



# High-Performance Computing at Nanoscale

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**Motivations.** Nanotechnology is a tricky business. Physical experiments at this level of precision are still difficult to do and are expensive. This research can be greatly accelerated using high-performance computing. Scientists model physical phenomena at the nanoscale level using complex computer codes, such as molecular dynamics. This eliminates physical experiments that would waste resources, enabling scientists to pinpoint the ones that are likely to succeed.

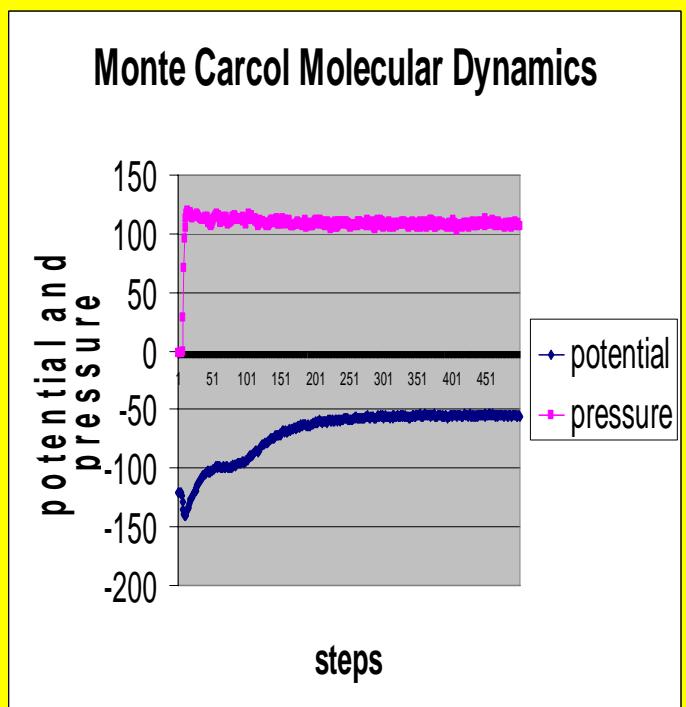
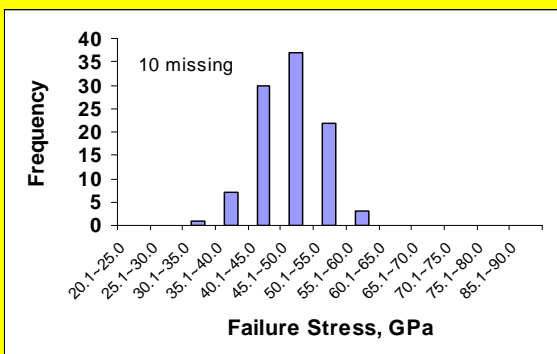
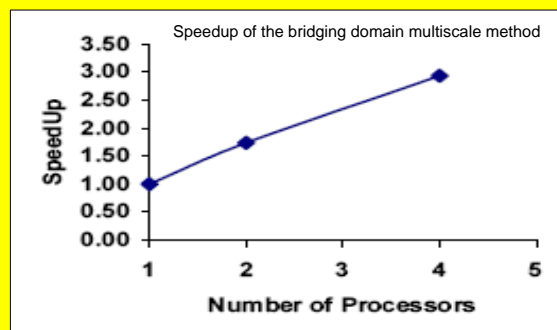
### Needs of high-performance computing in multiscale simulation:

1. Currently developed multiscale methods still have limitations on length and time scales. This issue can be solved by employing high-performance computing.
2. Concurrent multiscale methods are ready to be implemented with high-performance computing since they involve multiple length/time scale computations.

### Needs of high-performance computing in molecular simulation:

1. The Monte Carlo method is one of the candidates for high-performance molecular methods
2. Molecular dynamics is computationally intensive for molecular systems containing more than 10,000 atoms, which are still far smaller than the ones observed in the experiments.
3. High-performance computing, especially Grid computing, has potential on reliability analysis of nanoscale materials that requires numerous numerical tests.

Effect of randomly occurring vacancy defects on failure stresses of carbon nanotubes. The above figure shows the distribution of failure stresses when nanotubes have 10 missing atoms. Locations of vacancy can be arbitrary and 100 tests have been simulated with parallel computing.



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