SDSC's Trestles Provides Rapid Turnaround and Enhanced Performance for Diverse Researchers

New Supercomputer Delivers Increased Productivity, On-demand Access

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Jan Zverina

Trestles, a supercomputer launched earlier this year by the San Diego Supercomputer Center (SDSC) at the University of California, San Diego, is proving itself as a valuable resource for researchers across a wide range of disciplines, from astrophysics to molecular dynamics, who need access to computational resources with rapid turnaround.

In the seven months since its launch, more than 50 separate research projects have been granted time on *Trestles*. As the system is targeted to serve a large number of users, project allocations are capped at 1.5M SUs (service units, or single processor hours) annually on the new SDSC system.

"*Trestles* was designed to enable modest-scale and gateway researchers to be as computationally productive as possible," said Richard Moore, SDSC's deputy director and co-principal investigator the system, the result of a $2.8 million National Science Foundation (NSF) award. "It has attracted researchers from diverse areas who need access to a fully supported supercomputer with shorter turnaround times than has been typical for most systems. In addition, to respond to user requirements for more flexible access modes, we have enabled pre-emptive on-demand queues for applications which require urgent access in response to unpredictable natural or manmade events that have a societal impact, as well as user-settable reservations for researchers who need predictable access for their workflows."

With 10,368 processor cores, a peak speed of 100 teraflop/s, 20 terabytes memory, and 39 terabytes of flash memory, *Trestles* is one of several new HPC (high-performance computing) systems at SDSC. The center is pioneering the use of flash-based memory, common in much smaller devices such as mobile phones and laptop computers but relatively new for supercomputers, which typically rely on slower spinning disk technology.

"Flash disks can read data as much as 100 times faster than spinning disk, write data faster, and are more energy-efficient and reliable," said Allan Snavely, associate director of SDSC and co-PI for the new system. "*Trestles* uses 120GB flash drives in each node, and users have already demonstrated substantial performance improvements for many applications compared to spinning disk."

Three recent research projects, each allocated one million SUs on *Trestles*, include:

Climate Change: How Aerosols Affect the Air We Breathe At present, there are large uncertainties associated with the effects of atmospheric aerosols, fine solid or liquid particles suspended in the air. Atmospheric aerosols have both natural (e.g., volcanic eruptions, biomass burning and wind-blown dust from soils) and anthropogenic (e.g., combustion) origins and during their lifetimes undergo several transformations due to the interaction with solar radiation and gas molecules in the air.

By influencing the amount of solar radiation that reaches the Earth's surface as well as the formation of clouds, researchers believe that aerosols play a major role in the atmosphere with important consequences for global climate and the ecosystem. Atmospheric aerosols are also associated with adverse effects on human health, notably in the areas of respiratory, cardiovascular, and allergic diseases.

Researchers lack a complete understanding of the properties of aerosols and the chemistry that takes place on these particles, according to Francesco Paesani, assistant professor of chemistry and biochemistry at UC San Diego. "This incomplete knowledge of aerosol chemistry currently limits the possibility of making quantitative predictions about the future state of the atmosphere," said Paesani, who as PI is conducting this research under a grant from the NSF's Environmental Chemical Science Division. Paesani and his research group are also part of the NSF Center for Aerosol Impacts on Climate and the Environment (CAICE) established at UC San Diego.

Using *Trestles* as a resource, Paesani and his group have been developing computational methodologies to more accurately assess how particles in atmospheric aerosols directly affect air quality, and better understand their role in global climate concerns such as Earth's radiative balance and cloud formation. The Paesani group research interests focused on modeling chemical reactions on aerosol surfaces under atmospheric conditions, specifically the characterization of the molecular mechanisms that determine the dissociation of inorganic acids such as hydrogen chloride (HCl), nitric acid ($HNO3$) and sulfuric acid ($H2SO4$) on aqueous environments. They have been studying the dissociation of HCl in small water clusters as well as on ice surfaces under atmospheric temperature conditions.

HCl has been shown to play a critical role in chlorine activation reactions taking place at the surface of polar stratospheric clouds. Paesani's preliminary results indicate that the dissociation of HCl on ice surfaces is very rapid at all relevant atmospheric temperatures of 180 to 270 Kelvin (-135 to +25 degrees F). These results suggest that the ice surface does not simply serve as a static platform on which the reactants meet, but actually plays an active role in the reaction itself.

"Since our computational methodologies take into account the quantum nature of both electrons and nuclei using a 'first principles' approach, our molecular simulations are computationally highly expensive.," said Paesani, who recently published related research in the *Journal of Physical Chemistry*. "Having access to a powerful computing cluster such as *Trestles* has greatly benefited us."

Molecular Dynamics: Thermal Management in Microelectronics Simply put, heat and inefficient thermal management pose major barriers to the continued miniaturization and increased capabilities of microelectronics such as microchips, now used in everything from mobile phones and digital cameras to supercomputers and missile guidance systems.

Tengfei Luo, with the Massachusetts Institute of Technology (MIT), specializes in the study of thermal management in microelectronics. His supercomputer simulations show that the intrinsic thermal conductivity of polymer chains, widely used in thermal management, strongly depends on their structural stiffness, and that surface morphology can greatly influence the efficiency of heat transfer across interfaces, or connections. By contrast, "soft" chains, or less structurally stiff ones, tend to scatter more heat carriers and results in low thermal conductivity.

"Our research is focused on studying heat transfer mechanisms in many different materials, and in particular we are providing new insights into the selection of thermally conductive polymers and better thermal transporting interfaces, essential to the ongoing miniaturization of microelectronics," said Luo.

"We found *Trestles* to be a very versatile system, on which we could run a large number of smaller jobs simultaneously or perform larger simulations of more than 512 cores involving tens of thousands of atoms," added Luo. "Unlike other systems, we were able to use *Trestles* to run jobs for as long as two weeks, which is a very valuable feature for studying thermal transport. Our I/O-intensive first-principle calculations greatly benefited from the system's local flash memory, while improving the stability of our calculations. Plus the large memory (64GB) on each node helped us significantly for memory-demanding FP calculations."

Luo's latest research related to thermal management was published in the April 2011 issue of the *Journal of Applied Physics.*

Astrophysics: High-Energy Collisions of Black Holes In astrophysics, 'black holes' are formed when a massive star collapses with such gravitational force that not even light can escape from it. Black holes can be modeled using Einstein's theory of General Relativity in four dimensions (three spatial and one time). These equations are considered to be among the most complicated ones in all of physics, and it wasn't until almost 90 years later, in 2005, that breakthroughs in simulating black hole dynamics using numerical relativity were achieved. These recent advances have come about because of the availability of supercomputers having both large memory and strong computational performance.

Ulrich Sperhake, a theoretical astrophysics researcher with the California Institute of Technology (CalTech) as well as the Institute of Space Sciences at CSIC-IEEC, Barcelona, Spain, was recently allocated one million SUs on *Trestles* to further investigate high-energy collisions of black holes, with the goal of improving our understanding of the dynamics of these implosions.

"The purpose of our research is to identify the possibility of achieving numerically more robust and accurate simulations by using alternative formulations," said Sperhake, PI of the NSF- funded project, whose team has been studying black holes in three distinct areas of experimental and observational research: gravitational wave physics, Trans-Planckian Scattering, and high-energy physics. Sperhake plans to publish a detailed review of his numerical studies in those three areas. His most recent research was published in the May 20, 2011 issue of *Physical Review D.*

"Numerical simulations of black-hole binary space times in the framework of Einstein's theory of General Relativity, or generalizations thereof, require hundreds of processors and of the order of 100s of GB of memory," said Sperhake. "That is way outside the scope of workstations available locally, so the importance of having a computer cluster of the quality of *Trestles* cannot be overstated."

A TeraGrid/XSEDE Resource *Trestles* is appropriately named because it is serving as a bridge between SDSC's current resources such as *Dash*, and *Gordon*, a much larger data-intensive system scheduled for deployment in late 2011/early 2012. Like *Dash* and the upcoming *Gordon* system, *Trestles* is available to users of the NSF's TeraGrid, the nation's largest open-access scientific discovery infrastructure. TeraGrid is transitioning this summer to a new phase called XSEDE (Extreme Science and Engineering Discovery Environment), the result of a new multi-year NSF award.

Trestles is among the five largest supercomputers in the TeraGrid/XSEDE repertoire, and is backed by SDSC's Advanced User Support group, which has established key benchmarks to accelerate user applications and assist users in optimizing applications. Full details of the new system, including how to utilize on-demand access or user-settable reservations, can be found at http://www.sdsc.edu/us/resources/trestles/.

Media Contacts: Jan Zverina, SDSC Communications, 858 534-5111 or jzverina@sdsc.edu Warren R. Froelich, SDSC Communications, 858 822-3622 or froelich@sdsc.edu