

High Performance Computing System for Scientific Applications

Modern research institutes strive to offer smart computing systems to entertain robust applications modeled to address and solve eminent research problems being faced by the current scientific community. The central research institute in Pakistan dealing with various areas of Physics – NCP, emphasizes to compete with its small-scaled facility with other related research setups over the globe by deploying a computational cluster setup comprising of computing nodes having 56 physical as well as 24 virtual cores of CPUs serving under both serial and parallel fashioned batch queues. The virtual nodes are provisioned by private cloud using manual instance creation which will be automated in near future. Data persistence of the infrastructure running is governed by an IP SAN over iSCSI setup responsible to share its storage across the compute nodes involved. The state-of-the-art facility is dedicated to carry out the corresponding workflow simulations for the local research community spread across the various provinces of the country and is meant to operate round the clock without any foresee interruption. The user community of the cluster comprises but not limited to researchers working in the fields of Computational Condensed Matter Physics, Climate Modeling, Density Functional Theory, Computational Plasma Physics, and Semi-conductor Nanostructures. Software packages/compiler support is available for Intel Fortran, gcc, Quantum Espresso, Gaussian09, Mopac2012, Turbo mole, Wien2k, and Geant4 etc. The results produced making use of this facility by submitting user jobs over it looks comparable to the those obtain in the past using similar computational clusters hosted by other international institutes. NCP anticipates enhancing the performance and capacity of its deployed facility by scaling it further to incorporate GPUs as well in the near future, thereby widening its scope for other impending research problems/areas.

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