenges with Hatch was how to organize data. Specifically, pretty much every organization with scientific data has their own standard or format on how they store research data. Many of these organizations want to share data between each other, but they cannot decide how to merge the formats. Consider the following examples:

site	datetime	unique fish tag
TUC	02/16/06 19:08:15	3D9.1BF1E7919A
TUC	02/16/06 19:18:36	3D9.1BF1A998FA
TUC	02/17/06 18:21:03	3D9.1BF20E8FE2
...

Figure 2: A database representing for PTAGIS data

unique fish tag	DNA sequence
3D9.1BF1E7919A	ATGCTTAC...
3D9.1BF1A998FA	TTACGATC...
3D9.1BF20E8FE2	GTGGASCT...
...	...

Figure 3: A database representation for DNA data

In each of the examples above, the data is represented with **rows** and **columns**, much the same way someone would represent the data in a Microsoft Excel spreadsheet. These structures in a typical **relational database** (SQL, etc). are called **tables**.

The above examples are simplifications of the rows and columns in actual research data. But they highlight one of the biggest issues with data storage using relational databases: they require you to know the column names ahead of time. Not only that, but they require that you know the data types of the values that go in those columns, and once a table is created expecting a certain format, it is hard to change.

The problem with needing to know the structure of research data before designing databases, is that research data **is semi-structured**, at best. Once it does represent some structure, it often changes. For example, once researchers finally decide what columns and data types should go in the table in Figure 2, another researcher suggests more columns that should go in to the table.

This leads to endless edits to the database and program design by some software developer. The standard table format that everyone can agree on isn't useful to many researchers, because it usually leaves out a lot of other needed columns and fields.

A better approach is needed. Researchers, not committees, should decide how to store data. Data should be mergable based on common values in different tables (like the **unique fish tag** column in Figures 2 and 3. The person who inputs the data should decide how one particular

dataset is stored in a database, and should be able to choose to store the same data in a different table format, how they choose. There should be a simple tool that helps them do this.

The following sections describe different approaches to implementing a database design that enables data storage for dynamic or semi-structured data.

2.2 Relation Databases with table creations

This approach is the simplest and follows the concept of table creation for data sets pretty closely. Basically, for each input document in the form of a spreadsheet, a new SQL table is created. The columns names and type are determined from the headers and data values in the spreadsheet.

```
CREATE TABLE ptagis_doc1
(
    id int ,
    site char(50) ,
    read_data_time date ,
    tag char(50)
);
```

Figure 4: The SQL syntax for creating the table in Figure 2

The biggest problem with this approach with this approach is that each document in the database is a table. When searching for a specific document, the database typically searches for the table name. This search is linear, and with hundreds, thousands, or hundreds of thousands of documents, frequently searching the database to look for values would be infinitely slow and useless.

Another problem with this design, is that building an interface like a web gui would be difficult and complicated.

2.3 Relational Databases with tables for each datatype

Another approach is to create column tables for each data type, and let document tables just be collections of columns. Each of the document column values point to respective values in the column tables.

This allows for documents to have a dynamic amount of columns with variable data types. But there are two problems with this approach. First, for every value in every document in the database, they are put into one table (i.e. all values with a 'string' data type go into the 'string' table). With potentially millions of data values, each table becomes an overflowing bucket, and don't utilize the the advantages of storing multiple columns and values in one table. Searches for data would require lots of filtering for just the ones wanted for specific documents, and would be inefficient.

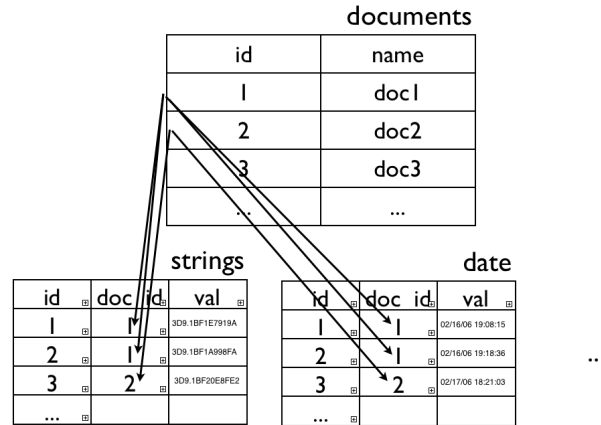


Figure 5: Document table as a lookup table

The other issue is that every retrieval of data from a document would require lot and lots of lookups. Data retrieval over significantly high data sets would quickly become very computationally intensive, and not practical.

2.4 CouchDB

When one thinks about the fundamental issues with storing, searching, and merging research data, a core issue is identified: data is semi-structured. This is what makes trying to use relational databases so hard. They were made for datasets where you knew the structure up front, and seldom wanted to change their structures.

The one assumption that Hatch makes about the data is that **there are rows and columns**. This is the only assumption Hatch makes. This leaves the database and interface designs free from whatever changes are needed by the users.

This is done by storing data in JSON format. The data is stored in an array of hashes, modeled exactly like how Ruby on Rails 3 returns records from its Active Record. This allows users to input data however they like, define delimiters for columns using Hatch Input Filters, and Hatch does the rest. It finds the most specific data type the values can be stored in, skips non-matching entries, and populates all the forms on the web pages according to the data. All without actually knowing the structure of the data.

This leads to the technical implementation of the Hatch Database.

2.5 Hatch Database

Since Hatch uses Ruby on Rails, there are lots of tools and libraries for using the standard relational database, via Rails' Active Record. In many/most cases, Hatch actually wants to stick to the relational database. With Hatch's internal database structured, order is important. For example, a user will always have a name, email address, etc. A document will always have a name and

an owner. But the data in the document is the semi-structured data. Hatch only wants to use CouchDB for that.

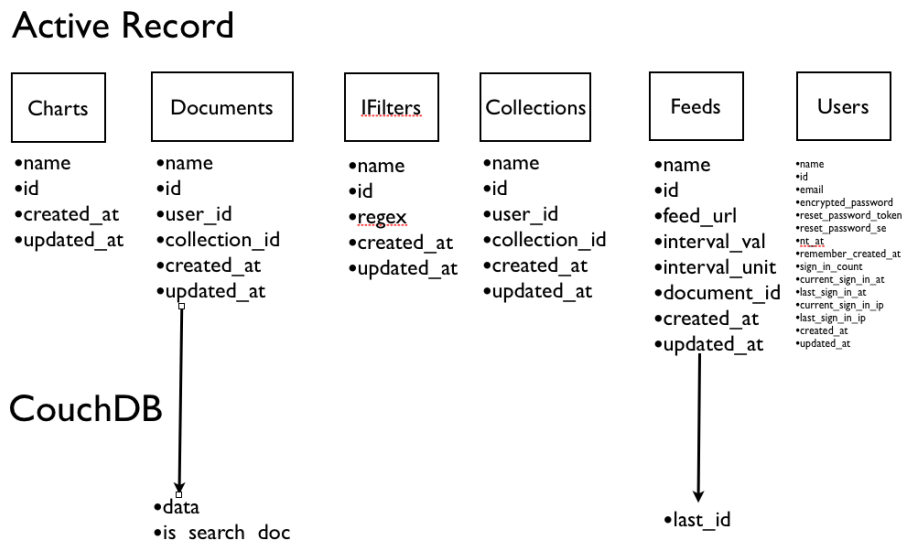


Figure 6: The Hatch relational - non-relational database hybrid

The result is a relation - non-relational database hybrid. Hatch uses traditional relational database columns when the columns are ubiquitous, and can add columns to a database entity (called scaffold) on the fly using CouchDB. For example, we create a scaffold called Documents. Document always have a name, id, and collection/folder they belong to. But, documents may have a data section, or they may not. That data section may have infinite columns and rows of data, that would match the flat file they came from (like an Excel file). Or document may have any other data that can be stored in JSON format. It is up to the Hatch interface, not database, to decide. And by allowing the interface to decide the structure and fields of data, Hatch is by extension allowing the user to decide how to format data.

Field	Value
_id	"Document-93"
_rev	"9249-b28848a4e69c5cbc17badd089f97757a"
data	<pre>[{ "date": "Sat Apr 28 07:11:34 PDT 2012", "l": 1357, "id": 9241 }, { "date": "Sat Apr 28 07:11:34 PDT 2012", "l": 1357, "id": 9242 }, { "date": "Sat Apr 28 07:11:34 PDT 2012", "l": 1357, "id": 9243 }, { "date": "Sat Apr 28 07:11:34 PDT 2012", "l": 1357, "id": 9244 }, { "date": "Sat Apr 28 07:11:34 PDT 2012", "l": 1357, "id": 9245 }, { "date": "Sat Apr 28 07:11:34 PDT 2012", "l": 1357, "id": 9246 }, { "date": "Sat Apr 28 07:11:34 PDT 2012", "l": 1357, "id": 9247 }]</pre>
last_id	9247

Figure 7: Typical representation of document data in CouchDB / JSON

Most Rails applications that use CouchDB completely replace Active Record with some library's version of it, like **couchrest's Active Model**. But if you replace Active Record, you lose tons of support for libraries that lots of Rails developers make, like pagination.

Hatch gets around this by using its database hybrid, using a Ruby library called **stuffing**. Stuffing is a link that ties Rails Active Record records with CouchDB documents. It allows for rapid prototyping in development, and is a nice, modest alternative to ripping out the guts of Active Record. Since the base model for database scaffolds are still Active Record, the huge amount of Rails Active Record based libraries still work.

3 Bibliography

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