Successful Educational Request

Title: Hennig's Course: Computational Materials Science Request Summary
Primary Field of Science: Materials Research
Resources Request Information:

- What percentage of the work you expect to do in this allocation will be the following types:
  - Production (actually doing research): 0%
  - Exploration/porting (preparing to do research): 0%
  - Education (teaching others to do research): 100%
- What percentage of the jobs you expect to run in this allocation will be the following types:
  - Submitted through command line/script: 100%
  - Submitted using Grid tools (such as GRAM): 0%
  - Submitted through a meta-scheduler: 0%
- Please estimate what percentage of the science runs you expect to perform in this allocation will be the following types:
  - Independent (a job that is not immediately connected to any other job - a job that is artificially broken into chunks by queue limits should still be placed this category): 100%
  - Independent but related (such as jobs that make up an ensemble or parameter sweeps): 0%
  - Tightly-coupled (multiple jobs that will run simultaneously): 0%
  - Dependent (multiple jobs such as in a workflow): 0%

Resource Requested: TACC Sun Constellation Cluster (Ranger)
Resource Requested Amount: 150,000 SUs
Resource Awarded Amount: 150,000 SUs

Abstract: This allocation request is to support my course MSE 5720 "Computational Materials Science" which will take place this Fall semester at Cornell University. The course is aimed at seniors and beginning graduate students and will introduce a variety of computational methods used in different fields of materials science. The course will take the students from the smallest scale of electrons and nuclei to properties of real materials, such as electronic structure, mechanical behavior, diffusion and phase transformations. The students will learn how to use a number of modeling methods relevant to a wide variety of materials, ranging from metals and semiconductors to ceramics and polymers to molecules and liquids. The topics include: Molecular dynamics simulations with empirical potentials, quantum mechanical ab initio methods for electronic structure, continuum methods such as finite volume and finite elements, and application to metals, semiconductors, molecules, nanostructures. Through lectures, hands-on labs, and discussions, the class will introduce the students to powerful computational methods and state-of-the-art simulation codes. We request an allocation of 150,000 SU to support the labs

and projects of the 30 registered students. In the labs the students will learn various computational tools such as density functional and quantum chemistry methods (Quantum Espresso and Gaussian), molecular dynamics (GULP, LAMMPS), and finite elements methods (OOF2). An allocation of 150,000 SU will ensure that the students can run these labs and an additional course projects and gain useful experience running parallel simulations on state-of-the-art supercomputers.