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Computational Steering with System X and the UVAG by Visually Analyzing Simulations Immersively in "Real-Time"

by

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Computational steering is not a new idea. Scientists have wanted to visually analyze their simulation data in "real-time" for many years but typically lack access to facilities and skills necessary to use these facilities. This goal is now possible with current technology and facilities at Virginia Tech. In the early 1990s Silicon Graphics Inc. (SGI) was the first to exploit the idea of "real-time" data visualization and coined the phrase "visual computing". Although visual computing was available, most universities continued to primarily focus on High Performance Computer (HPC) simulation ("number crunching") and data visualization was typically not integrated into the problem solving environment. Chronologically, researchers must first create HPC simulation results before any data visualization is realized. Hence HPC resources became the focus and data-visualization was accomplished by the individual researchers at their desktop computers weeks later. Although this process provides scientific insight post mortem, it does not provide researchers the ability to interact, manipulate, and change the boundary conditions using visual data analysis ("visualization") tools in real-time. This real-time visual data analysis is related to the idea of computational steering because it puts the applied scientist in the loop much the same as a pilot in a flight simulator. It can also be argued that computational steering can be used to help minimize compute cycles, because researchers can determine when to terminate "bad" jobs or continue the simulation until results converge. But to do so requires applied scientists extend their analytic-numerical skills to include scientific visual data analysis ("visualization") and universities must rethink how HPC resource can be integrated with data visualization to create a more powerful problem-solving environment. Because real-time visual data analysis is important, the next-generation of researchers have adopted new information technology skills that go beyond traditional numerical modeling and we are witnessing a renewed interest in data visualization and computational steering. This renewed interest in computational steering is also motivated by the advent of affordable High Performance Computing (HPC) systems such as the Virginia Tech System X [1]. The advent of Tera-scale computing creates tera-scale n-dimensional data sets that exceed capabilities for desktop data visualization tools and is the motivation for this concept paper. Researchers must either downsize their tera-scale simulations to continue to use their current desktop data visualization paradigm or a real-time computational steering system can be implemented in n-dimensions in an immersive virtual environment such as a CAVE. Such a system constitutes a powerful new problem-solving environment.

There are few scenarios that have effectively combined simulation and visualization into a problem-solving environment. One scenario exists here at Virginia Tech. This is the research of Dr. Diana Farkas in the Department of Materials Science and Engineering. She created her own molecular dynamic simulation code that runs for long periods of time on various HPC systems that predict properties associated with large 3D nanostructures [2]. Once created, simulation output is studied post mortem by using different visual methods. In addition to viewing traditional 2D slices at desktop computers, 4D (3D with time as the fourth dimension) visual data analysis tools were used from an immersive point of view in Virginia Tech's CAVE, a resource of the University Visualization and Animation Group (UVAG) [3]. Researchers at the UVAG, under the direction of Dr. Ron Kriz, developed 4D visualization tools in collaboration with Dr. Farkas and NCSA in 1997, that harnessed the immersive power of a CAVE system to study nanostructures interactively, D_Atomview [4,5]. These tools extend the post mortem analysis with visualization in 4D interactive virtual environments, which can now be extended to a "real-time" scenario. These interactive 4D visualization tools have advanced nano-structure research due to the unique nature of being able to be surrounded ("immersed") and to visually interact within the 4D data [6,7].

Both Dr. Farkas and the UVAG have continued to explore new technologies. Dr. Farkas is researching new areas that are always pushing the boundary of computational power needed to solve larger more realistic simulations. The UVAG has developed the Diverse Adaptable Display System (DADS) that currently operates the CAVE projection system [8]. The DADS system is a new generation of Linux-cluster visualization systems that have replaced the SGI computer system, which has powered the CAVE at Virginia Tech for the past seven years. The DADS system provides more power for visualizing larger 3D nanostructures predicted by Dr. Farkas than the current SGI system, and costs several orders of magnitude less than a new SGI system. Dr. Farkas's 3D nanostructure simulations are currently being implemented to run on System X. System X provides a several orders of magnitude increase in computational ability compared to previous resources [1]. With System X, DADS, and D_Atomview we have three existing pieces needed to implement a computational steering system. Currently these research projects are not connected. This concept paper is written to connect these areas of research and provide a computational steering prototype here at Virginia Tech.

Currently the code that Dr. Farkas uses for her simulations is being modified to run on the new System X resource. System X will provide Dr. Farkas with larger datasets in shorter amounts of time. As part of the analysis of these new datasets, the current D_Atomview 4D immersive visualization tool may be used. D_Atomview has recently been modified to view the larger datasets. D_Atomview has also been modified to read remote data in real-time. Hence, D_Atomview was designed with computational steering in mind. Adapting D_Atomview to work in concert with System X in real-time is a feasible task and would provide a working computational steering model.

We propose collaboration between the UVAG, Dr. Farkas, and the System X team to provide a computational steering example as proof of the power of Virginia Tech resources for scientific research. Not only will the System X's power be demonstrated, but the ability to harness its power for "real-time" scientific visual data analysis will also be demonstrated. This could lead to increased research activity, optimized usage of Virginia Tech computing resources, new research discoveries, grants, and will help increase awareness of resources available for researchers here at Virginia Tech. In order to accomplish this goal managers and developers will need to work in close collaboration.

References:

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