ANUPAM-Adhya SUPERCOMPUTER

The ANUPAM-Adhya supercomputer is being used by scientists and engineers of BARC in solving computationally intensive problems in diverse fields ranging from physics, chemistry and engineering.

One **application** that uses ANUPAM-Adhya is :

Molecular Dynamics Simulation : This simulation is carried out by setting up a box consisting of a number of particles. Then, assuming certain starting values of positions and velocities of atoms, the equations of motion are solved iteratively with a small time step, with the new iteration utilizing the results of the previous cycle. The parallelization is done on calculating the net forces on the atom at each time step and the values of atomic coordinates are passed between processors for each iteration. This involves minimum communication and can be scaled very nicely with more number of nodes.

….. and many more !!

Parallel architecture used: MIMD (Multiple Instruction Multiple Data), distributed memory. ANUPAM-Adhya consists of two independent interconnection networks – a primary network using Infiniband and a secondary network using Gigabit Ethernet. The Infiniband network is used for inter-process communication by jobs and Network File System I/O. The Gigabit Ethernet network is used for installation and management tasks. 50% non-blocking.

Tools used: OpenMPI, MVAPICH and MVAPICH2

www.barc.gov.in/publications/nl/2012/2012010209.pdf

www.barc.gov.in/publications/nl/2000/200012-01.pdf