Quarterly Progress Report
Date of Report: 07/15/2011

Award Number: DE-EE0004449

Project Title: Unconventional and Renewable Energy Research Utilizing Advanced Computer Simulations (UT)


Recipient Organization: SCI Institute, University of Utah
72 south Campus Drive, Room 3750
Salt Lake City, Utah 84112

Partners: Chris R. Johnson, PhD
Martin Berzins, PhD
Ross Whitaker, PhD
Mike Kirby, PhD
Cost Sharing Partner: University of Utah

Technical Contact: Chris R. Johnson, PhD
72 south Campus Drive, Room 3750
Salt Lake City, Utah 84112
(801) 585-1867
crj@sci.utah.edu

Business Contact: Edward Black
72 south Campus Drive, Room 3750
Salt Lake City, Utah 84112
(801) 585-1867
ed@sci.utah.edu
Project Objective:

The ability to develop science-based and validated computational tools to simulate and facilitate the development of clean, highly efficient energy systems of the future requires innovation in several key computational science technologies, including scientific data management, scientific visualization, scientific software environments, and scientific computing. The overall objective of this work is to leverage our expertise and experience in both scientific visualization and complex science-based simulations toward the accurate and robust simulation of science-based phenomena in the area of unconventional and renewable energy research. This work is aimed at garnering a better understanding of science-based phenomena in energy research and also the advancement of the Uintah software system. The Uintah software system accommodates the massive amounts of data and advanced algorithmic, software, and hardware technologies required to deal with the enormity and complexity of the simulation data in this area of research. To accomplish these goals, we are creating new numerical and visualization techniques needed to assess the uncertainty of the simulation, extend the Uintah scientific problem-solving environment for large-scale simulation of science-based systems, and integrate and extend the data provenance infrastructure of Uintah to systematically capture provenance information and track simulation parameter studies.

Background:

Science-based development of clean and efficient energy systems often involves modeling and simulations of fluid flows, chemical reactions and mechanical properties within heterogeneous media. As part of our DOE-funded (1997-2009) Center for Simulation of Accidental Fires and Explosions (C-SAFE), we created the Uintah scientific problem-solving environment. Uintah is a parallel software environment for solving large-scale computational mechanics and fluid dynamics systems, and has particular strengths when dealing with systems that require large deformations, fire simulation, and fluid-structure interactions. Uintah, general-purpose, fluid-structure interaction code has been used to characterize a wide array of physical systems and processes encompassing a wide range of time and length scales - from microseconds and microns to minutes and meters. Complex simulations require both immense computational power and complex software. Typical
simulations include solvers for structural mechanics, fluids, chemical reactions, and material models, which are efficiently integrated to achieve the scalability required to perform the simulations. Uintah scales to cores by using a novel asynchronous task-based approach for challenging AMR applications. Novel parallel computing algorithms, on both CPUs and GPUs, are needed when simulating large-scale complex science-based energy systems. In moving beyond petascale, it will be necessary to make use of GPU-like architectures as the ongoing convergence between GPUs and multi-core CPUs continues. Task-based codes like Uintah are very well placed to exploit such architectures.

The challenge for finite element type simulations is that the memory access patterns are not well suited for the cache coherency required for efficient operations on streaming architectures. The problem becomes worse for the sparse systems associated with large simulations, and performance improvements over CPU implementations have been limited. An alternative is to take advantage of the geometric configuration of unstructured meshes, and to invent compact, efficient data structures that allow SIMD processing of individual cells and subsequent SIMD assembly of cell computations and mapping onto global degrees of freedom in the solution. The problem becomes more challenging for algorithms that are effective on multi-GPU clusters, such as the NVIDIA cluster at the SCI Institute. We anticipate the need for hierarchical domain decompositions that provide sufficient computational density and efficient communication. This work will pursue GPU and GPU-cluster based algorithms for numerical simulations of combustion using both generic linear solvers and specialized solutions that directly map unstructured and structured domains onto streaming architectures.

The system must also provide data visualization capabilities that allow interaction and analysis of the simulated data. The SCI Institute is an international leader in scientific visualization research. The PI, Chris Johnson, co-leads the DOE Visualization and Analytics Center for Enabling Technology (DOE-VACET). In this work we are leveraging our expertise in large-scale visualization research and development toward the seamless integration of high-end visualization techniques with simulation results of science-based energy systems. Additionally we are exploring the use of higher fidelity visualization with methods based on the use of high-order mesh elements.

With large computational simulations there is substantial uncertainty inherent in any prediction of science-based systems. A number of factors contribute to uncertainty, including experimental measurements, mathematical formulation, and the way different processes are coupled together in the numerical approach for simulation. Tracking of and analysis of this uncertainty is critical to any work that will truly impact the creation of future energy systems.

Exploration of large-scale scientific systems using computational simulations produces massive amounts of data that must be managed and analyzed. Because of the volume of data manipulated, and the complexity of the simulations and analysis workflows, which are iteratively adjusted as users generate and evaluate hypotheses, it is crucial to maintain detailed provenance (i.e., audit trails or histories) of the derived results. Provenance is necessary to ensure reproducibility as well as enable verification and validation of the simulation codes and results. In order to manage large-scale simulations and the analysis of their results, we will use systems such as the VisTrails software (http://www.vistrails.org), an open-source provenance management and scientific workflow system that was designed to support the scientific discovery process, to guide us in building "hooks" into Uintah for provenance systems.
Accomplishments:

Uintah Software System:

In applying the Uintah software framework to new energy problems we have attempted to improve the scalability of the code on large numbers of cores and have begun to investigate using Uintah on new problems and on GPU architectures. In the second quarter of the year we have made a major improvement to the software that has made it possible to scale the software to 196K cores and have undertaken scaling studies that have demonstrated how the software does indeed scale.

The major improvement made under NSF grant funding has been to move to a hybrid execution model. The standard message passing paradigm that Uintah initially operated under was that any data that needed to be shared to a neighboring core must be passed via MPI. For multi-core architectures, the process of passing data that is local to a node is both wasteful in terms of latency from MPI sends and receives and in the duplication of identical data that is shared between cores. For these reasons we have moved to an architecture in which only one copy of global data is stored per node in Uintah’s data warehouse. The task scheduler now spins off tasks to be executed on, say, nc cores using a threaded model, which results in the memory used in a single shared data warehouse being a fraction of only 1/nc of what is required for multiple MPI tasks, one per each of the nc cores. Figure 1 shows dramatic memory saving and even more dramatic memory decrease when the MPICH buffer sizes are constrained. The memory saving from eliminating the duplication of data within a node allows us to expand the scope and range of problems that we have been unable to explore up until now. This architecture also offers the possibility of being extended to spin off tasks to be executed on other types of processors, such as GPUs, in the near future.

These improvements in memory use enabled DOE NETL project work on two scaling studies of both weak and strong scaling to be carried out, showing that Uintah scales to 196K cores non DOEs Jaguar architecture. In weak scaling (horizontal lines) the problem size per core is constant, while
in strong scaling (solid diagonal lines) the problem size is fixed and the number of cores varies. The first scaling study involved the simulation of the transport of two fluids with a prescribed initial velocity of Mach two. For this problem, the conservation of mass, momentum, and energy equations were solved for two inviscid fluids. The fluids exchange momentum and heat through the exchange terms in the Navier-Stokes equations. An explicit time stepping method was used to solve the governing equations. The scaling results are shown in Figure 2.

![AMR ICE: Scaling](image)

**Figure 2**: Scaling results from the first study

The second scaling study involved a full-physics simulation of an explosive array during detonation. In this simulation, a high-pressure wave travels through an array of explosives. The wave causes each container to detonate as it passes through, thereby increasing the energy within the explosion. This combined fluid structure interaction problem is representative of the type of simulation that is the basis for a new proposal. The full Navier-Stokes equations combined with the equations of motion representing the solid material along with a chemistry model representing detonation are solved using an explicit time stepping method for both the fluid and solid components. The strong and weak scaling results are shown in Figure 3.
Uncertainty Visualization

During the third quarter of our project, postdoctoral research fellow, Dr. Joel Daniels and research scientist Dr. Kristin Potter, continued working on creating a new software framework for visualizing and assessing uncertainty called QuizLens.

QuizLens

The improved ability of visualization procedures in generating impressive representational imagery from complex scientific datasets is driving the use of virtual environments. As visualizations go beyond data presentation for promotional tasks and decision-making scenarios, it becomes increasingly important to understand and convey the existence of uncertainty. To this end, knowledge of the uncertainty that accompanies data and is incurred throughout the visualization process, is mandatory.

QuizLens provides an interactive exploration framework in which users navigate their dataset using an uncertainty lens to affect local visualization views of the data within the global context. The goal of this work is to gain a better understanding of surfaces by exploring the space in which the surface may possibly lie. Data exhibiting fuzzy surface boundaries include medical images and scientific simulations. The domain experts wish to understand characteristics of the surfaces, such as the range of possible surface location, the probability of the surface at any given point, as well as statistical information such as the most likely position.

To facilitate the understanding of surface position, we are developing a visualization tool using the idea of multiple lenses. Common problems found in visualizations are information overload and visual clutter. This is especially true for uncertainty visualizations which add indications of qualitative information to existing visualization techniques, which can quickly become overwhelming. Multiple linked windows is one solution for this problem, however such an approach suffers from the loss of context and discontinuity in that one must investigate many windows to get a full
understanding. Our method takes the strength of the multi-window approach, but places the many windows as lenses within the original visualization. This provides a contextual viewpoint as well as provides the user with an interactive tool which can switch between various display methods designed to highlight specific data features.

A prototype of our interactive system, QuizLens, is in-process, and to date we have developed four lenses as well as the contextual visualization. The global display consists of an isosurface rendering of the data, with tunable transfer functions to allow the user fine control over the look of the visualization (4). A high-level focus lens clears away data unnecessary for the current exploratory task, such as removing tissue between the user’s viewpoint and the region of interest, as shown in Figure QuizLensFocus. Three more lower level lenses have been implemented which aim to give the user a better understanding of the uncertainty of the surface. The probability slice lens (5, a) displays the probabilities of a selected region and projects those probabilities onto a 2D slice. The fuzzy lens (5, b) renders the selected tissue as a fuzzy volume, modulating opacity with the amount of uncertainty at each point. Finally, the uncertainty contours lens (5, c) projects contours of the uncertainty onto a 2D slice, thus showing the maximal location of the tissue, as well as the probability of the surface colormapped through opacity.

Progress and Status:

- Personnel - There were no changes in personnel during this reporting period.
- Equipment - No equipment was purchased during this reporting period.

Scope issues:

There are no scope changes.

Figure 4: Context: A global display of the data using an isosurface rendering. The tunable transfer functions allows the user fine control over the look of the visualization. High Level Focus: A high-level focus lens clears away data unnecessary for the current exploratory task, such as removing tissue between the user’s viewpoint and the region of interest.
Figure 5:  (a) The probability slice lens displays the probabilities of a selected region and projects those probabilities onto a 2D slice. (b) The fuzzy lens renders the selected tissue as a fuzzy volume, modulating opacity with the amount of uncertainty at each point. (c) The uncertainty contours lens projects contours of the uncertainty onto a 2D slice, showing the maximal location of the tissue, as well as the probability of the surface colormapped through opacity.

**Budget and Schedule Status:**

There are no budget nor schedule status changes.

**Patents:**

There are no patent applications attached to this award.

**Publications / Presentations:**

**Publications**
M. Berzins, Q. Meng, J. Schmidt and J. C. Sutherland DAG-Based Software Frameworks for PDEs. Accepted for HPSS Workshop, Europar 2012, Bordeaux August 2011.

Q. Meng, M. Berzins, and J. Schmidt Using Hybrid Parallelism to Improve the performance of Uintah. Accepted for Teragrid 2011 Conference, Salt lake City, July 2011. ACM


Additionally, two publications were accepted pending revisions and were recently submitted for final acceptance.

**Presentations**
Martin Berzins, *Uintah a scalable computational framework for hazard analysis.*, FEMTEC Conference Lake Tahoe May 2011 (Invited Talk)

Chris Johnson, *Biomedical Computing*, International Conference on Simulation Technology, Stuttgart, Germany, June 2011 (Keynote Presentation)


Chris Johnson, *Visualizing Uncertainty*, Dagstuhl Visualization Workshop, Waden, Germany, June 2011

Chris Johnson, *Visual Computing*, TEDx, Salt Lake City, June 2011


**Uncertainty Visualization Seminar Series** Since the start of the second quarter, the Uncertainty Visualization Seminar Series has meet approximately every other week. Over the last quarter, the following presentations were given:
- Kristi Potter presented *A prototype for Material Models*.
- Tobias Martin, Guoning Chen and Suraj Musuvathy presented *Extraction and Harmonic Parameterization of Topology-Consistent Midstructures* .
- Josh Levine presented *Exploring Large Scalar Data using Hixels*.

**Plans for Next Quarter:**

**Uintah Software System:**

The next stage of this work is to consider how to better weak scale this complex fluid structure interaction problem. This work is ongoing now. In the second half of this year we will be in a position to run more advanced simulation studies of our target problem.

Also both to respond to industry needs for executing codes GPUs and also in preparation for hybrid architectures such as the proposed DOE Titan system, we are beginning an investigation of GPU approaches and have hired a new staff member to undertake this work. So far we have only undertaken some feasibility studies but will focus on this for the second half of 2011.

As part of finding new Uintah applications, we have begun work with John McLennan on a challenging problem on flow through nanopores. We have investigated how Uintah might be applied to this and we are now helping McLennans group to run simulations.

**Provenance Enabling Uintah**

We are reviewing applicants for the software development position that will work toward the implementation of VisTrails into the Uintah framework.
Uncertainty Visualization

The continuation of the work will refine the existing lenses, add more lenses as needed, and create a pointer to allow for direct data access, refining the exploration from a large-scale, global overview, through various local lenses, to small-scale data information. We will also be testing the system out on multiple datasets.