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Prepared for the U.S. Department of Energy  
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Contractor for the U.S. Department of Energy  
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# Hanford Site Composite Analysis Technical Approach Description: Integrated Computational Framework

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*Kevin J. Smith, Ph. D.*  
*February 2017*

## APPROVAL PAGE

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~~MODELING ATMOSPHERIC TRANSPORT~~ INTEGRATED COMPUTATIONAL FRAMEWORK <sup>REV</sup>

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Date

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5/30/17  
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## Terms

CA	composite analysis
DAS	disposal authorization statement
DBWA	databased-backed web application
DOE	U.S. Department of Energy
EMDT	electronic modeling data transmittal
ICF	integrated computational framework
QA	quality assurance
QA/QC	quality assurance and quality control

## 1 Introduction

The U.S. Department of Energy (DOE) in DOE O 435.1 Chg. 1, *Radioactive Waste Management*, requires the preparation and maintenance of a composite analysis (CA). The primary purpose of the CA is to provide a reasonable expectation that the primary public dose limit is not likely to be exceeded by multiple source terms that may significantly interact with plumes originating at a low-level waste disposal facility. The CA is used to facilitate planning and land use decisions that help assure disposal facility authorization will not result in long-term compliance problems; or, to determine management alternatives, corrective actions, or assessment needs if potential problems are identified.

A CA is not prepared to demonstrate current compliance; rather, its purpose is to model potential future exposure events. In other words, a CA is a DOE planning tool, used to provide a reasonable expectation that DOE public radiation protection requirements will be met over the long-term after the DOE site achieves its projected end state. Furthermore, the CA is a prerequisite to acquire and maintain an operational Disposal Authorization Statement (DAS) for low-level waste disposal facilities and to achieve closure of tank farms.

CAs are closely linked with performance assessments for specific disposal facilities, which DOE uses to demonstrate that there is a reasonable expectation that the performance objectives will be met for a given facility. CAAs may be documented in a companion report to the performance assessment, or integrated in the same report with a PA. At the Hanford Site, with numerous separate disposal facilities and tank farms, the CA has been developed and maintained as a separate document that includes all facilities contributing to dose at a specific boundary for supporting performance assessments for several low-level waste disposal facilities at the Hanford Site.

The currently maintained CA for the Hanford Site is documented in PNNL-11800, *Composite Analysis for Low Level Waste Disposal in the 200 Area Plateau of the Hanford Site*, and the subsequent Addendum 1 (PNNL-11800-Addendum-1, *Addendum to Composite Analysis for Low Level Waste Disposal in the 200 Area Plateau of the Hanford Site*). The annual summary report for this CA for fiscal year 2015 reached the determination that an update to the Hanford Site CA is necessary based on information reviewed for fiscal year 2015 as well as information presented in prior annual status reports. DOE has initiated work to develop a revised CA followed a phased approach with planning, scoping, and analysis phases. The scoping phase will culminate in the development of a detailed technical approach for preparing the revised CA. This technical approach description document presents the approach for the integrated computational framework (ICF) as one facet of the overall technical approach. This is a companion document to a series of other technical approach description documents for various facets of the revised CA.

## 2 Overview

This technical approach document describes the proposed design for an ICF to support efficient calculations to generate, and maintain, the updated CA. The proposed design is expressly developed to meet the scope of the updated CA, as defined in the key aspects identified in Table 1 of CP-60649, *Summary Analysis: Hanford Site Composite Analysis Update*.

The CA is divided into a series of modeling efforts that each focus on one problem domain; examples include the Inventory database, waste form release models, vadose zone flow and transport models, aquifer flow and transport models, and dose calculators. This division is useful conceptually, because different modeling techniques are appropriate for different problem domains. This partition is also useful from the point of view of project management, because each unit of work requires specialized expertise.

While each partition represents a complicated collection of data and operations on that data, it is sometimes useful to think of them collectively as a series of connected blocks or *facets*. In this construct, information generally flows unidirectionally from an upstream facet as input to the next, downstream facet; for example, results from the vadose zone and transport models generally condition and constrain the aquifer flow and transport models. These model facets are discussed in detail in the following companion technical approach documents:

- CP-60195, *Hanford Site Composite Analysis Technical Approach Description: Radionuclide Inventory and Waste Site Selection Process*
- CP-60410, *Hanford Site Composite Analysis Technical Approach Description: Waste Form Release*
- CP-40605, *Hanford Site Composite Analysis Technical Approach Description: Vadose Zone*
- CP-60406, *Hanford Site Composite Analysis Technical Approach Description: Groundwater*
- CP-60409, *Hanford Site Composite Analysis Technical Approach Description: Groundwater Pathway Dose Calculation*

The signal flow between the facets is shown in Figure 1.

While the above approach is convenient, it is nevertheless important to employ a system that unifies work, aggregates results, and prevents errors in the handoff of data during transition. This is particularly important for quality assurance (QA), since upstream errors are likely to have a compounding effect on downstream operations. Furthermore, the computational runtimes associated with modeling runs can last weeks; an upstream error can easily create a project bottleneck, waste resources, and risk cost overrun. During the scoping phase, the ICF was proposed as a system that would address the above concerns by performing the following services:

1. Automate and enforce QA procedures where possible;
2. Store data and results;
3. Handle and track the transfer of information between modeling efforts; and
4. Provide a platform for communicating results.

The ICF is thus analogous to the CA's nervous system; it relays information among model facets and provides users with a platform for saving and viewing state information, visualizing results, and enforcing QA. The ICF is shown schematically as the gray box in Figure 1 and the lines connecting the various model facets. This document first describes how the ICF supports the flow of information between the various CA components and then details the technical approach to the ICF's design itself.

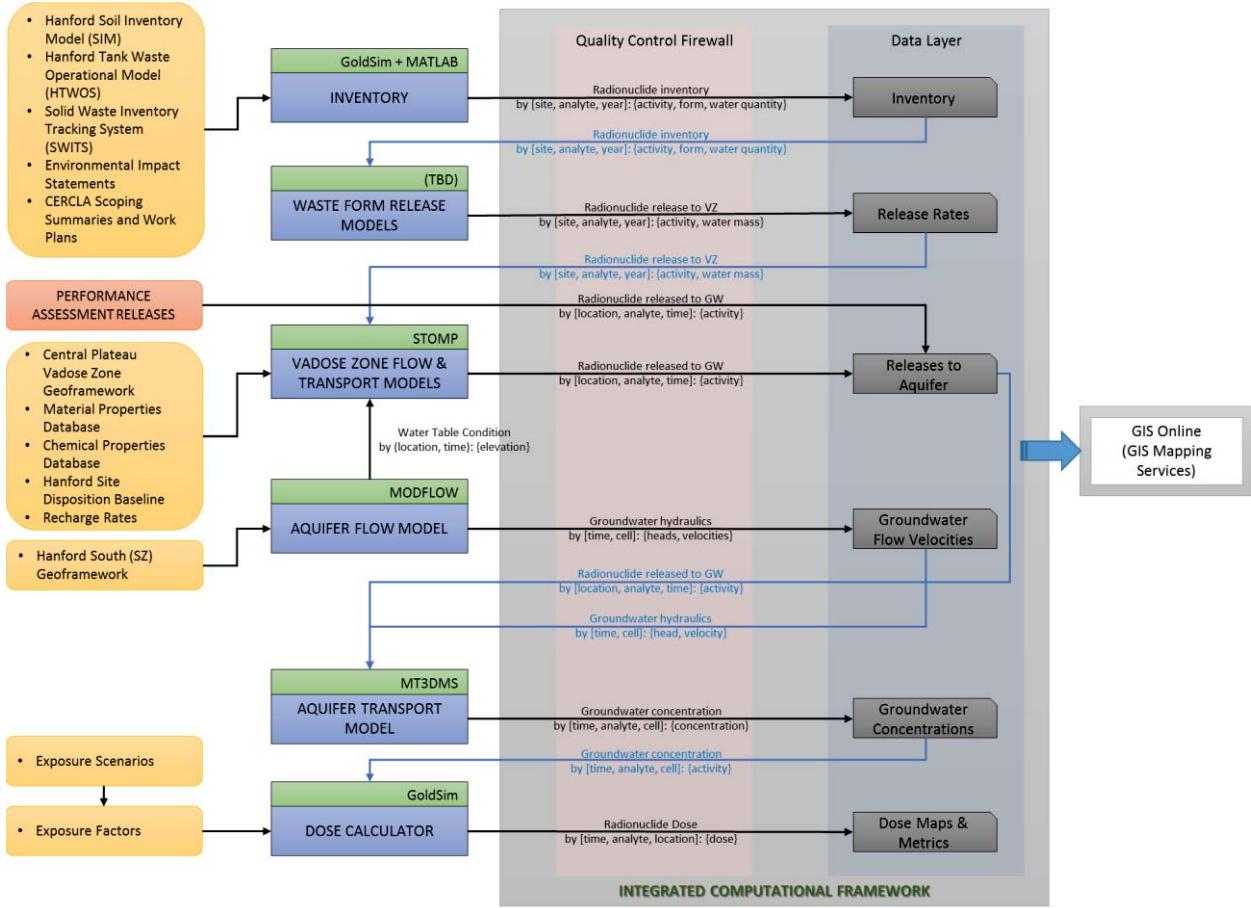


Figure 1. Composite Analysis Component Diagram (Preliminary)

### 2.1.1 Information Persistence

One complete cycle through the CA's workflow generates a large volume of data in the form of model results, reports, and QA documentation. Occasionally, a new discovery or observation precipitates a change for one facet and triggers a new cycle through all downstream facets. For example, field activity may result in an update to the geoframework model that provides new information about the aquifer, thus triggering an update to the groundwater flow and transport models. Likewise, the exposure calculations must be rerun since they depend on the groundwater facets.

These dependencies mean that it is important for the ICF to track the pedigree of data, as well as how one facet's results are related to other facets. The ICF handles this by storing data packages and run information (such as the user, state of QA checks, etc.) in a relational database. This method allows related results to be retrieved and inspected on demand; the ICF thus functions as a memory system.

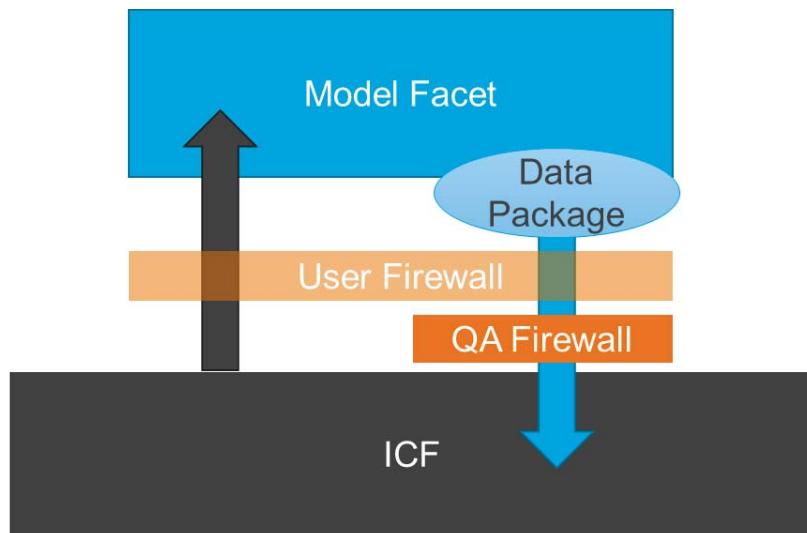
### 2.1.2 Information Transmission

Each facet has its own defined set of inputs and outputs with differing indexing; keeping track of all of them simultaneously leads to a growing multiplicity of state information and risks transcription errors due to the high volume of information that is passed through the CA. The ICF deals with this problem abstractly by working with and storing encapsulated *data packages*, which are a group of a facet's model data and metadata. Model data includes input files, run conditions, and model outputs; metadata might include things such as timestamps, user information, and a report of hardware qualifications.

Rather than chaining model facets in series and sending outputs directly from one facet to another, the ICF interacts with each facet independently and stores only qualified data centrally. This strategy emphasizes modular development; since the ICF does not depend on the details of the model facets themselves, components may be developed, maintained, or added independently.

The relationship of a model facet to the ICF is shown conceptually in Figure 2.

Once a user has completed a unit of work, a data package is created and sent through firewalls that restrict user access and enforce QA and data integrity. Data is logged in the ICF and available to other facets only if its data package conforms to specifications and QA checks described in the companion document CP-60411, *Hanford Site Composite Analysis Technical Approach Description: Automated Quality Assurance Process Design*.



Note: The ICF (black box) supports the flow of information (arrows) from a common repository to each model facet (blue box). The ICF's design treats model facets independently (only one is shown here); data is sent to the ICF in the form of a data package (blue oval) through a series of firewalls that enforce security and assure quality. Data not passing QA checks cannot be submitted to the ICF.

**Figure 2. Relationship of a Model Facet to the ICF**

### 3 Components

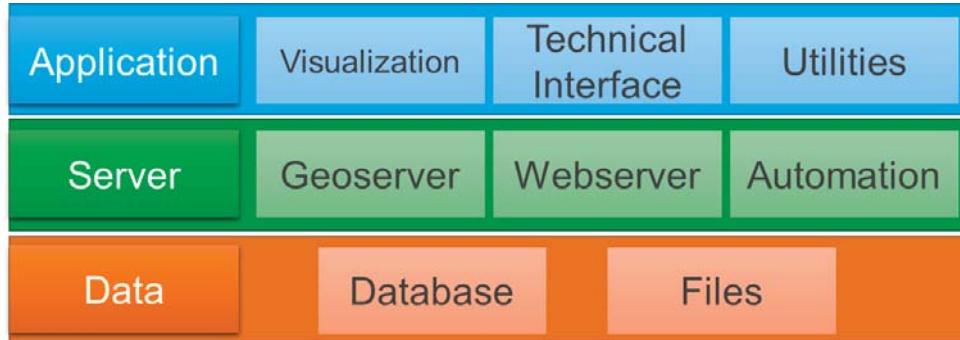
The previous section described the ICF from a functional perspective by considering how it interacts with model facets. This section describes the components of the ICF itself and details how each component will be implemented.

The primary objective of the ICF is to provide a CA state machine that supports QA enforcement. We have settled on an approach that supports the development of database-backed web applications (DBWA) for the following reasons:

1. The user may only interact with data through a series of controlled applications.
2. QA checks may be applied whenever data is entered to the system.
3. A web-based platform is device independent in that users can access the ICF through any major web browser.

4. The developers maintain all hardware; updates are automatically pushed out to the user through their web browser.

The above approach divides the ICF into three layers, as shown in Figure 3. Since the primary unit of the ICF is data in form of state information, the foundation is composed of a database and file system. Access to this layer is highly restricted to enforce data integrity. The server layer (green) is composed of programs that relay information to and from the data layer. Users may only interact with the ICF through the application layer (blue), which provides the user with a series of web pages. The remainder of this section describes these layers in detail.



Note: Information is stored in the data layer (orange) as entries either in a relational database, or as related files in a file archive. A group of servers and scripts (green) act as the intermediary between users and the data layer. Users interact with the ICF through the application layer (blue), which is primarily a collection of secure web applications.

**Figure 3. The ICF's Functional Layers**

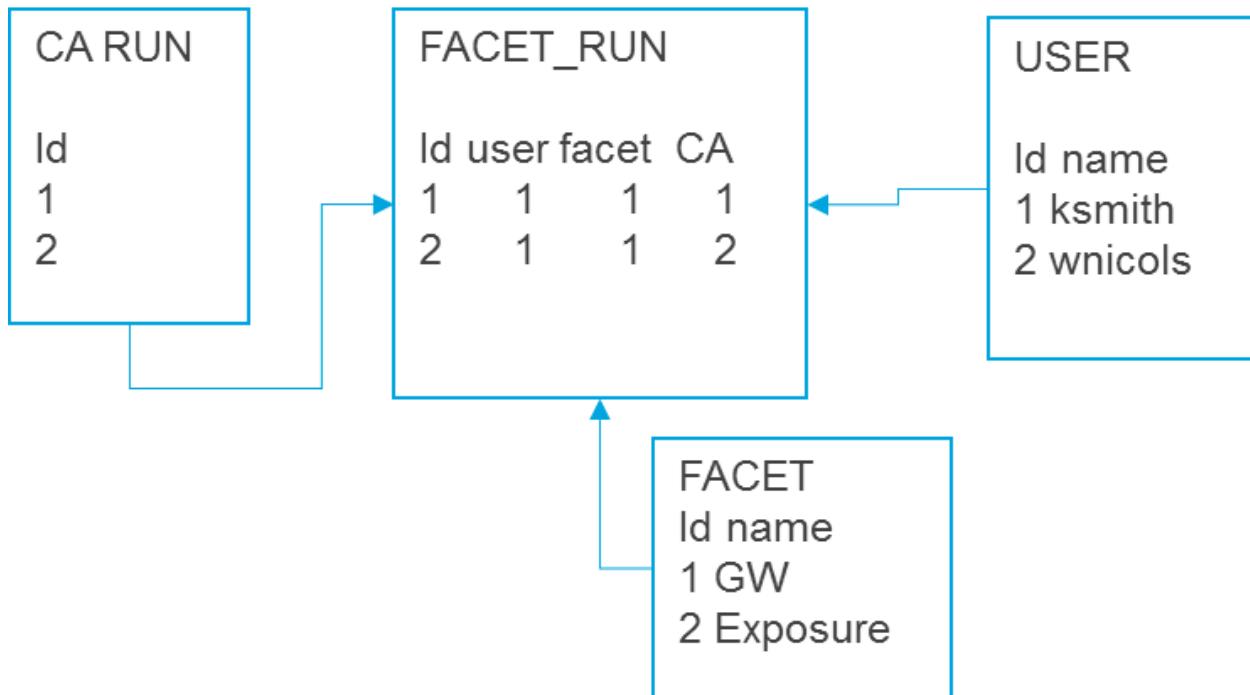
The data layer acts as the foundation of the ICF. It stores and relates state information such as run history, user permissions and activity, parameters, facet data packages and metadata. Given the large volume of data required for one full iteration of the CA, the data layer is split into two sections: a file archive, and a database. The file archive stores large files that must be retained but are seldom needed once they are first used; this includes model input files, model results, and other objects from facet data packages. The database stores data package headers and metadata, key parameters such as material properties, and user information and activity.

### 3.1.1 Database

The ICF database backend will be PostgreSQL with PostGIS for geospatial data (waste site boundaries, shapefiles, etc.). The database is designed as a collection of related tables, as shown in Figure 4. The specific design of the database in part depends on the findings of the other technical leads during the scoping process that led to this technical approach description, so the database design will be specified during the first step of the analysis phase, once the other technical approaches have been finalized. At a minimum, the database will house tables supporting the following:

- User information
  - User roles
  - User role assignments
  - User activity
- Internal activity logs

- Material properties (this includes radionuclides and decay pathways)
- Geoframework data
- Waste Sites
- Waste Site Boundaries
- CA Revisions (a run id corresponds to a CA revision number)
- Model Facets
  - Model Facet Runs
  - Model facet data packages
    - Metainformation
    - Pointers to the file archive where large data is stored
    - Hash (checksum or similar) of associated data to ensure data has not been corrupted
  - Model Facet QA status and reports
- An inventory of the ICF File Storage



Note: The actual design depends on the findings of the other technical leads during the scoping phase, which are discussed in companion technical approach documents; the database design will be finalized during the development phase.

**Figure 4. Example Schematic of the Relational Database that will Track CA Information**

### 3.1.2 File Storage

CA data is often many gigabytes in size and is thus too large to reside conveniently in a database and most data retained during a model run is only seldom needed once it is initially used. Furthermore, a byproduct of the algorithms employed by many of CA's numerical solvers is that output file size is often not determined until run time. The ICF's data layer also contains a file system that can store data of this type.

Files are stored in directories labeled by their associated run IDs that generated by the database when a user submits a data package; this information is stored as "pointers" in the database. Users thus only interact with file storage indirectly; retrieval is handled by the ICF.

### 3.1.3 Data Packages

As described previously, each model facet run has an associated data package that encapsulates its data output. While the data package identifier and header information is stored in the database, the data package contents are stored in the file archive. When data is loaded into the archive, the ICF will compute a hash of the data and store it in the database along with a pointer to the data. Later, when a user retrieves the data package, the hash will be recomputed and checked against the record to ensure that the associated data has not been modified.

Since the structure of a facet's data package depends on that facet's technical approach, the various data packages will be designed during the first steps of the ICF's implementation to be completed once all the CA's technical approaches are finalized.

### 3.1.4 Development Plan

This document outlines the overall technical approach to the development of the ICF. The specific functional requirements and detailed database structure of the data layer depend on the technical approaches of the various model facets, since they determine the quantity and quality of associated data. The implementation of the data layer thus begins with the design of the database and follows the following prescription:

1. Develop a list of functional requirements given the findings of the QA technical approach; these define the constraints under which the data layer must operate and the QA operations that it must enforce.
2. For each model facet:
  - a. Develop a data package specification
  - b. Design the database tables supporting that specification
3. Design a template for the file structure.
4. Develop documentation detailing the findings of steps 1 and 2; this will be the design specification of the data layer.
5. Develop a test plan with tests for each functional requirement in step 3.
6. Implement the design specification by coding the database.
7. Run the tests in step 4; this will result in a completed test report.
8. Deploy the data layer.

9. Compile Technical Documentation.

## 3.2 Server Layer

The ICF will contain a collection of programs offering services linking the user to the data layer; these are grouped by function:

- **Web Server** (*Apache*<sup>1</sup>): posts and returns web content depending on HTTP requests sent by the user through the Application layer.
- **File Server** (*Samba*<sup>TM2</sup> or similar): serves files.
- **Geospatial Server** (*Geoserver*<sup>TM3</sup>): serves geospatial content depending on HTTP requests sent by the user. This is for visualization of data on maps: shapefiles, GeoJSON objects, etc.
- **Database Server** (*PostgreSQL*): hosts a connection to the PostgreSQL<sup>TM</sup>
  - **Django**<sup>TM4</sup>: A Python<sup>®5</sup> framework for developing the application layer.
  - **QA Scripts**: Each facet will have QA checks, which can be automated;<sup>6</sup> these programs perform these tasks and help to inventory facet data packages.
  - **Data Processing**: These are routine data operations that can be scripted; for example, converting MT3DMS output (the output of the groundwater transport model, implemented in the MT3DMS software) into geospatial layers hosted by the geospatial server.

The server layer's role as an intermediary between the database and the user provides an opportunity to tailor the available applications in the applications layer to the user's status. Programs performing these functions comprise a user firewall; for example, users with "admin" privileges will have access to the core database tables, while anonymous users will have read-only access to a very small subset of web applications. Likewise, the server layer will trigger QA checks when a user with write privileges submits a model facet data package to the data layer.

### 3.2.1 Development Plan

The specific functional requirements and detailed structure of the server layer depend on the technical approaches of the various model facets, since they determine the actions that can be automated. The implementation of the server layer thus begins with the design of the miscellaneous scripts and follows the following prescription:

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1. Develop a list of functional requirements for QA automation given the findings detailed in the QA technical approach.
2. For each model facet:
  - a. Develop functional requirements for the programs assisting data processing.
  - b. Develop functional requirements of the web utilities (to be implemented in Django) given the functional requirements of the application layer, described below.
3. Develop documentation detailing the findings of steps 1 and 2 and identify the hardware needed to support the requirements of the server layer. This step results in the design specification of the server layer.
4. Develop a test plan with tests for each functional requirement in step 3.
5. Implement the design specification by coding the server layer.
6. Run the tests in step 4; this will result in a completed test report.
7. Deploy the server layer.
8. Compile Documentation.

### 3.3 Application Layer

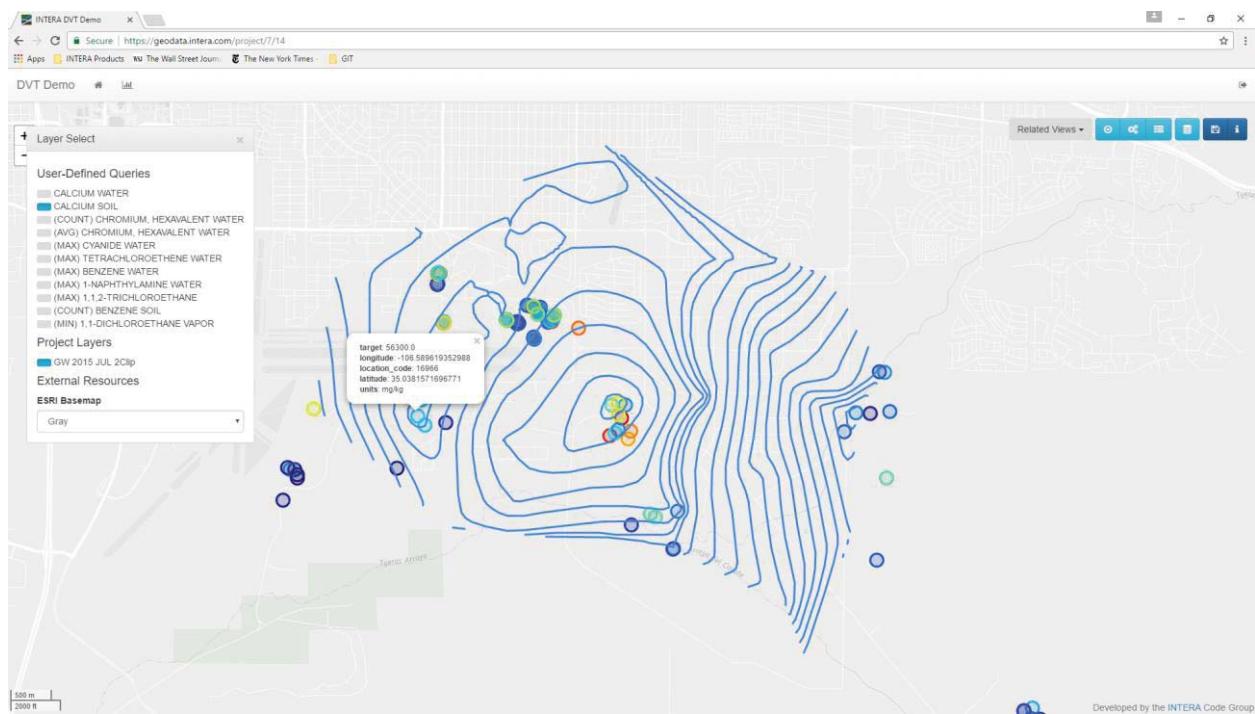
Users interact with the ICF through the Application Layer, which is a series of web-based applications. These are a collection of secure web pages written in HTML and JavaScript®<sup>7</sup> and served by the Server Layer.

#### 3.3.1 An Example: The ICF Prototype

During this scoping phase, we found that there is a need for applications that present geospatial information such as groundwater contours, site locations, maps, etc. We built a prototype (a screenshot is shown in Figure 5) with a simple set of geospatial layers to demonstrate this functionality. In the example below, the user logs into a website and is presented with an interface that allows them to explore interactively views associated with data groups. The same approach will be adopted for the ICF; however, the available views will be set by the needs of the various model facets.

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<sup>7</sup> JAVASCRIPT is a trademark and brand of ORACLE AMERICA, INC.



Note: This is a screen shot of a demo that was built as part of the ICF scoping phase. Here, various geospatial objects are charted on a map; the user can interact with the objects to find detailed information.

**Figure 5. One Example of an ICF Application in the Application Layer**

### 3.3.2 Application Layer Requirements

Through the development of the prototype, we learned that the Application Layer must offer the following views at a minimum (note that some of these views are accessible only to users with elevated privileges):

1. User login/logout
2. For all CA runs:
  - a. A means of viewing dosage over time on a map
3. For the active CA run:
  - a. A means of viewing the status of the model facets; these must include the QA status.
  - b. A means of notifying facet leads (e-mail or similar) when activity is required.
4. For each CA model facet, a series of pages supporting visualization useful to the leads of that facet.
5. A means for inspecting the data layer directly (admin only).
6. A series of publicly available web pages that offer aggregate/summary information.

### 3.3.3 Development Plan

The specific functional requirements and detailed structure of the application layer depend on the technical approaches of the various model facets, because they determine visualization needs. The

implementation of the application layer thus begins with the design of the views supporting visualization and follows the following prescription:

1. Develop a list of functional requirements for QA views given the findings detailed in the QA technical approach.
2. For each model facet:
  - a. Develop functional requirements for views assisting data processing.
  - b. Develop functional requirements for views supporting visualization.
3. Develop documentation detailing the findings of steps 1 and 2 incorporate this into the design specification of the server layer. This step results in the design specification of the visualization layer.
4. Develop a test plan with tests for each functional requirement in step 3.
5. Implement the design specification by coding the application layer. Applications supporting QA will be given priority, followed by data entry and finally visualization.
6. Run the tests in step 4; this will result in a completed test report.
7. Deploy the application layer. Applications will be deployed piecewise once they pass testing.
8. Compile User Documentation.
9. Compile Technical/Code Documentation.

## 4 Technical Characteristics

The ICF will be deployed as a virtual machine and will have the following technical characteristics:

- **OS:** Ubuntu 16
- **Database:** PostGres + PostGIS
- **Servers:**
  - **Web:** Apache/Django (via mod\_wsgi)
  - **File:** Samba
  - **Geospatial:** Geoserver
  - All custom server-side code will be written in Python
  - All client-side code will be written in HTML/CSS/JavaScript. The following libraries will be used:
    - JQuery.js (application functionality)
    - Bootstrap.js (layouts, etc.)
    - Plotly.js (scientific plots; time series, charts, etc.)
    - Leaflet.js (mapping)

We elected to deploy the ICF as a virtual machine because it is easy to schedule periodically backups of the entire system and its state. Backups will be stored in a minimum of two off-site locations. The virtual machine will be hosted on a server maintained by INTERA.

## 5 Quality Assurance and Quality Control

PRC-MP-EP-53107, *Hanford Composite Analysis Project Management Plan*, Appendix B (“Hanford Site Composite Analysis Quality Assurance Plan”) specifies the QA/QC requirements for the CA update, noting the importance of QA/QC to this project:

“A critical aspect of preparation of the revised Hanford Site Composite Analysis is quality assurance and quality control (QA/QC). This Project-Specific Quality Assurance Plan documents the plan for QA/QC for the project that is consistent with CHPRC plans and procedures that implement DOE requirements, EPA guidance, and adds additional project-specific requirements deemed necessary to facilitate delivery of a successful product.”

Guiding principles are provided in the project QA plan (Section 1.2 of Appendix B), including that QA/QC controls will address three key areas:

1. Software quality and control – to ensure use of only software that meets DOE requirements for use under a graded approach.
2. Data quality and control – to promote fully traceable development of model input parameters from traceable and qualified data.
3. Application quality and control – to promote fully traceable calculations using numerical software in which inputs are traceable to data (basis information), code use is traceable to inputs, and outputs are traceable to code use.

Software quality and control are to be addressed through the application of procedure PRC-PRO-IRM-309, *Controlled Software Management*, which implements requirements of DOE O 414.1, *Quality Assurance* (NQA-1-2008, *Quality Assurance Requirements for Nuclear Facility Applications*; NQA-1a-2009 addenda, *Quality Assurance Requirements for Nuclear Facility Applications*), for software used for modeling and calculations in the CA. Software QA documents will be prepared for the ICF at an appropriate quality level under a graded approach.

Data quality and control are addressed through provisions of the project QA plan, including the designation of a data configuration manager for the CA update project, maintenance of data configuration control, and requirements for the use of electronic modeling data transmittal (EMDT) forms to document submittal and review of all data configuration items utilized in the updated CA.

The companion technical approach description document for automated QA (CP-60411) identifies the approach for application quality and control will be managed within the ICF described in this document.

## 6 Conclusions

The ICF is a collection of DBWA and server scripts that provide a platform for automating and enforcing QA procedures, storing and tracking CA state information, and visualizing results. The ICF aims to minimize errors by handling the transfer of information between CA modeling facets. Users primarily interact with the ICF through a series of secure web pages and access is controlled through permission groups set at the database level.

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