

Superlinear speedup on NANCO - the new RBNI cluster computer

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There have been many arguments over the value of centralised high performance computers (HPC) over local workstations. Israel came late to HPC because of export license politics and our original public facilities became outdated quickly. The revival of HPC in the rest of the world during recent years was also slow to percolate here.

However, after many years of no local academic access to a high performance computer, RBNI at the Technion purchased NANCO for computations in nanotechnology in late 2006. It is a 128 dual-core processor (2.2 GHz AMD Opteron) LINUX cluster with a fast VOLTAIRE interconnect based on DDR Infiniband, provided by SUN/EMET. It has been fully operational since mid-summer, with a good range of compilers and MPI for parallelization. Details about NANCO can be found at <http://phycomp.technion.ac.il/nanco>

One of the first projects to be completed on NANCO is a study of its speedup statistics for a molecular dynamics simulation of the elastic constants of argon. Up to a million particles have been modeled (using only 6.25 % of the machine) but the extensive statistics are for 1/4 million, equivalent to a 21.6nm sample. Using MPI with spatial decomposition runs of 2500ps took 177,330 seconds for 4 processors and only 76,366 for 8. For 16(20) processors times of 48280(42428) seconds indicate that 16-20 is an optimal number of processors to get good parallelization and a less than 24 hour turnaround. Details of the code can be found at

<http://phycomp.technion.ac.il/pavelba/Compphys/Project/Project.html>

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