PARAM Shavak - Case Study

Introduction

PARAM Shavak

Param Shavak machine PARAM Shavak - solution, aims to provide computational resource (Capacity building) with advanced technologies to perform high-end computations for scientific, engineering and academic programs to address and catalyze the research using modelling, simulation and data analysis. This initiative is expected to create HPC aware skilled workforce (Capability building) and for promoting research by integrating leading-edge emerging technologies at grass root level. As the scope and complexity of computational needs continue to increase at colleges universities, professors and administrators are compelled to seek appropriate and affordable solutions. PARAM Shavak provides the computing power necessary to keep academic institutions on the leading edge in today's competitive market at affordable cost. This system is meant for research organizations and academic institutions that are on the verge of adopting HPC culture in their institutions/organizations. Besides a handful of value additions from C-DAC, the system comes with most of the features that can be found in a full blown HPC clusters job schedulers, compilers, parallel libraries, mpi, resource managers, some of the commonly used HPC applications in engineering scientific domains etc.

PARAM Shavak - Supercomputer in a box with unbound performance features:

- HPC system in a table top model.
- Powered with minimum two multicore CPUs, each with at least 10 cores along with either one or two cores or GPU accelerator cards.
- Phenomenal for academic, scientific and research institutions that are on the verge of adopting high performance computing culture.
- Equipped with indigenously developed software technologies by C-DAC for HPC applications in academic and scientific domains.
- Easy to deploy solution with minimal data-centre infrastructure.
- Pre-loaded with parallel programming development environment.
- Customizable as per the user hardware and software requirements.
- 2.3 TF and above computing power.
- Scalable model.
- Access to C-DAC PARAM Yuva II at National PARAM Supercomputing facility for computations on a larger scale as per the NPSF usage policy.
- Support for C-DAC's Reconfigurable Computing System technology to speed up applications through hardware.
- Resource for parallel programming, training and workshops.
- Affordable computing environment for the faculty, students – both undergraduate and post graduate PhD scholars

System Requirements:

Hardware Overview

Following are the hardware configuration details of PARAM Shavak –

Node	
Processor	Dual socket Intel Xeon E5-2600 v2 series/ with 10 cores each with minimum 2.2 GHz clock speed with min. specfp2006_rate of 580
RAM	64 GB ECC DDR3 1866 MHz RAM in balanced configuration
Network	Two 1GbE network ports
Accelerator's Slot	2 x16 PCI-E Gen3 slots for GPU/co-processors
DVD	One number internal DVD RW/DVD combo
HDD	4 x 2 TB SATA/NL-SAS disks with support for hardware RAID 0,1 and 5 Configured with RAID 5 Total usable space 5.456TB o 1.455 TB for System, applications o 4.0 TB for user home
Graphics	On board or add-on card for visualization
Monitor	19'' TFT LCD monitor along with USB keyboard and mouse
Accelerator	i. Intel Xeon Phi 3120A/3120P card (Max 2) or ii. nVidia K20/K40(Max 2) series

Software Overview

Following are the software requirements for PARAM Shavak.

System Software Details

OS	CentOS 6.5
Drivers	MPSS/CUDA
Tools	ONAMA, CHReME
Libraries	mpich2, Intel®
Compilers	GCC, Intel®
SDK	Netbeans
Job Scheduler	Torque
Monitoring Tool	Ganglia

PARAM Shavak System Architecture

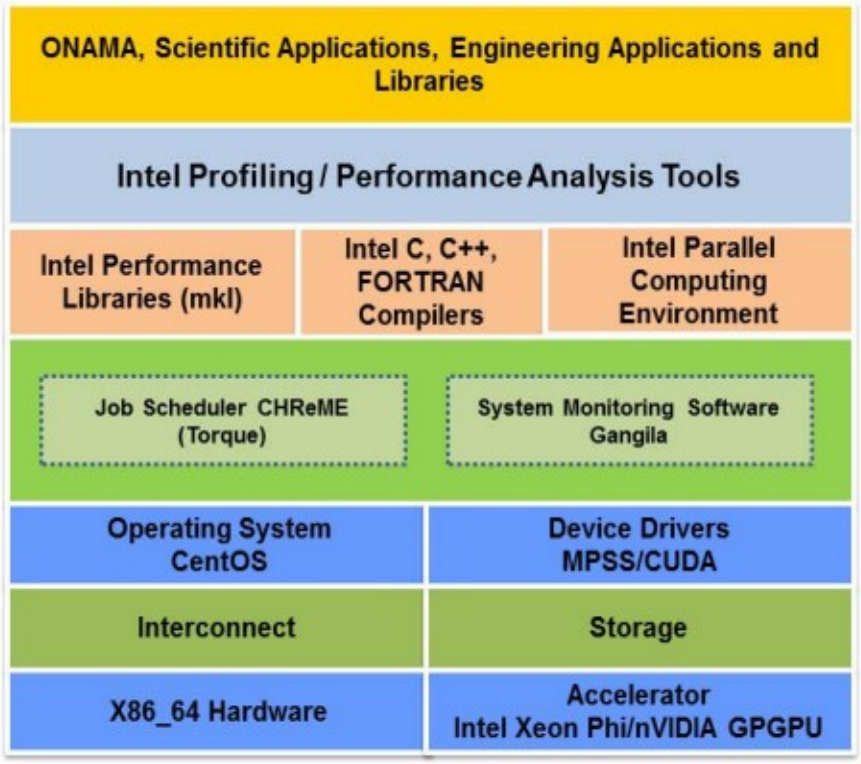

Figure 1 - PARAM Shavak Software Architecture Block Diagram

Tools in PARAM Shavak

Onama

ONAMA is an integrated software and hardware solution for future technocrats/engineers, providing them a platform for a quantum leap to gain an indepth understanding of High Performance Computing (HPC). This is an integrated package comprising of a well-selected set of parallel as well as serial applications of scientific and engineering domain and is useful across various engineering disciplines.

ONAMA provides a great opportunity for networking amongst industry experts, professors, faculties, research scholars and students to work in multi-disciplinary areas of engineering and to incorporate the latest technologies in high-end computing.

Features:

- A well selected set of parallel as well as serial applications and tools across various engineering disciplines. In addition to this it consists of accelerator enabled applications in several domains namely molecular dynamics, bioinformatics, life sciences and physics.
- Onama comes with built-in applications and execution model which allows the execution of desired applications with minimal efforts.
- It also provides access to various libraries like parallel libraries, performance libraries and engineering domain specific libraries that can be used to develop programs to solve the user's problems.
- Onama offers unique opportunity to the faculty members of the engineering colleges to go beyond their conventional teaching practices and experiment with innovative learning techniques.

CHReME

To access Linux-based HPC environments, scientists and researchers require expertise in Linux and HPC, which is something many do not have. CHReME empowers users with an intuitive GUI to exploit HPC resources and provides a layer of abstraction to shield them from the complexity of accessing HPC resources. This enables them to concentrate on their core research/scientific work. CHReME's Web Interface makes clusters of different magnitude easy to manage and monitor, which makes things easier for the HPC systems administrator while enabling researchers and scientists of varied domains to carry out their scientific simulation with minimal efforts.

Features

- User friendly web based GUI to access various HPC resources.
- Simplified and secure access to the HPC resources from the remote machine.
- Secure credential specific access on web through https.
- Optimum utilization of HPC system's resources and resource reservation.
- Creation, submission, monitoring and management of jobs through GUI. Jobs are submitted through industry standard cluster schedulers at the backend.
- Personalized job list and job status information.
- Graphical representation of the cluster resources and jobs.
- Timely e-mail notification regarding job status.
- Portal provides a layer of abstraction to the end users by freeing them from the command line mode of execution in addition to providing benefits to the end users to focus on their scientific domain areas

HPC Applications

The term high performance computing (HPC) refers to any computational activity requiring more than a single computer to execute a task. Computer clusters are used to solve advanced computation problems. Computational Science – and with it the associated computational resources and HPC technology – has now established itself as the third pillar of scientific enquiry alongside theory and experiment.

HPC has the capacity to handle and analyze massive amounts of data at high speed. Tasks that can take months using normal computers can be done in days or even minutes. It can be used to model and solve highly complex problems across a range of high value sectors.

Uses are diverse and examples include DNA sequencing, weather forecasting, quantum chemistry, fluid dynamics, etc…

- HPC applications available on PARAM Shavak include:
- Bio-informatics: mpiBLAST
- Molecular Dynamics: GROMACS, LAMMPS, NAMD
- Weather forecasting and Oceanography: WRF, MOM
- Quantum Chemistry: NWChem, ABINIT
- Materials Science: Quantum Espresso
- CFD: OpenFOAM

For more detailed information about HPC Applications, refer the HPC Applications user manual in the path /opt/manual of PARAM Shavak.

PARAM Shavak Security

PARAM Shavak incorporates following measures of security.

- **TripWire:** PARAM Shavak incorporates TripWire which serves as a host based intrusion detection system. It is useful for detecting intrusions after the event, it can also serve many other purposes, such as integrity assurance, change management and policy compliance.
- **SSH:** Terminal CAPTCHA is implemented for better security of PARAM SHAVAK against brute force attacks.
- **Strong Password policy:** Following password policy is implemented in PARAM Shavak o Minimum 8 characters
    1. Combination of alphabets, special characters and numbers.
    2. At least one upper case character (A-Z)
    3. At least one lower case character (a-z)
    4. At least two special characters (!@#$%^&*)
    5. At least 2 numbers (0-9)
- Operating System and services are hardened in order shield the system against Common Vulnerabilities and Exposures.