

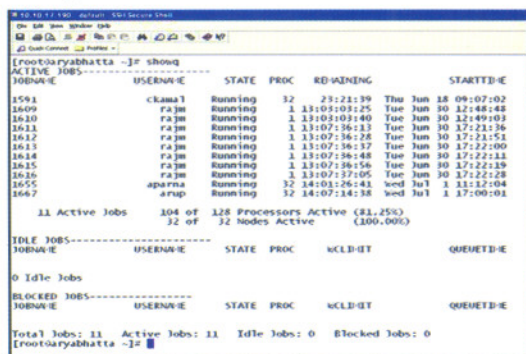
I.1 Scientific Computing and Software Development at RRCAT

A) Commissioning of Computing Server Ganak-1 (गणक-1)

Itanium2 based, HP 3600 series server (Dual core, Dual processor, 1.6 GHz Itanium2, 64-bit processor server with 16 GB RAM & 18 MB L3 cache) named as 'Ganak-1' has been commissioned for scientific computing applications. This server has been configured with 64-bit Red Hat Enterprise Linux (for Itanium IA64) version 5.2 operating system. Fortran compilers - g77, gfortran, Intel fortran (ifort) and C compilers - gcc, g++, Intel C compiler (icc) are installed on this server. Intel Math Kernel Library, version 10, is also available on this server.

B) Advanced job scheduling system for HPC cluster 'Aryabhata':

An advanced job scheduling system has been devised and configured on High Performance Computing Cluster 'Aryabhata' using 'Torque' and 'Maui'. HPC clusters are mainly used for parallel applications but all system resources (CPU, Memory, Disk etc.) are not always fully utilized by parallel applications. The job scheduling system of 'Aryabhata' has been configured in such a way that sequential applications can run along with parallel applications, without degrading performance of parallel applications.



JOBNAME	USER@NODE	STATE	PROC	RES-WINING	STARTED-TIME
1591	ckama1	Running	32	23:21:39	Thu Jun 18 09:07:02
1609	ra3m	Running	1	13:05:03:25	Tue Jun 30 12:48:48
1610	ra3m	Running	1	13:05:03:40	Tue Jun 30 12:49:03
1611	ra3m	Running	1	13:07:36:13	Tue Jun 30 17:21:36
1612	ra3m	Running	1	13:07:36:25	Tue Jun 30 17:21:51
1613	ra3m	Running	1	13:07:36:37	Tue Jun 30 17:22:00
1614	ra3m	Running	1	13:07:36:48	Tue Jun 30 17:22:11
1615	ra3m	Running	1	13:07:36:56	Tue Jun 30 17:22:19
1616	ra3m	Running	1	13:07:37:05	Tue Jun 30 17:22:28
1655	aparna	Running	32	14:01:26:41	Wed Jul 1 11:12:04
1647	arup	Running	32	14:07:14:38	Wed Jul 1 11:00:01

11 Active Jobs 104 of 128 Processors Active (81.25%)
32 of 32 Nodes Active (100.00%)

0 Idle Jobs

0 Blocked Jobs

Total Jobs: 11 Active Jobs: 11 Idle Jobs: 0 Blocked Jobs: 0

Fig.I.1.1: Queue of advanced job scheduling system on Aryabhata cluster.

C) Scientific Compilers and Libraries:

Absoft Pro Fortran compiler version 10.2 is installed and configured on Xeon based Linux server with graphical fx3 debugger. This is a Fortran 90/95/2003 compatible compiler and supports OpenMP & all available SSE3 Instructions.

Absoft Fortran 90/95 compiler version 9.0 is installed and configured on IBM P5+ server 'Avantika' with graphical fx2 debugger. Pre-configured BLAS, LAPACK90, ATLAS and PLplot (2D & 3D) graphics libraries are also configured with this, Fortran 90/95 compatible, compiler.

Lahey/Fujitsu Linux64 Fortran Pro (LF64 Pro) compiler version 8.1 is installed & configured on Xeon based Linux server. Wisk, Winteracter graphical packages, BLAS & LAPACK v4.0 libraries are also configured with this Fortran 90/95 compatible compiler.

IMSL Fortran numerical libraries for Absoft version 5.1 is also configured on Xeon based Linux server. The IMSL Fortran Library is a complete collection of mathematical and statistical algorithms which integrates the IMSL F90 Library, Math & Stat and Fortran 77 libraries into a single, cohesive package.

D) Auto Parallelization Software for multi processor and multi core Linux servers:

Auto parallelization software 'Vast-F/ Parallel' has been installed and configured on Intel Xeon and IBM P5+ based Linux servers. This software tool automatically converts serial code into code designed for multi-core or multi-processor systems using Absoft Fortran compiler and carries out additional optimization. Code re-structuring is done automatically and the original source code files are retained in unmodified form. VAST-F/ Parallel also provides OpenMP support. VAST-F/ Parallel 7.0 x64 Linux is used on Intel Xeon Linux multiprocessor server and VAST-F/ Parallel LinuxPPC is used on IBM P5+ based Linux server for auto parallelization.

E) Porting of user programs:

ADF bundle with HPMPPI (Amsterdam Density Functional, version 2008 - a FORTRAN program for calculations on atoms and molecules) has been successfully ported on 'Aryabhata' cluster.

F) MATFOR Graphical Library on Linux:

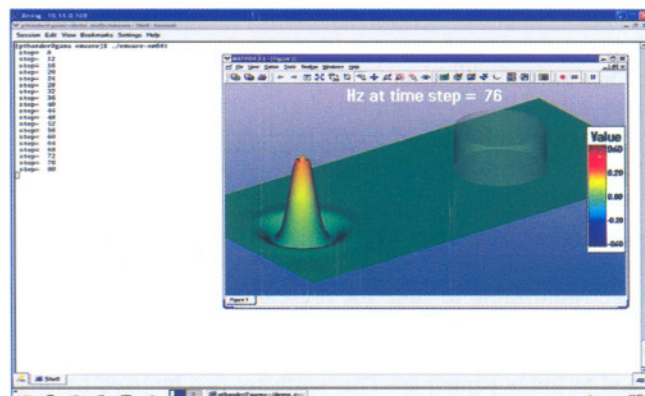


Fig.I.1.2: Example of 3D graphical plot using MATFOR software at user's Desktop.

MATFOR Graphics Library is installed and configured on Xeon based Linux server and it can be accessed from user's desktop. This graphical library contains high-level graphical procedures that support x-y plot, vector plot, contour, mesh plot, surface plot, isosurface plot, streamline, slicing plot, molecules plot etc.

MATFOR Graphics Viewer displays high quality graphs without the need of Windows programming and graphics initialization.

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