

## **Instant-On Simulation Delivery: Helping TeraGrid Achieve Its Wide and Open Strategic Goals**

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**Background:** The National Science Foundation's TeraGrid high-performance computing (HPC) network provides extensive support for massive computational science, typically conducted by scientists highly trained in HPC. TeraGrid's strategic plan [1] requires the engagement of a much larger and more diverse community of researchers and educators in computational science discovery and learning.

The unmet needs of this broader community, not now using TeraGrid to advance their science and engineering through computational learning and discovery, are four-fold. First, these users need modest, not massive, allocations of HPC to conduct their science. Second, they need to replace their weeks-long computational runs on a desktop computer with an HPC run taking just minutes. Third, most want to run well-defined workflows rather than develop their own codes. Fourth, education involves many student uses of simulation that are repetitive, thus archiving and reusing results would free TeraGrid computational resources while supporting education well. Running a code with the same input as before would return the archived results rather than using computational time.

**This Project:** We will develop, test, and deploy a new "instant-on" computing capability on nanoHUB.org, which will host TeraGrid-approved codes and workflows with results-archiving and reuse that is connected to a portion of TeraGrid configured for queue-less, instant-on, interactive parallel computing.

**Intellectual Merit:** With the above enhancement, the HUBzero platform [2] that powers nanoHUB.org [3] with over 7,000 annual simulation users will be able to manage the interaction of simulation runs with TeraGrid resources to achieve short elapsed times for short runs and to manage allocation of access among the potentially very large number of users. HUBzero will also support data exploration and results reuse. The software developed for this project will become part of the core HUBzero platform and redeployed on dozens of other science gateway sites built on the same platform.

**Broader Impact:** TeraGrid will meet the needs of an expanded community of users. The science gateway will hold a TeraGrid community allocation and contain only pre-approved codes and workflows. Gateway users would neither individually request TeraGrid resources nor run arbitrary codes. This environment would serve both the users and TeraGrid management well. Wider use of TeraGrid will result in new high-value science with a broad set of scientific publications.

### **References**

- [1] "TeraGrid 2008 Science Highlights," p. TG03 at <http://www.teragrid.org/news/docs/SH08.pdf>
- [2] Michael McLennan (2008), "The Hub Concept for Scientific Collaboration," <http://hubzero.org/resources/12>
- [3] Gerhard Klimeck, Michael McLennan, Sean B. Brophy, George B. Adams III, Mark S. Lundstrom, "nanoHUB.org: Advancing Education and Research in Nanotechnology", IEEE Computers in Engineering and Science (CISE), Vol. 10, pg. 17-23 (2008), free pdf from Purdue Library (<http://docs.lib.purdue.edu/cgi/viewcontent.cgi?article=1079&context=nanodocs>).