Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Characterizing Large-Scale Computational Physics TIMOTHY WILLIAMS, Argonne National Laboratory — Large-scale computational physics calculations typically share some of a number of basic characteristics:

- Brute-force approaches: Atomistic molecular dynamics, particle-in-cell plasma physics, particle-mesh cosmological simulations, DNS of turbulence, lattice QCD, Monte Carlo, ...
- Wide range of relevant scales: Angstroms to millimeters in molecular dynamics, ion/electron cyclotron period to seconds or minutes in plasmas, galaxy to observable universe in cosmology, high Reynolds number turbulence, ...
- Obvious need for yet larger scale: higher resolution, larger simulation domain, more particles, ...
- Code is named, parallel, community, long-lived (but evolving).

This talk views the computational physics landscape from the perspective a physicist who has worked at three DOE large-scale computing centers: the Argonne Leadership Computing Facility, the (former) Advanced Computing Laboratory, and NERSC. The "usual suspects" at the large-scale end of computational physics are remarkably persistent, even in the face of an ever-increasing definition of large-scale.

Timothy Williams
Argonne National Laboratory

Date submitted: 11 Nov 2010 Electronic form version 1.4