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SDSC Awarded NSF Grant for Triton Shared Computing Cluster Upgrade

'Triton Stratus' to provide interactive computing and cloud scaling for researchers

The National Science Foundation (NSF) has awarded the San Diego Supercomputer Center (SDSC) at UC San Diego a two-year grant worth almost $400,000 to deploy a new system called *CC* Compute: Triton Stratus* as an enhancement to the existing *Triton Shared Computing Cluster* (TSCC) campus High-Performance Computing (HPC) platform.

The grant, which was made under auspices of the National Science Foundation's Campus Cyberinfrastructure (CC*) program, runs until mid-2021 and includes funding for new on-campus capabilities as well as credits for commercial cloud computing services.

Triton Stratus will provide researchers with improved facilities for utilizing emerging computing paradigms and tools, namely interactive and portal-based computing, and scaling them to commercial cloud computing resources. Researchers, especially data scientists, are increasingly using tools such as Jupyter notebooks and RStudio to implement computational and data analysis functions and workflows.

Triton Stratus will establish a pool of new compute nodes dedicated to Jupyter and RStudio, providing researchers with higher performance technology and better system response times. Moreover, the project will investigate and deploy techniques for packaging tested notebooks and sending or "bursting" them to commercial cloud services for greater scale or throughput.

These tools are part of a general trend in research computing toward web-based and graphical interfaces for accessing HPC systems, especially for attracting newer generations of researchers and data scientists. *Triton Stratus* will allow exploration of the emerging hybrid

model of on-premise cluster computing resources, coupled with commercial cloud computing services.

The new capability is expected to be operational by the second quarter of 2020.

“When we polled our user community, researchers were very excited about improved capabilities for working with Jupyter Notebooks and RStudio and there was interest across the entire spectrum of scientific disciplines,” noted Ron Hawkins, TSCC Program Manager and Principal Investigator for *Triton Stratus*. “We are appreciative that the NSF has seen fit to fund this system enhancement and we look forward to the scientific progress that will ensue from it.”

SDSC’s Robert Sinkovits, Subhashini Sivagnanam, and Mary Thomas are co-PIs on the award.

Triton Stratus leverages the strong commercial momentum in cloud computing and underlying technologies. The worldwide public cloud services market is projected to grow 17.5 percent in 2019 to total $214.3 billion, up from $182.4 billion in 2018, according to research and advisory company Gartner, Inc. The fastest-growing market segment will be cloud system infrastructure services, or infrastructure as a service (IaaS), which is forecast to grow 27.5 percent in 2019 to $38.9 billion, from $30.5 billion in 2018. The second-highest growth rate of 21.8 percent will be achieved by cloud application infrastructure services, or platform as a service (PaaS).

“This significant award is part of SDSC’s multi-pronged hybrid cloud strategy,” said SDSC Director Michael Norman. “The NSF has recognized the significant growth in commercial cloud services and the advantages that they offer the greater research community, and SDSC is answering that call via multiple funded projects.”

“This project will let us investigate and understand a number of dimensions, including the right balance of on-premise and cloud resources, the best modes for scaling or bursting to cloud platforms, and new models of interactive research computing,” added Hawkins.

“*Triton Stratus* will enhance the Materials Virtual Lab’s use of Jupyter notebooks and TSCC for various tasks, including setting up high-throughput DFT (density functional theory) calculation workflows, the analysis and extraction of materials properties, the insertion and querying of processed data into databases, and the rapid prototyping of neural network and other machine learning models,” said Shyue Ping Ong, associate professor of nanoengineering at UC San Diego’s Jacobs School of Engineering, and the lead principal investigator of the MVL.

Through machine learning of large data sets, the MVL studies and designs materials for energy storage (e.g., rechargeable lithium-ion batteries), energy efficiency (e.g., phosphors for solid-state lighting) and structural materials for extreme environments.

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