Application Domain: Design and functioning of nanoscale systems / Self-assembly and fabrication of nanoscale systems

Problem: Computational Nanotechnology has led the development of the field and has motivated the current effort on experimental verification and fabrication technology. Continued success in this field requires progress in our ability to simulate more complex systems and guide the development of experimental and fabrication efforts. Two key steps are central to the success of this effort:

a. Furthering our ability to simulate simple nanoscale structures to complex systems so that simulations can impact design of these systems.

b. Fabrication of nanoscale systems almost certainly will depend upon self-assembly. Self-assembly is a poorly understood process and progress is critically dependent on our ability to simulate self-assembling systems and to develop rules by which target system fabrication can be achieved.

Benefit: As stated previously, computational nanotechnology has led the development of this field and continued progress is critically dependent on extensive and ubiquitous simulation capability. Lack of these capabilities will mean development by a trial and error experimental with consequent diminished chances of success. Further, we may have little idea of the causes of failure of nanotechnology to live up to its potential.

Algorithmic technique(s):

a. Classical molecular dynamics
b. Quantum molecular dynamics
c. Quantum transport
d. Quantum chemistry
e. Discrete system dynamics and thermodynamics
f. Self-assembly processes

Is there a "tipping point" i.e., is the application area not feasible now but that will take off once some measure of computer performance reaches x?

Most emphatically, yes. While simulations have motivated the initial development of nanotechnology and the realization of potential, continued success depends on ability to extend simulation capability to nanoscale systems. This capability will allow simulations to impact design of systems. Lacking this capability, the field is likely to plateau while this capability would provide a second surge.

In terms of computer performance, current resources allow us to perform "one of" type simulations of simple structures. We need to get to the point of being able to perform parametric design and optimization studies of nanoscale systems both for functioning and fabrication.

HEC driver/requirement:

Why is _high end_ computing needed for progress?

Without high end computing and its associated resources, there is faint hope of achieving the state goals for computational nanotechnology and the associated goals for the field and the realization of potential.

What are the high performance computational capabilities or capacities required to enable this application?

Current capability allows us to perform "one of" computations that require special queues, or special times when large resources can be blocked. For impact, these simulations need to become routine and ubiquitous.

Is your agency likely to be able to provide computers to satisfy this requirement? If not, why not?

Current roadmaps indicate that such resources will not be available. We will not have the budgets to motivate vendors to develop the next generation machines that would be required.