Nanostructure Modelling on Parallel Systems

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CENG 471 Parallel Computing

What is Nanostructure Modeling?

- Nanostructure modeling is the computation of the positions and orbitals of atoms in arbitrary nanostructures.

Why is Nanostructure Modeling Important?

- Accurate atomic-scale quantum theory of nanostructures and nanosystems fabricated from nanostructures enables precision metrology of these nanosystems and provides the predictive, precision modeling tools needed for engineering these systems for applications including advanced semiconductor lasers and detectors, single photon sources and detectors, biosensors, and nanoarchitectures for quantum coherent technologies such as quantum computing. The tight-binding model based upon the Linear Combination of Atomic Orbitals (LCAO) method provides an accurate atomistic theory for nanostructures.

Why Parallelize Nanostructure Modeling?

- The tight-binding method is ideal for modeling small nanostructures. However, for modeling nanostructures with more than 25,000 atoms, the method is impractical on sequential computers due to long run times. Significant improvements in run time can be achieved through parallelization.

How is the Parallelization Realized?

- There are two parts to parallelizing this problem: creating the structure; and solving the Hamiltonian equation. The structure is created geometrically. We parallelize this by dividing the structure into layers. Communication is across layers. The starting point is a cubic structure that encompasses the desired nanostructure; the structure shape is created by pruning away the excess. We parallelize solving the Hamiltonian with PARPACK. The parallel implementation can handle arbitrary nanostructure shapes through an input file specification procedure.

Hamiltonian equation

- In physics and mathematics, Hamilton's equations is the set of differential equations created by William Rowan Hamilton.
- Hamilton's equations provide a new and equivalent way of looking at classical mechanics.

Hamiltonian equation

- Generally, these equations do not provide a new, more convenient way of solving a particular problem but rather they provide deeper insights into the structure of classical mechanics in general and its connection to quantum mechanics that arise in Hamiltation mechanics, but also in many other related and sometimes apparently not related areas of science.

How is the Parallelization Realized?

- Once the atom positions are determined, then the Hamiltonian is determined. Once the Hamiltonian is known, it is diagonalized to find the electron Eigen energies and Eigen states, i.e. the electron energies and charge distribution at each atom site. This is parallelized with PARPACK.

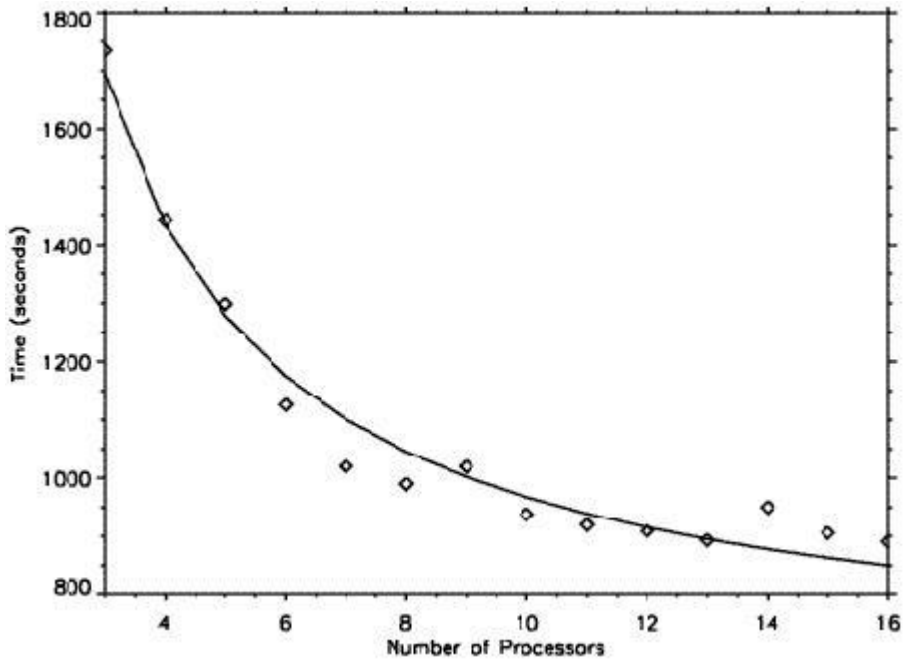
ARPACK SOFTWARE

- ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.
- ARPACK software is capable of solving large scale symmetric, nonsymmetric, and generalized eigenproblems from significant application areas.

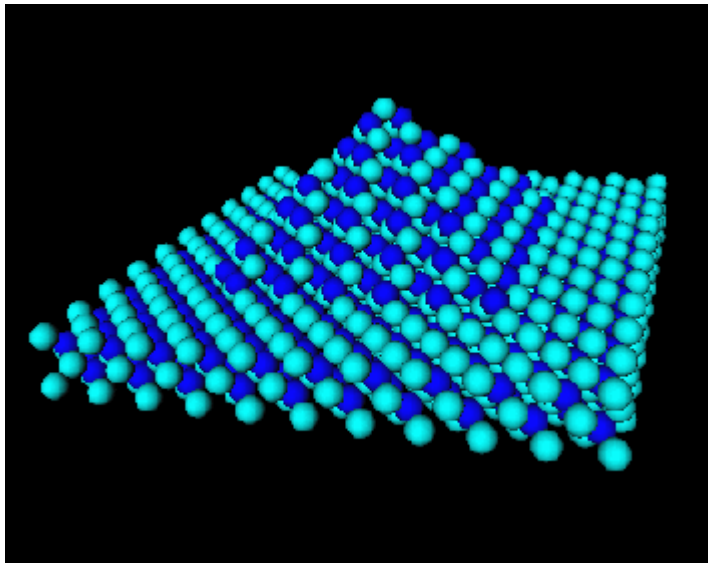
What is the Performance of the Parallel Code?

- We ran the code on the NIST NBS Cluster of 500Mhz Pentium III processors. Each processor has a Gigabyte of memory. For the structure consisting of three concentric spheres with diameters 3, 4, and 5 lattice units, the timing data closely matches the formula: T = 655.7 + 3116.0/N. T is execution time (in seconds), and N is the number of processors. The non-parallelizable computation time is 655.7 seconds; while the parallelizable portion of the computation uses 3116.0 seconds. Thus the portion of the code that was directly parallelizable with PARPACK is almost 83%.

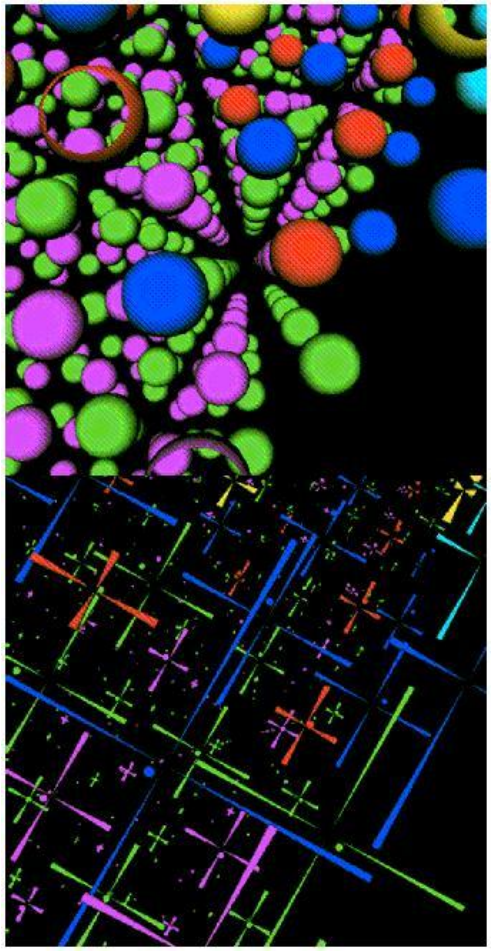
Execution time versus number of processors for concentric spheres problem



Pyramid structure.



Atoms (top) with Orbitals (bottom).



Concentric spheres