Visual Data Analysis as an Integral Part of Environmental Management

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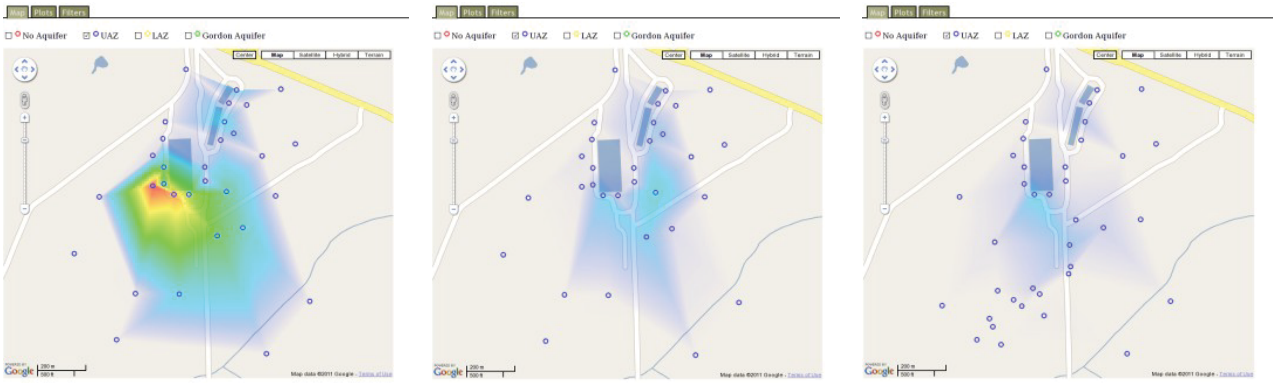

Fig. 1. Plan view map of the oil and groundwater U-238 contamination at Savannah River Site (SRS F-area, upper aquifer zone) in (a) 1994, (b) 2001 and (c) 2008, displayed in a web browser as a Google Maps bitmap overlay created in *VisIt* [1].

Abstract—The U.S. Department of Energy's (DOE) Office of Environmental Management (DOE/EM) currently supports an effort to understand and predict the fate of nuclear contaminants and their transport in natural and engineered systems. Geologists, hydrologists, physicists and computer scientists are working together to create models of existing nuclear waste sites, to simulate their behavior and to extrapolate it into the future. We use visualization as an integral part in each step of this process. In the first step, visualization is used to verify model setup and to estimate critical parameters. High-performance computing simulations of contaminant transport produces massive amounts of data, which is then analyzed using visualization software specifically designed for parallel processing of large amounts of structured and unstructured data. Finally, simulation results are validated by comparing simulation results to measured current and historical field data. We describe in this article how visual analysis is used as an integral part of the decision-making process in the planning of ongoing and future treatment options for the contaminated nuclear waste sites. Lessons learned from visually analyzing our large-scale simulation runs will also have an impact on deciding on treatment measures for other contaminated sites.

Index Terms—Visual analytics, high-performance computing, data management, parallel rendering, environmental management.

1 Introduction

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In an effort to provide computational infrastructure for environmental management solutions, the U.S. Department of Energy (DOE) created the Advanced Simulation Capability for Environmental Management (ASCEM) initiative, a multi-year program that involves geologists, hydrologists, physicists and computer scientists from various national laboratories, including Pacific Northwest National Laboratory (PNNL), Savannah River National Laboratory (SRNL), Los Alamos National Laboratory (LANL) and Lawrence Berkeley National Laboratory (LBNL). ASCEM is envisioned to be a state-of-the-art approach for integrating data, software and scientific understanding to improve subsurface contaminant fate and transport simulations used to support environmental management decisions.

The goal of this program is to develop models, simulation software and visual analysis tools for the evaluation of measured and simulated data with respect to nuclear waste, waste products, and other contaminants in soil and ground water. Historical data from

existing contamination sites is taken into account to calibrate soil and water flow models and to verify simulation results. The simulation code is then used to extrapolate this data into the future, incorporating different treatment options. The ultimate goal of the simulation and analysis of the resulting data is to arrive at a decision about potential future closure of the site. This is usually equivalent to ending environmental treatment measures.

Due to the complexity of the underlying data models developed by the geologists and physicists teams, it is often necessary to employ high-performance computing (HPC) methods both for the simulation and for the subsequent visual analysis of the data.

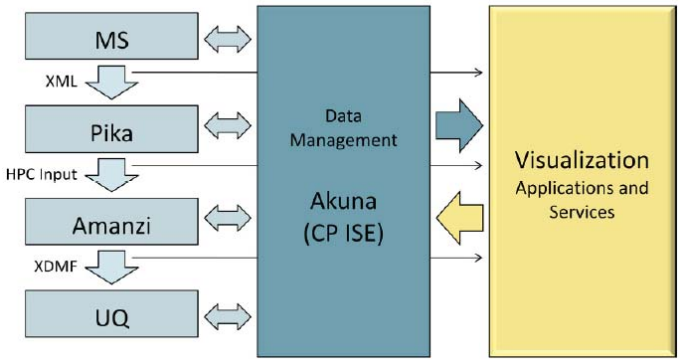

Fig. 2. Data flow graph for graphical user interface (Akuna) designed by Core Platform Integrated Software Environment Team (CP ISE) and Visualization. Model Setup (MS) data is fed into Parameter Estimation software (Pika), which controls HPC simulation (Amanzi code), followed by Uncertainty Quantification (UQ).

While a data management team has developed a graphical user interface to control the workflow (Figure 2), the visualization team has provided the visual data analysis infrastructure for analyzing the field data. Other team members have added verification tools for model setup and uncertainty quantification. These tools are invoked by Akuna (integrated graphical user interface).

The main challenge for visual data analysis in this program is the aggregation and integration of data from various sources, including site characterization and modeling output. This enables decision-makers to draw conclusions regarding potential outcomes for various treatment options, and for predicted states of contamination in the future, ultimately leading to closure of the site once contamination levels have reached values below a certain threshold.

The main contribution of this article is the description of visual analysis tools which were developed using the VisIt [1] framework using HPC infrastructure, and the methods that were used to aggregate and display sparse, measured field data.

2 Field Data and Modeling

2.1 Use Case Site Data and Modeling

For the ASCEM project, two contamination sites have been selected as use cases: one is located near Aiken, South Carolina, the other one is near Richland, Washington. In the first phase of the study, the teams have obtained field data from current and previous measurements at selected well sites. We found the main challenges to be in the sparseness of the data, the different coordinate systems they were represented in, and the heterogeneity of the selected sites.

The Savannah River Site (SRS) is located in south-central South Carolina, near Aiken, approximately 100 miles from the Atlantic Coast. It covers an area of approximately 800 square kilometers (300 square miles) and contains facilities constructed in the early 1950s to produce special radioactive isotopes. SRS has approximately 172 million cubic meters of groundwater, soil and debris contaminated with metals, radionuclides and organics [2] as a result of previous on-site disposal practices.

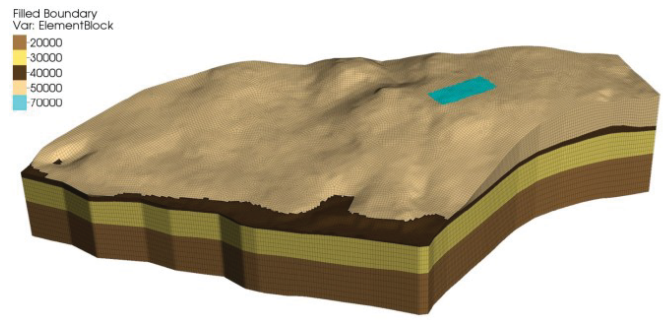

Fig. 3. SRS F-area contamination site (unstructured, hexagonal mesh, 25 ft. resolution) [3]. Hydrostratigraphic layers are colored according to the number of mesh elements given in the legend.

The SRS F-Area Seepage Basins consist of three unlined, earthen impoundments that received approximately 7.1 billion liters (1.8 billion gallons) of acidic, low-level waste solutions. The acidic liquid waste plume currently extends from the basins to an area with a radius of 600 meters (Figure 3). The terrain and subterranean aquifers feature a downgradient in the direction of a nearby creek [3].

The Deep Vadose Zone (Hanford Site) is located near Richland, Washington [4]. It is an area of 1517 km^2 (586 mi^2) in size, located in a sparsely populated area in the rain shadow of the Cascade Mountains, adjacent to the Columbia River (Figure 4). The site was used for Plutonium production for over 40 years. Production was suspended in the late 1980s in the aftermath of the Chernobyl accident. The data obtained at the site includes contamination information from wells in this zone.

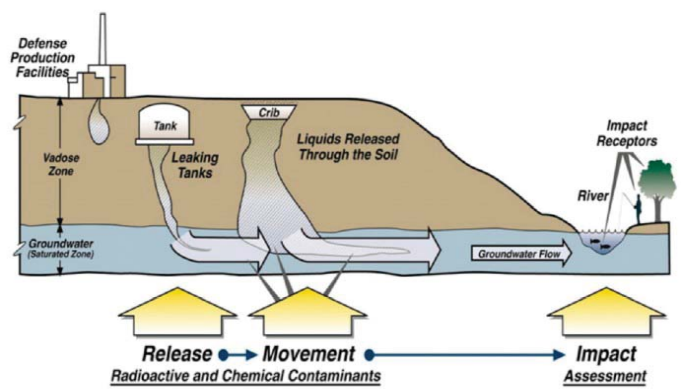

Fig. 4. Schematic diagram of waste discharge at the Hanford Site Vadose Zone and the Columbia River [3].

2.2 Visualization Framework

Our approach centers around leveraging the capabilities of the VisIt visual data analysis and exploration application. VisIt is a free, open-source, interactive, parallel visualization and graphical analysis tool for viewing scientific data [1]. It features an extensible design and supports approximately 300 types of file loaders. It is widely used because of its interactive visual analysis capabilities.

This approach allows us to take advantage of a production-quality, petascale-capable visual data analysis application that supports a diverse set of visualization and data analysis operations and that can run effectively on diverse platforms ranging from laptops to the world's largest supercomputers.

2.3 F-Area Database Visualization Techniques

The primary motivation for developing this visualization application was the need for a simple an intuitive way to select a well, contaminant and year from the data set and to display the result of the database search in a geospatial and temporal context. Using the Google Maps application interface (API), we are able to provide the user with a graphical representation of the geographic location of the well sites in their geographical context. In Google Maps, the user can switch between a map view and an aerial image view.

We use the Google Maps API, because it provides a programmable web interface for adding additional information layers to the base map display. For the SRS F-area we display the sites of wells that were used to obtain contaminant concentration data over the course of several decades (if data is present for a specific year), and the actual concentration of selected contaminants for a specific year. This allows us to perform a quick spatiotemporal visual analysis of the site for specific contaminants.

Data from over one hundred monitoring wells used for site characterization and modeling is currently available. The key datasets used are briefly described below:

- Concentration database, which includes 44 measurements of ion concentration and other wellbore parameters collected during 1990-2009. These data were retrieved from 145 monitoring wells and from three different aquifers in the Atlantic Coastal Plain: the Upper Aquifer Zone (UAZ); the Lower Aquifer Zone (LAZ); and the Gordon aquifer.
- Depositional database, which includes information about depths of stratigraphic (depositionally-related) units, particle size distribution, lithology (physical characteristics of rock and soil, such as porosity and mineral composition), well coordinates, well depths, and well screen zones (areas where well screens and filters are used in monitoring wells).
- Hydrostratigraphic database, which includes the coordinates of the base of the stratigraphic units that have common hydrological characteristics determined from wellbore data (aquifers).
- Lithostratigraphic database, which includes the coordinates of the base of the lithologic units defined on the basis of distinctive and dominant sediment characteristics, such as sand, silt, or clay.

We store these data in a PostgreSQL database, which is an open-source relational system that has flexible search capabilities and serves as a back-end to the visualization tools.

In order to enable display of the wells' geographic location in Google Maps, to query the data, and to display results in terms of graphs and tables, we adapted a JavaScript plotting package called FLOT. We also developed an AJAX-based user interface which allows users to plot the layout of the wells on a map and select one or more wells either by clicking on the well icons or by interactively selecting all the wells in a spatial range within a bounding box on the map.

For the depositional database we display the particle size distribution for the selected well as well as lithological information, i.e., porosity and mineral composition. For the concentration database we display a list of measured quantities of ions, also known as analytes. Users can plot a graph of concentration over time for any listed analyte for the selected wells. Additionally, for a given aquifer and analyte users can overlay a contour plot of the analyte concentration as measured by all the wells screened in that particular aquifer for any calendar year in the measured range.

To generate the contour plots we used the graphical capabilities of the VisIt server. Upon selection of the aquifer, analyte and year, all concentration data for every well satisfying the selection criteria are retrieved from the database and passed via an AJAX call to the VisIt server along with the geographic coordinates of the wells.

Conceptually, the data sent consist of an array where each element is a triplet of the form <latitude, longitude, and value>. In addition, the geographic coordinates of the southwest and northeast corner of the visible portion of the Google map as well as the width and height in pixels of the map display area are sent to the VisIt server.

Upon receiving the data, the VisIt server launches a Python script which generates a Delaunay triangulation and a contour plot, as shown in Figure 1. We chose a Delaunay triangulation as a method for interpolation, because it linearly interpolates between the data points located at the well sites. Compared to other interpolation techniques or other scattered-data methods, this seemed to be a natural choice, because no radius-based attenuation can be assumed around the wells and the best way to interpolate between two points in an unknown subterranean structure seems to be a straight line. It should be noted that this method does not take lithological information into account, which will be the subject of future research.

Finally, we generate an image the size of the map display area and return it to the web interface which overlays it on top of the map using the Google Map API.

2.4 F-Area 3-D Visualization Techniques for Selected Contaminants over Time (Animation)

As this work focuses on the visual display of historical data, the starting point centers around loading such data into VisIt. Here, we first obtained raw field data from scientists working at the site. The data formats include plain text (comma-delimited), GDAL GeoTIFF images [5], and ESRI Shapefiles [6]. We loaded most data types into VisIt with the included readers. However, we had to construct a custom plug-in to read in comma-delimited plain text files with a specific layout describing the depositional environment as recorded in wellbores at the site. Other plain text files record concentration values for contaminants measured at specific depths within each monitoring well or describe the subsurface coordinates of impermeable lithologic surfaces that form aquifer boundaries. Georeferenced true-color aerial photographs and Digital Elevation Model (DEM) terrain data were loaded as GDAL GeoTIFF images. ESRI Shapefiles loaded into VisIt contain vector data defining roads and structures.

Some datasets required processing prior to being loaded into VisIt. For example, not all observation wells were sampled with the same temporal frequency or resolution. Thus, concentration values were averaged on an annual basis. Also, in order to apply elevations from the DEM topography to the aerial photographs, we had to resample the DEM to match the pixel resolution of the photographs. We managed to subset all datasets to be within the same spatial extent.

Once we had loaded the datasets into VisIt, we created plots from each dataset. A "Data-Level Comparison" allows for two datasets to be associated with each other in such a way that the variables from one dataset can be applied to the other. We used this tool to associate the elevation values from the DEM with the aerial photograph on a pixel-by-pixel basis. Then we visualized the aerial photograph using a Truecolor plot in VisIt with 55% opacity and gave it a 3D perspective by applying the Elevate operator using the associated elevation values (Figure 5). This was desired by the geologist because of the three-dimensional structure of the aquifers and hydrostratigraphic layers, which could not be seen in the Google Maps interface described previously (Section 2.3).

We used a Pseudocolor plot to visualize the concentration values, varying the color from white to red by using a range of concentration values from 0 to 400 pCi/L. Prior to drawing the plot, we subset the concentration values using the Threshold operator to confine the measurements within a particular aquifer defined by the depth at which the measurements were recorded. Subsequently, we created a surface from those values by applying a Delaunay triangulation. We chose to use a Delaunay triangulation, because it avoids errors typical for other types of interpolation, such as Shepard's, Sibson's or Hardy's method [7]. We also applied a Delaunay triangulation to the lithologic information that defines a particular aquifer boundary and gave the resulting surface the color green.

We rendered the monitoring wells with a Filled Boundary plot. We applied a Geometry operator called Tube to the wells to give them a tube-like appearance in the visualization. We colored the tube segments according to their respective depositional layer, as indicated by the legend in the lower right corner of Figure 5. We also created a Label plot using the well ID values from the monitoring wells. We subset the well labels to reduce clutter and applied the Transform operator to raise the labels to the tops of the wells.

VisIt has a feature that allows the recording of all the commands used to open databases, create and modify plots, modify legend attributes, and add text annotation. Once all the commands were collected, we copied them into a Python script that can be called from the VisIt command line interface (CLI). The Python script can also be invoked at the same time as VisIt.

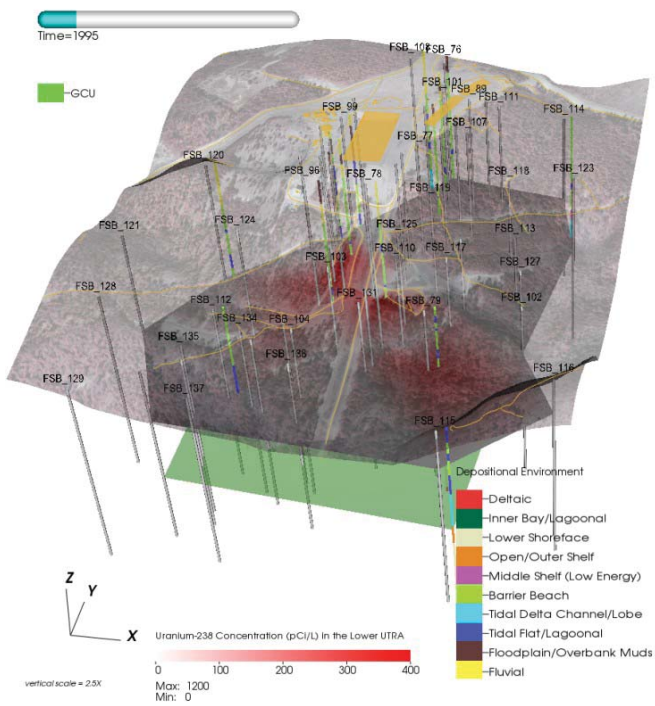

Fig. 5. 3-D visualization (computed in VisIt) of Uranium-238 plume migrating through the subsurface of the F-area. The animation this still image is taken from includes an aerial image with elevations applied from a digital elevation map, wells that have information about the depositional environment (lithology with respect to depth), buildings, structures, and roads (in yellow/orange color), and the lower boundary for the GCU aquifer (green). It also shows Uranium-238 concentration as a pseudocolor plot (white to red).

2.5 Visualization Techniques for Soil Desiccation

Soil desiccation is being tested by the Department of Energy as a method of reducing the downward movement of contaminants in the subsurface region between the ground surface and the water table (i.e. the vadose zone). We inject dry nitrogen in one well and extract it from another in order to desiccate the region between the wells. Subsurface monitoring is critical to understand when and where desiccation occurs.

One method we are testing for monitoring subsurface desiccation is electrical resistivity tomography (ERT). The electrical resistivity of soils is governed by properties that are modified during desiccation, such as saturation, ionic strength, and temperature. We use changes in resistivity to infer when and where changes in saturation, ionic strength, or temperature are occurring during desiccation. The primary advantage of using ERT over point measurements is that ERT can be used to estimate resistivity away from the sensor locations, providing a capability to 'see' everywhere in space and time with the instrumented region.

To do this, we installed vertical arrays of electrodes within monitoring wells surrounding the target desiccation zone. A series of current injections and corresponding voltage measurements over electrode pairs provides a data set which is tomographically inverted to produce an estimate of subsurface resistivity. In monitoring mode we repeat this process on a regular schedule to image desiccation induced changes in resistivity with time.

The visualization of the Hanford Site (deep vadose zone) comprises of a mix of volume outline for context, and a combination of isocontours and slicing planes to represent contamination data.
We show the outline of the volume with a low opacity value to provide geometrical context for our visualizations. We then add a slicing plane through the center of the volume to provide contextual information. Finally, the isocontours illustrate the conductivity information within the volumetric data.

Furthermore, we add annotations to effectively inform the scientists of which areas the data was collected from. In Figure 6, for example, the purple markers contain the electrode locations. The green and yellow wells show where the injection and extraction sites were placed. Finally, the red and blue wells contain the logging and sensor information for the Deep Vadose Zone.

We used VisIt to render these images and to create an animation that shows the progression of subsurface bulk connectivity over time.

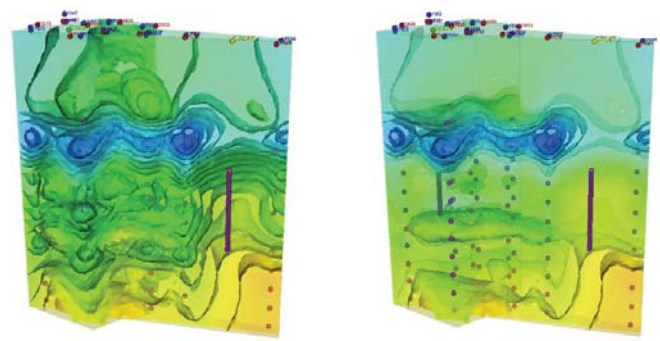

Fig. 6. (a) Absolute subsurface bulk conductivity during desiccation (logarithmic space). (b) Same as (a), but near zero regions removed to better emphasize the larger changes in conductivity.

3 Results

3.1 F-Area 2-D Visualization

Figure 1 shows the Uranium-238 concentration as measured by all the wells screened in the Upper Aquifer Zone (Google Maps overlay). The sequence of images (Figures 1a-c) shows the concentration measured in 1994, 2001 and 2008, respectively.

The images indicate that the overall concentration of the selected isotope drops with time, but the extent of the plume and the direction of movement follow the terrain structure. It should be noted that the Delaunay triangulation does not take the actual subsurface structure of the soil and aquifers into account, which is mainly due to lack of accurate subterranean data. However, according to geologists and hydrologists the data obtained from strategically placed wells provide a good approximation, and the underlying model is a reasonable representation of the actual site.

The response time of the server for this interactive application is the sum of data base retrieval, generating place marks on Google Maps, loading the map from the Google server, launching VisIt, producing a Delaunay triangulation of the contamination data for a selected contaminant and time step, returning the image to the server and displaying it as an overlay on Google Maps. This process, which also depends on network load and latency, is usually completed within a few seconds.

The main innovation in this Google Maps interface is the fact that the user is enabled to quickly select a spatiotemporal subset of the

data set, access a data base, and generate visualizations for further visual analysis. We accomplish this tight coupling between user interface, scientific data management, and visualization by using a combination of JavaScript, AJAX, Google Maps API (version 3), and VisIt.

3.2 F-Area 3-D Visualization

The images in Figure 7 are taken from an animation of the changes in concentration of a contaminant plume through time in a section of the F-Area site. The concentration surface only represents one measurement location per well, all from within the same aquifer. The concentration values have been reduced to an annual average, and thus each time step in the animation represents one year. The top surface in Figure 7a-c is a semi-transparent aerial photograph. Elevations from a topographic surface have been applied to give it a 3D appearance. The z-axis (elevation) has been exaggerated by 200%. Roads and structures such as the rectangular waste tank and nearby buildings have been included as landmarks.

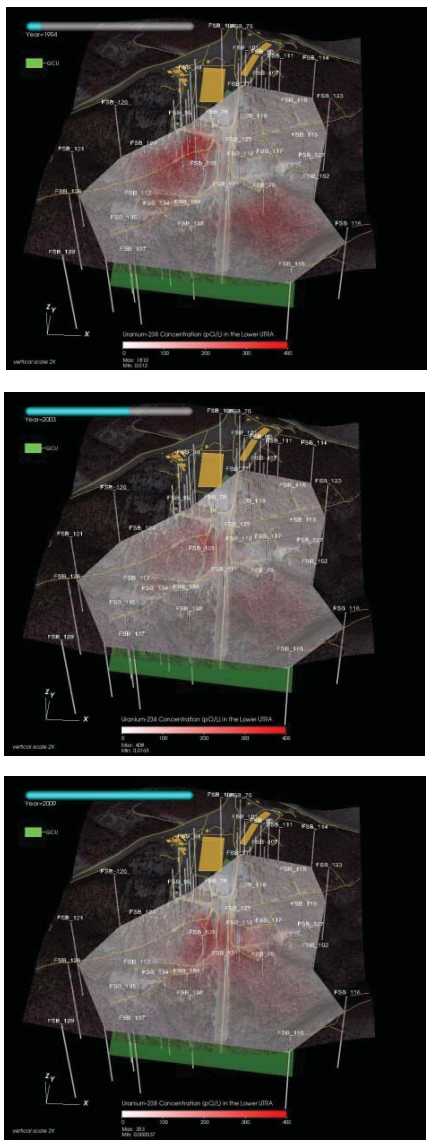

Fig. 7. Evolution of Uranium-238 concentration in one aquifer at three different time steps displayed as a white-to-red surface.

Gray linear tube-like features with labels at the top are monitoring wells where contaminant concentrations are measured. The white-to-red surface illustrates the varying concentration of Uranium-238 within a specific aquifer. This surface is created from a Delaunay Triangulation of the annual mean of the measurements taken from the monitoring wells within a particular aquifer zone. The green surface is a lithostratigraphic impermeable clay layer that is the lower boundary of the aquifer in which the measurements were taken.

All visualizations were created on a MacBook Pro with a 2.66 GHz Intel Dual Core i7 processor, 8 GB 1067 MHz DDR3 RAM, and Mac OS X 10.6.6. The animation from which images for Figure 7 were taken was created using 17 time frames, one for each year in the range of 1993-2009, and each frame took less than a minute to create. Multiple copies of each frame were used to lengthen the time of the final animation.

3.3 Deep Vadose Zone Visualization

The Deep Vadose Zone data collected at the Hanford site measures two major points of interest: absolute bulk conductivity and percent difference of the bulk conductivity measured from January 2011 to April 2011.

Figure 6a shows a visualization of the logarithm of the absolute bulk conductivity. To attain this visualization we employed a rainbow color map on evenly spaced isocontours with a cross sectional view through the middle of the volume to provide context. In Figure 6b, we prominently emphasize larger changes of bulk conductivity by removing the near zero regions.

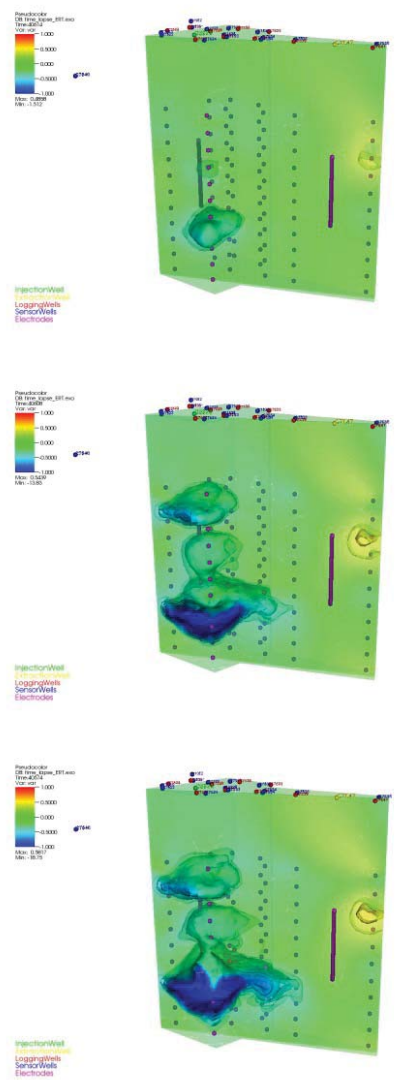

Fig. 8. Deep Vadose Zone: Differences in bulk conductivity. (a) Time step 8, (b) time step 32, and (c) time step 44.

Figure 8 highlights the differences in bulk conductivity to capture the growth of the plume in the Deep Vadose Zone. Figures 8a-c show different stages of the plume for various time steps.

The algorithm was executed on a MacBook Pro 2.66 GHz i7 with 4 GB RAM, and it has also been tested on a Linux/Ubuntu 10.10 system with 16 core Intel processor and 24 GB of RAM. Both scenes (Figures 6 and 8) were animated (all time steps followed by camera rotation), and the animations took 12 minutes for a 30 seconds movie (Figure 6, 750 frames, 0.96 s/frame) and 287 minutes for a 90 seconds movie (Figure 8, 2,250 frames, 7.65 s/frame), respectively, on a MacBook Pro. The difference in performance is due to the fact that the second movie (Figure 8) made extensive use of transparency. On the given PC, the second animation took approximately 90 minutes to compute (0.48 s/frame), which is due to faster I/O and a higher core count.

4 Impact

4.1 F-Area: Lessons Learned

Before the visualization system was in place, the underlying field data, which was acquired over the course of approximately thirty years, came in a variety of formats, ranging from hand-written notes to electronic records and spread sheets.

In a first step, an experienced geologist aggregated the data from various sources, averaged measurements over time to obtain annual values, discarded erroneous data, e.g., negative concentration values, eliminated or averaged duplicates, and used linear interpolation to calculate values for a small number of points. The coordinates in the datasets had varying spatial references and we applied coordinate transformations to standardize all to a locally-defined projection.

In order to prepare the data for visualization, we consolidated it in a single database, which was then fed into VisIt for visualization. In addition to the Delaunay triangulation of the contaminant concentration data for a given depth and year, we also assigned colors to wells and hydrostratigraphic layers.

As a result of this effort, not only our database was in a much better state, but the visualization for the first time allowed us to look at the data in an aggregated form and to study contaminant fluid transport in an intuitive way in a three-dimensional representation over time.

Instead of looking at isolated data of selected contaminants, e.g., Uranium-238, for individual wells, we were now able to see concentration data for this isotope for all wells at the same time in the form of animation.

We made several observations while looking at the data. One finding was that certain measures for mitigation that were performed on site during the data acquisition period (three decades) had a profound impact on the extent of the subterranean contaminant plume. The installation of a concrete lid on the pool prevented new rain water from entering the site and temporarily reduced the inflow of contaminated ground water into a nearby aquifer.

Also, the effect of a previous pH treatment on the pH level of the water in the wells was clearly visible in the rendered animation.

The results from these animations helped us to better understand fluid transport at the given site (Savannah River F-Area) and will aid in generating new and improved models for extrapolating contaminant transport into the future.

The Akuna user interface, which was discussed in section 1 (Figure 2), helps in this endeavor, because it integrates data management, mesh generation, parameter estimation, modeling, high performance simulation and visualization tools.

4.2 Hanford Site: Observations and Usage of Visualization Tools

For the Hanford Deep Vadose Zone, the observations and lessons learned were very similar to those from the F-area.

Due to the somewhat more sparse nature of measured field data, the resulting visualization is not quite as rich as the one generated for the F-area. For instance, the data obtained from the site contained mainly measurements of conductivity using electrodes to study desiccation over time. Nevertheless, we found the visualization to be very useful for studying the progression of the desiccation process in 3-D. In particular, VisIt's animation features allowed us to study this process over time.

We also found that the given visualization, when compared to visualizations generated using other tools popular among earth scientists, such as TecPlot [8], takes advantage of the full feature set available in VisIt, allowing us to change colors, transparencies, plot types (contour plots vs. volume rendering), etc., in a much more interactive and flexible way. VisIt's parallel rendering capabilities allowed us to render and interact with the data in real time.

Another interesting occurrence while working with the data was the fact that another earth scientist, who saw the visualization of the conductivity measurements, asked if the system could be used to visualize data for the same site, but from a different source, in this case ground penetrating radar.

Having corroborating techniques to study the same site greatly enhances the validity of the analysis and measurement work. Figure 9 shows a visualization generated for measurements obtained for the Deep Vadose Zone at Hanford from ground penetrating radar.

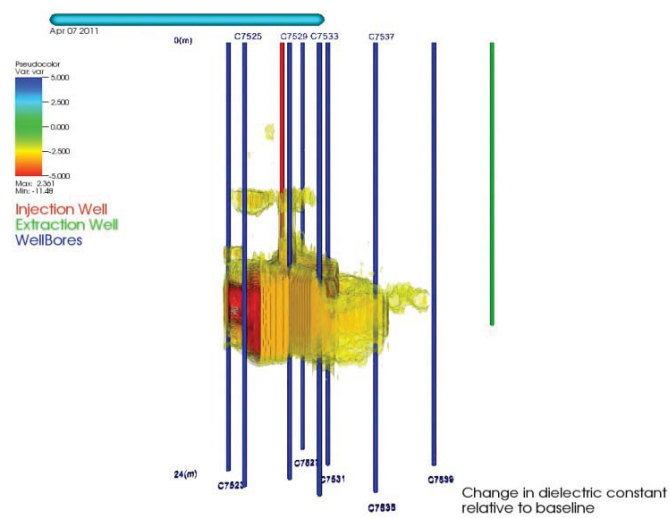

Fig. 9. Ground penetrating radar (Hanford site).

One of the key benefits we got from using the visualization system was the ability to look at the same area with different techniques and verify scientific results by being able to visually compare results. This helped us solidify the results and conclusions and will potentially aid in generating improved simulations.

5 Conclusions

We have demonstrated that by bringing together experts from a variety of domains, including geology, hydrology, physics, and computer science, we can develop an integrated system that helps scientists make well informed decisions regarding environmental management. Visual analysis, along with data management and uncertainty quantification, is one of the key elements in the ASCEM project.

We have presented a set of tools that was designed to help geologists, hydrologists and physicists determine the extent of soil and water contamination from radioactive isotopes from measured data and to develop models that will be used to predict the future progression of a contaminated site with respect to these contaminants.

We have overcome challenges with respect to sparse data representations, different coordinate systems found in historical data, data management, user interface integration, and computational complexity.

We have formulated specific questions regarding the length of necessary treatment. Our visual analysis tools have an impact on answering these questions. As an example, we selected specific contaminants for our analysis that have a long half-life or can be harmful to the environment due to their acidity. One result from the visual analysis was the observation that the overall concentration of certain contaminants (U-238) drops over time, but the extent of the plume expands.

In order to protect a nearby creek, the hydrology team determined that it is necessary to treat subsurface water for pH by injecting an alkaline solution into the ground near the aquifers. A possible outcome of the visual analysis will be to determine how long this treatment is necessary and at what point in time in can be stopped.

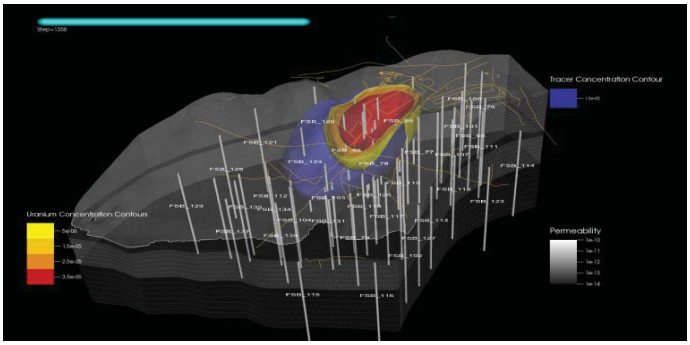

Fig. 10. F-area: High-Performance Computing Simulation of Uranium-238 Concentration under F-area basin.

Figure 10 shows the result of an initial simulation run for the F-area nuclear waste disposal site. The parameters for the model, such as mesh size, mesh resolution, etc., were obtained from studying visualizations of the F-area field data using the integrated Akuna user interface.

Accurate predictions of future developments at the selected sites will require more detailed models and many more additional simulation runs. This is still work in progress and an upcoming challenge for the entire science team.

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