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

Cem Ozdoğan

Department of Physics, Middle East Technical University, Ankara, Turkey

Abstract

Carbon nanotubes with their remarkable mechanical and electronic properties play a major role in the design of next generations nanoelectronic and nonoelectromechanical devices [Special issue, Physics World, June 2000]. 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 ($O(N^3)$) [Rep. Prog. Phys. 60 (1997) 1447]. In this work we have compared our O(N) [Computational Material Science 12 (1998) 157] 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) [www.epm.ornl.gov/pvm/] 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.

Joint work with Gülay Dereli(Department of Physics, METU)

ozdogan@newton.physics.metu.edu.tr

A Neutron Diffusion Equation Solver Using Object Oriented Technique

Mehmet Yılmaz Peker

Informatics Institute, Istanbul Technical University

Abstract

In this paper, a general neutron diffusion differential equation solver is presented. Object Oriented Technique (OOT) in the solver was implemented. OOT was chosen because of maintainable, reusable and efficient. The solver has capabilities of solving two dimensional and multi-regional one group neutron diffusion equations. It has also capabilities of solving reflective and vacuum boundary problems. To solve many engineering problems is used larger programs. OOT is suitable for writing such a large program. The most important feature of the solver is that it has all benefits of Object Oriented Technique.

oint work with Hasan Saygın(Informatics Institute and Nuclear Energy Institute,Istanbul Technical University, Turkey)

myp@be.itu.edu.tr

A Visual Nuclear Fuel Management Driver

Mehmet Yılmaz Peker

Informatics Institute, Istanbul Technical University , Turkey

Abstract

Fuel Management Calculations in the nuclear technology are very complicated processes. As in so many other fields of endeavor, complex computer programs are used to carry out state-of-the-art design calculations. These calculations are cumbersome. Therefore, A visual model describing nuclear reactor core behavior is necessary to understand easily. The Visual Nuclear Fuel Management Driver get explaining the basic principles of nuclear fuel management understood by students as a teaching tool. Different nuclear fuel types can be defined in this driver. By using these different nuclear fuel types, nuclear core is modelled in the visual environment

oint work with Hasan Saygın(Informatics Institute and Nuclear Energy Institute, Istanbul Technical University, Turkey)

myp@be.itu.edu.tr