Stokes systems, which can exhibit poor convergence in absence of effective preconditioners. The emergence of GPU-based architectures offers dramatic hardware acceleration of many scientific computation tasks. Therefore it is natural to try to take advantage of GPU acceleration for many sparse matrix calculations, including Stokes systems. While achieving peak performance on sparse matrices is usually a challenge, we focus on enabling GPU support within one of the most popular sparse linear algebra and PDE library: PETSc (Portable Extensible Toolkit for Scientific computation). In this talk we will discuss our approach to enabling GPU acceleration for sparse matrix calculations, preconditioning, and the implications for Stokes solvers.

WebViz: A web-based collaborative interactive visualization system for largescale data sets

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With larger, faster, and more affordable multi-core and massively parallel computers coming to the market and with the introduction of general purpose GPU computing, the number and size of data sets being produced by the scientific community is on a steep rise. Additionally, with the rise of digital communication technologies, it is more and more common for scientists to engage in international collaborations across large geographical distances. To make sense of the large amount of data now being produced and to make collaboration between scientists easier, a new paradigm for data visualization is necessary. We propose that collaborative visualization tools and a web-based approach to data visualization is an attractive solution [Woodward et al., 2007; Damon et al., 2008; Greensky et al., 2008; McLane et al., 2009].

We have created a web-based application for multi-user collaborative visualization called WebViz. Our web application allows users in geographically disparate locations to simultaneously and collectively visualize large data sets (on the order of gigabytes) over the Internet. Furthermore, by providing data visualization services "in the cloud," users all around the world can leverage our service regardless of their local compute capabilities.

WebViz leverages asynchronous java and XML (AJAX) web development paradigms via the Google Web Toolkit (http://code.google.com/webtoolkit/) to provide remote users with a web portal to LCSE's (http://www.lcse.umn.edu) large-scale interactive visualization system already in place at the University of Minnesota. LCSE's custom hierarchical volume rendering software provides high-resolution visualizations on the order of 15 million pixels and has been employed primarily for visualizing data from simulations in astrophysics, geophysics, and computational fluid dynamics [Porter, 2002; Porter et al., 2002; Greensky et al., 2008; McLane et al., 2009].

In the current version of our WebViz application, we have implemented a new, highly extensible back-end framework built around HTTP "server push" technology. This design allows us to provide a rich collaborative environment and a smooth end-user experience. Furthermore, the web application is almost completely platform independent and is accessible via a variety of devices including netbooks, iPhones, and other web- and javascript-enabled cell phones.

Features in the current version of WebViz include: the ability for (1) users to launch multiple visualizations, (2) a user to invite one or more other users to view their visualization in real-time, (3) users to delegate control aspects of the visualization to others and (4) engage in collaborative chat and instant messaging with other users. These features are all in addition to a full range of visualization functions including 3D camera and object orientation/position manipulation, timestepping control, and custom color/alpha mapping.

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Molecular Paleoclimatology: Quantum Chemistry and the History of the Earth's Atmosphere

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The history of the composition of the Earth's atmosphere is one of the most important problems of our time. As the human race considers the possibility of planetary engineering to mitigate the potential effects of CO_2-induced global warming, clearer insight into the history of atmospheric PCO_2 and global temperature is required. For example, if PCO_2 values were 20 times higher at times in the geologic past, it may be premature to worry about anthropogenic increases in PCO_2 a factor of two above Pleistocene-Holocene values, which are anomalously low from the point of view of geologic history. Two major techniques for determining the history of atmospheric PCO_2 are the chemically based. The first depends on the isotopic composition of carbon incorporated into soil minerals during their growth. The second depends on the isotopic composition of boron incorporated into marine minerals during precipitation. Both methods depend crucially on knowing the equilibrium constant for isotope exchange between minerals, aqueous, and gas phases. There are major uncertainties in these equilibrium constants which strongly affect geochemical estimation of the history of PCO_2 in Earth's atmosphere. Here, I describe how quantum chemistry techniques can be used to reduce this uncertainty and make more reliable estimates of PCO_2 values.

Ab initio molecular dynamics and quantum chemistry techniques are used to calculate the structure, vibrational frequencies, and carbon-isotope fractionation factors of the carbon dioxide component [$CO_2(m)$] of soil (oxy)hydroxide minerals goethite, diaspore, and gibbsite. We have identified two possible pathways of incorporation of $CO_2(m)$ into (oxy)hydroxide crystal structures: one in which the C^{4+} substitutes for four H^+ [$CO_2(m)_A$] and another in which C^{4+} substitutes for (Al^{3+},Fe^{3+})+H^+ [$CO_2(m)_B$]. Calculations of isotope fractionation factors give large differences between the two structures, with the $CO_2(m)_A$ being isotopically lighter than $CO_2(m)_B$ by≈10 per mil in the case of gibbsite and nearly 20 per mil in the case of goethite. The reduced partition function ratio of $CO_2(m)_B$ structure in goethite differs from $CO_2(g)$ by<1 per mil. The predicted fractionation for gibbsite is>10 per mil higher, close to those measured for calcite and aragonite. The surprisingly large difference in the carbon-isotope fractionation factor between the $CO_2(m)_A$ and $CO_2(m)_B$