SCIENCE GRID THIS WEEK

May 10, 2006

Calendar / Meetings

May

8-10, NSDI '06: 3rd Symposium on Networked Systems Design & Implementation, San Jose, California

10-12, GGF17: The 17th Global Grid Forum, Tokyo, Japan

10-12, Geoinformatics 2006, Reston, VA

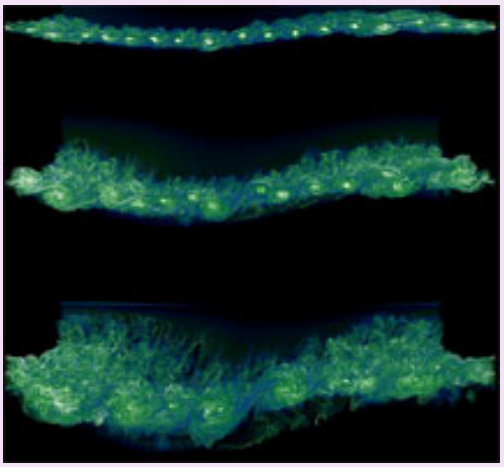
15-18, TERENA Networking Conference 2006, Catania, Italy

16-19, CCGrid06: 6th IEEE International Symposium on Cluster Computing and the Grid, Singapore

16-19, Grid Asia 2006, Singapore

Full Calendar

Image of the Week

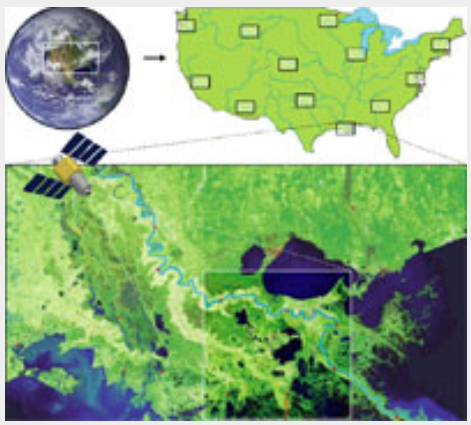


Simulation of turbulent flow. (Click on image for larger version.)
Image Courtesy Paul Woodward and David Porter, University of Minnesota

Scientists at the University of Minnesota studying turbulent

Feature Story

CLEANER's Vision for the WATERS Network

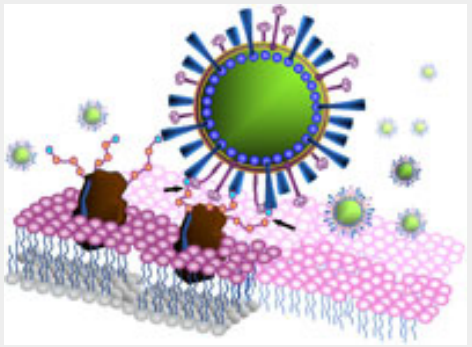


Hypothetical scope of the WATERS Network.

As population levels and the rate of urban development rise, our society grows increasingly concerned with balancing the need to maintain water supplies of adequate quantity and quality for human use with preserving the integrity of aquatic ecosystems. Common practices associated with modern living often negatively impact the environment. Commercial fertilization of agricultural fields can result in significant run-off of nutrients and microorganisms into nearby surface waters. In some U.S. cities, untreated stormwater, containing substantial loadings of pathogens and chemicals, is discharged into the nearest body of water. And along some major U.S. rivers, drinking water intakes are located downstream from wastewater treatment plants. Because many of these issues are tied to where people live and work, scientists and engineers must also factor in social and economic impacts when considering solutions to these problems.

The goal of CLEANER, the Collaborative Large-Scale Engineering Analysis Network for Environmental Research, is to transform and advance the scientific and engineering knowledge base in order to address the challenges of complex, large-scale,

EGEE Grid Attacks Avian Flu



Neuraminidase, one of the two major surface proteins of influenza viruses, facilitating the release of virions from infected cells.
Image Courtesy Ying-Ta Wu, Academia Sinica.

During April, a collaboration of Asian and European laboratories has analysed 300,000 possible drug components against the avian flu virus H5N1 using the EGEE grid infrastructure. The goal was to find potential compounds that can inhibit the activities of an enzyme on the surface of the influenza virus, the so-called neuraminidase, subtype N1. Using the Grid to identify the most promising leads for biological tests could speed up the development process for drugs against the influenza virus.

One of the targets of existing drugs today on the market is viral neuraminidase, an enzyme that helps the virus to proliferate and infect more cells. As this protein is known to evolve into variants if it comes under drug stress, drug resistance becomes a potential concern in case of an influenza pandemic.

The challenge of the in silico drug discovery application is to identify those molecules which can dock on the active sites of the virus in order to inhibit its action. To study the impact of small scale mutations on drug resistance, a large set of compounds was screened against the same neuraminidase target but with various, slightly different structures. With the results from the in silico

convection in giant stars are exploring remote computation and visualization using the TeraGrid. Twice in 2005, the scientists demonstrated a prototype computational steering, visualization and data-analysis pipeline that produced volume-rendered images at a rate of up to one second per frame streamed directly from the Pittsburgh Supercomputing Center. A turbulence simulation was run on computing resources at PSC, and the results were displayed remotely using the TeraGrid network.

Learn more...

Statistic of the Week

2,000

Number of computers used for four weeks in April to search for possible drug components to treat the avian flu virus H5N1. Three grid infrastructures were used in the search: AuverGrid; EGEE; and TWGrid.
Source: EGEE Press Release

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Office of Science/ U.S. DOE

human-stressed environmental systems. To understand these complex situations, scientists and engineers need to collect and integrate real-time data from watersheds, rivers, estuaries, coasts and cities throughout the country, and environmental engineers must integrate information from the laboratory or a single field site with information from larger, more geographically diverse observatories. It is only now, with the advent of grid computing, new data-mining techniques, and novel wireless sensors, that researchers are in a position to answer cutting-edge questions about hydrologic and environmental phenomena.

Full article

Grids in the News

Grid Takes Aim at Ills
Grid Computing Planet, May 9, 2006
By Paul Shread

Grid computing projects have sprung up in recent months to address pressing issues such as avian influenza and global warming.

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Vanderbilt engineers to help Air Force use Global Information Grid
Vanderbilt Press Release, May 8, 2006

Frustrated with cell phone dead zones, busy signals, e-mail spam, endless voice mail loops and other exasperating aspects of technology?

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Grid seeks bird flu cure
Silicon.com, May 5, 2006
By Stefanie Olsen

Scientists in the UK and Asia have deployed a computing grid to find a potential cure for Avian flu.

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UK computer Grid plays its part in fight against avian flu
ElectronicsWeekly.com, May 3, 2006

screening, researchers can predict which compounds and chemical fragments are most effective for blocking the active neuraminidases in case of mutations.

Full article

Re-Engineering the Research Process


Jim Myers, NCSA

One could argue that scientists have been slowly losing the capabilities that enabled the scientific revolution. Hundreds of years ago, the top minds in any given culture had access to the overwhelming majority of their culture's knowledge. There wasn't that much data to go around, and thinkers tended to congregate at the intellectual epicenters. They all used a common format—text and drawings, even if it did mean you had to speak several languages. And they all used a very limited set of tools. Mostly, they had their brains, pencils, and benefactors.

That systemic view is something we've lost, locking up knowledge in a variety of tools and databases and individual disciplines. Cyberenviron-ments—integrated, end-to-end software systems that will make cyberinfrastructure as accessible and usable as Web browsers made the Internet—mitigate that loss. They'll give researchers the ability to make connections across the whole of human knowledge and to have the global perspective that enabled their forebearers' revolutionary advances.

Cyberenvironments support the re-engineering of science and engineering research processes. Part of their role will be to provide an easy-to-use interface to local and shared instruments, sensor arrays, data stores and data sets, computational systems, networks, scientific and engineering applications, data analysis and visualization tools, and services, all within a secure framework.

By Richard Wilson

Computers in 11 UK universities and research laboratories have been employed in the fight against avian flu.

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Full article

This article, written by Jim Myers, originally appeared in the May issue of NCSA's Access Online.