# Order–N Parallel Tight Binding Molecular Dynamics: Application to the Carbon Nanotubes

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Carbon nanotubes with their remarkable mechanical and electronic properties play a major role in the design of next generations nanoelectronic and nonoelectromechanical devices. Depending on their chirality carbon nanotubes could be conductor, semiconductor as well as insulators. Using Order–N (O(N)) parallel tight binding molecular dynamics method we have studied the structural stability and energetics of carbon nanotubes. In classical tight binding calculations standard matrix diagonalization algorithms have a complexity that grows as cube of the system size ($O(N^3)$). In this work we have compared our O(N) algorithm with $O(N^3)$ algorithm on sequential computer. Then parallelization technique is applied to O(N) TBMD program. Our system contains 8 computer having celeron processors with fast ethernet and PVM (Parallel Virtual Machine) library. The results for sequential and parallel runs are compared and assured that they are the same both in numerical accuracy and in physical aspects. Our results show that parallelization technique is beneficial because of the nature of the O(N) algorithm. We will report our results of speed up, efficiency and the system size studies. In present situation, parallelization together with O(N) algorithm proves to be very effective and favorable.

## References

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