I.1 Scientific Computing and Software Development at RRCAT

A) Visualization and Virtual Reality Facility:

3D Visualization and Virtual Reality facility is commissioned with HP Z800 Graphics Workstation, Stereo Projection System, Front Projection Screen, Stereo Emitter and Stereo Eyewear. Users can visualize their 3D applications using the EON Studio software suite. EON Studio 7.0 software suite has been installed with node lock license on a Graphics Workstation having two quad core Intel Xeon 3.20 GHz processors, 32 GB memory and NVIDIA Quadro FX4800 graphics card with 1.5 GB memory.

Users can load, view and optimize 2D and 3D files with creation of immersive environment, connectivity with Virtual Reality peripherals, stereoscopic viewing etc. Addition of
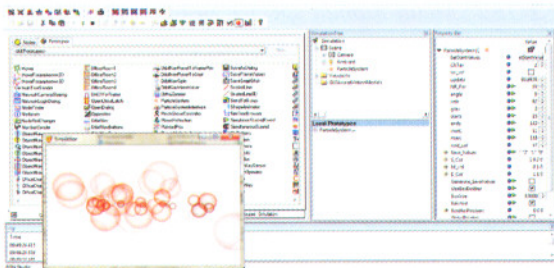

Fig. I.1.1: Development Environment of EON Studio.

Real-Time Physics, Kinematics, Collision, Gravity and Friction is also possible in user applications. Inclusion of numerous human characters in the environment is also possible without heavy requirements on rendering capacity. The software adds life-like animations.

Visual effects which create ultra-high quality and flexible shading are also available. The development process includes importing 3D objects, usually originating from various modeling tools like 3ds max, Light wave etc., or from CAD systems such as Solidworks, AutoCAD etc.
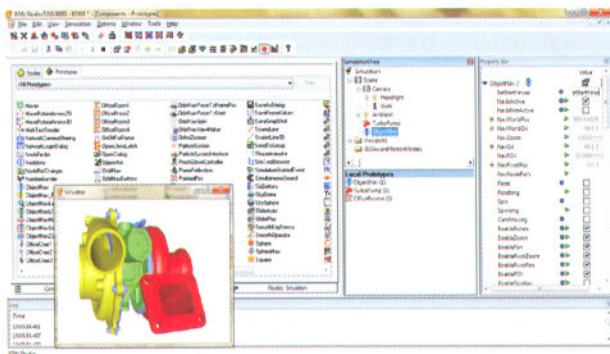

Fig. I.1.2: Object Navigation of a turbine pump.

Behaviour can be easily associated with the models through intuitive graphical programming interface and scripting available in EON software. EON applications can

Fig. I.1.3: Visualization of a turbine pump.

also be integrated in other tools that support Microsoft ActiveX components, such as PowerPoint, Word etc.

This facility can be used for 3D visualization of designed components, simulation, virtualization of complete assembly etc. Various file formats are supported by the software for importing 3D objects in this environment.

B) Performance analysis of HPC Linux cluster of multi-core node using NAS Parallel Benchmark (NPB):

Performance analysis of HPC Linux Cluster using multi core/ processor machines based on Intel Xeon processor and InfiniBand interconnect has been carried out using NAS Parallel Benchmark (NPB). NPB an open source software,
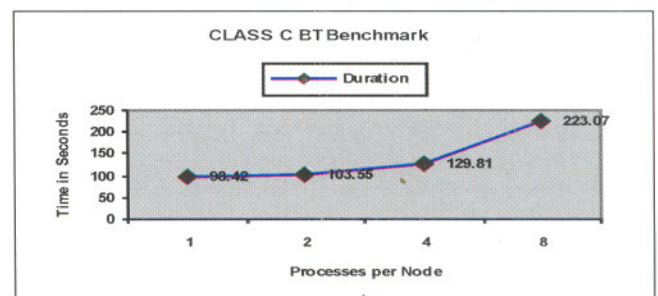

Fig.I.1.4: Class C Block Tridiagonal (BT) benchmark of NPB for 16 process application.

developed by NASA Ames Research Centre, USA, provides a set of eight programs and covers all major performance evaluation parameters applicable while benchmarking parallel machines. In this analysis the number of processors have been varied from one to eight (1, 2, 4, 8) for a common application (class C) for all the eight benchmark programs of NPB.
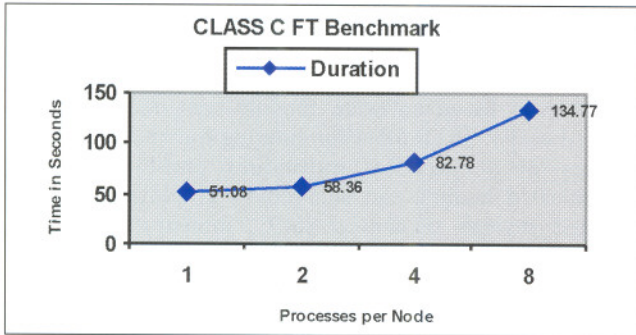
Fig. I.1.5: Class C 3D FFT Partial Differential Equation (FT) benchmark of NPB for 8 process application.

We used homogenous distributed memory based 16 nodes cluster, Mellanox PCI express MT25418 HCA and HP BLc 4X DDR IB switch for interconnecting nodes, Linux 2.6.18-128 as operating system, MVAPICH2 with Intel FORTRAN and C/C++ compilers as Inter Process Communication (IPC) library, HP ProLiant BL460c blade server with eight cores (two quad core) as node of cluster for this analysis.

The results of all these tests (indicated graphically in above figures) show that communication between cores of two nodes are faster than communication between two cores of the same node, in case of Infiniband interconnect. The best performance of HPC cluster with Infiniband interconnect can be achieved by selecting lower number of processors per node.

C) Augmentation of centralized computing server setup:

Two Intel Xeon based computing servers named as "amogh-2.rrcat.gov.in" and "amogh-4.rrcat.gov.in" have been commissioned with two Intel Xeon 2.93/ 2.00 GHz quad core processors, 16/ 10 GB memory for scientific computing and engineering applications. Red Hat Enterprise Linux Server release 5.4 is used as operating system for these two servers.

Intel FORTRAN and C compiler version 11, Absoft FORTRAN Compiler version 10.2.0, Lahey/Fujitsu v8.1a Linux64 Fortran compiler, MATH Kernel Libraries version 11, Intel Threading Building Blocks (tbb) for Intel C compilers, MATHEMATICA 7, IMSL version 9 are available in these server for advanced computing applications. User applications namely CST STUDIO SUIT 2009, CNTech, Flair and Fluka are also made available for computing and engineering applications.

D) Porting of user programs:

As per requirement of users, various software packages are successfully ported on computing servers and clusters.

Parallel software package LS-DYNA version 971 R4.2.1 with Inter Process Communication library OpenMPI-1.2.5 is ported successfully on 'Kshitij-1' HPC cluster. The software was successfully tested for user application.

Parallel version of CRYSTAL09 is ported successfully on 'Aryabhatta' cluster using OPENMPI version 1.4.3 and Intel FORTRAN compiler version 11.1. This package performs ab intio calculation of the ground state energy, energy gradient, electronic wave function and properties periodic systems.

Sequential application Tracy2 is also successfully ported on Intel Xeon Linux server. This program does the computation of off-momentum particle (i.e. electrons) loss in presence of multi-polar magnetic field error.

E) Training and hand-on sessions conducted at User Hall:

Five days training with hands-on session was organized on Virtual Reality & Visualization Software - EON Professional from 6th Sept. to 10th Sep. 2010.

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I.2: Development of Information Systems at RRCAT

A) Design, development and implementation of EAGLE (Electronic Assessment - Grade Logger and Editor) software:

EAGLE - Electronic Assessment Grade Logger and Editor software was designed, developed and released on RRCATInfonet for on-line assessment of APARs. This is an authenticated web based software for calculation of grade and writing of remarks electronically for Annual Performance Appraisal Report (APAR) of employees. The appraisal form as well as the remark entry interface has been made available digitally, to ease out the task of evaluation of grade and remark writing procedure. The evaluation process became more convenient by simple mouse clicks in comparison to the paper
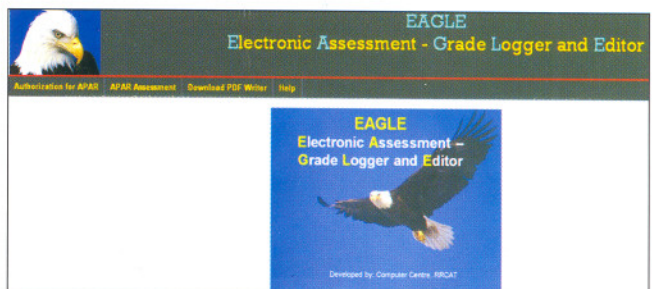

Figure I.2.1: EAGLE Software on RRCATInfonet.