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


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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:

Uncertainty Visualization:

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. During the second quarter of our project, newly-hired postdoctoral research fellow, Dr. Joel Daniels, worked on creating a new software framework for visualizing and assessing uncertainty called QuizLens; a tool that aids the user in gaining knowledge of the uncertainty accompanying visualized data.

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. Our method employs a user-controlled portal that focuses on a region of interest and deploys multiple visualization lenses. The user is able to toggle between the different uncertainty lenses to choose an appropriate display method for the region of interest. This approach to uncertainty visualization addresses many challenges, including visual clutter, arbitrary emphasis on uncertain regions, and the displacement of multiple visualization techniques in separate windows.

We demonstrate the utility of the QuizLens framework through the exploration and visualization of a segmented brain ensemble. This dataset describes the probabilities of point locations belonging to each of eleven different segmentation types: background, cerebrospinal fluid, fat, muscle, skin, skull, connective tissue, lesion, as well as grey, white, and glial matters. The data is composed by accumulating the tissue classifications assigned to a point location across multiple segmentation results from a scanned brain to determine probability statistics.

Scientific Visualization

In Progress

Uintah Software System:

Over the past three months, the work on Uintah Software has progressed considerably, and it focuses on two main capabilities. First, to ensure that Uintah can continue to run increasingly large problems of application types now and in the future. Second, to extend the applicability of Uintah to new problem classes that are appropriate to energy applications. In the previous report, we mentioned that parts of the code (the data warehouse) were being rewritten to make it possible to run Uintah with less memory per core. The restructuring of the software to run in a mixed threads/MPI model is now complete and has made it possible to reduce the memory that Uintah needs by 90%, effectively increasing the problem size per core by a factor of 10. This work is in the process of being submitted to the 2011 Teragrid Conference.

This development is also an important step in making Uintah work on GPU architectures, which will be essential for future activities. The scalability experiments for this case have been run on...
Figure 1: QuizLens allows the user to browse local uncertainty information within a global context. Above, the user culls the volume rendering of the skin tissue probability in order to locally visualize the maximal boundary surface of the skull (left). This isosurface is extracted using dual contouring, and colored according to the variance of probability values in the neighborhood of each vertex. The visualization tasks of the global environment and uncertainty lens can be controlled independently of each other, displaying the connectivity tissue isosurface within the grey-matter volume render (right).

The Jaguar and Kraken computers at Oak Ridge as part of the INCITE allocation. These machines have 224K and 112K cores, respectively.

The second area of work is to continue to prepare Uintah for new applications related to the energy field. A number of these applications involve implicit methods for time-stepping and therefore require solutions for large systems of equations. Although Uintah uses state-of-the-art solvers such as Hypre and PetSc from DOE Labs, attempts to run these codes have not been successful. In order to resolve this, we have begun a study of linear-equations scalability, and preliminary results have identified areas where performance improvements are needed.

Algorithm Development: Solving PDEs on GPUs

In Progress

Progress and Status:

- Personnel - No new hires were made during this reporting period.
- Equipment - No equipment was purchased during this reporting period.

Scope issues:

There are no scope changes.

Budget and Schedule Status:

There are no budget nor schedule status changes.
Patents:

There are no patent applications attached to this award.

Publications / Presentations:

Since the award is new, there are no publications resulting from this award at this time. There are several current submissions.

- **Chris Johnson**
  Presentation: *Large-Scale Visualization*
  Sandia National Laboratories on January 20, 2011.

- **Chris Johnson**
  Presentation: *Uncertainty Visualization*
  Texas A&M University on February 24, 2011.

- **Chris Johnson**
  Distinguished Lecture: *Image-Based Modeling, Simulation, and Visualization*
  Hong Kong University on March 1, 2011.

- **Martin Berzins**
  Presentation: *Uintah a Scalable Computational Science Framework for Hazard Analysis*
  SIAM Conference on Computational Science and Engineering on March 2, 2011.

- **Chris Johnson**
  Distinguished Lecture: *Visual Computing: Making Sense of a Complex World*
  University of Pittsburgh on March 25, 2011.

Uncertainty Visualization Seminar Series Since the start of the second quarter, the Uncertainty Visualization Seminar Series has met approximately every other week. Over the last quarter, the following presentations were given:

- **Jeff Phillips**
  Presentation: *There is uncertainty in your uncertainty.*

- **Fangxiang Jiao**
  Presentation: *Review of uncertainty analysis and uncertainty visualization in Diffusion Tensor Imaging (DTI).*

- **Liang Zhou**
  Presentation: *Transfer function combinations.*

- **Shreeraj Jadhav**
  Presentation: *Uncertain 2D Vector Field Topology.*

- **Mike Kirby**
  Presentation: *Overview of the stochastic Galerkin and stochastic collocation methods*
Plans for Next Quarter:

Uncertainty Visualization: QuizLens

Still in the initial stages of development, QuizLens currently supports exploration of the maximal boundary surfaces for the different tissue types, demonstrated in Figure 1. These screen captures illustrate the embedded uncertainty visualizations within the global environment and the ability to customize the local visualization tasks. These customizations include toggling between different aspects or computations of the uncertainty information as well as culling away the global visualization. Our uncertainty lenses reduce prohibitive visual clutter, maintain global context while locally informing, and support user-tuned uncertainty emphasis. To further emphasize these advantages, several additional localized visualization tasks are under development, including: (1) three-dimensional glyphs that measurably convey uncertainty information; (2) control sliders that affect the emphasis of uncertain versus certain regions of the data; and (3) the management of multiple lenses within the environment.

Algorithm Development

In the area of GPU processing, over the next quarters we will work toward extending the 2D fast iterative method to 3D tetrahedral meshes, finalizing the 3D GPU Eikonal solver with homogeneous anisotropic material.

Provenance Enabling Uintah

The provenance effort will focus on using the VisTrails (www.vistrails.org) provenance system to provide provenance capabilities within the Uintah system. Our first scoping meetings are taking place this quarter and will result in a timeline and more specific scope of work.