

# **MOLECULAR BIOPHYSICS UNIT**

UGC Centre for Advanced Study

INDIAN INSTITUTE OF SCIENCE BANGALORE: 560 012, INDIA

Dear Sir/Madam,

Date: 23/09/2019

Subject: Request for quotation for a high performance cluster

The Biological Sciences Division intends to purchase a high-performance computational cluster having a peak performance of **approximately 3 teraflops (double precision floating point)** per compute node. The CPU proposed should support double precision floating-point operations per second. In the evaluation, preference will be given to system with higher extensibility (ease of adding new nodes to cluster in future). Server chassis/ enclosure-based solutions, with redundant power supplies, and capable of getting mounted on standard 42U (19") rack is desirable. Also, each of the server nodes should be individually serviceable without shutting down the other server nodes. Proposed servers should be installed with the necessary schedulers, drivers and connectors for running and monitoring MPI based jobs.

Following are item wise specification. Only core components are cited below and the bidders are expected to also quote for and supply the necessary unlisted accessories (e.g. LAN, Rail, Software etc) that will be required for setting up the complete solution.

- 1) Master Node: A separate master node with the following specifications.
  - a. Dual x86 64 bit processor capable to meet a minimum rated of 2.9 TFlops per node.
  - b. Minimum 192 GB 2933 MHz, balanced memory configuration
  - c. 1.92TB \* 4 SSDs on RAID 5
  - d. RAID CARD with min. 1GB cache with RAID 1/5 support
  - e. Dual Gigabit LAN ports
  - f. Omnipath/EDR Infiniband Adapter, 100 Gbps with necessary cables
  - g. IPMI / Remote management features
  - h. Redundant power supplies
- 2) Storage: Parallel File System Lustre or GPFS with the necessary I/O nodes with redundant features / no single point of failure. 800 TB usable capacity post RAID 6 in (8D + 2P) and formatting. The storage system should operate at 10 GB/s throughput for 100 % write. A minimum of 3% of the total usable capacity to be

factored for Meta Data in addition to 800 TB. The meta data need to be configured with enterprise grade SSD in RAID 10.

RAID 1 / RAID 6 for Metadata as we

Onsite spares: Minimum 2% onsite spares of each disk type

- 3) **Compute Nodes:** Cluster with no less than **24 nodes** with the following specifications per node.
  - Dual x86 64 bit processor capable to meet a minimum rated of 2.9 TFlops per node.
  - Minimum 384 2933 Mhz, Balanced memory configuration
  - 960GB SSD
  - Dual Gigabit LAN ports
  - Omnipath/EDR Infiniband adapters with necessary cables
  - Redundant Power Supplies
  - IPMI / Remote management features
- 4) GPU Compute Nodes (V100): 4 GPU cards with following specifications node.
  - Dual Intel Xeon 6240 processors, 18 Core, 2.6 Ghz
  - Minimum 768 GB 2933 Mhz, Balanced memory configuration
  - 2 \* 1.92 TB SSD on RAID 1
  - Dual Gigabit LAN ports
  - 4 \* NVIDIA V100 GPU Card with 32 GB memory on NV Link
  - Omnipath/EDR Infiniband adapters with necessary cables
  - IPMI / Remote management features
  - Redundant Power Supplies
- 5) GPU Compute Nodes (Turing T4): 4 GPU card with the following configuration
  - Dual Intel Xeon 6240 processors, 18 Core, 2.6 Ghz
  - Minimum 384 GB 2933 Mhz, Balanced memory configuration
  - 2\* 1.92 TB SSD on RAID 1
  - Dual Gigabit LAN port
  - 4\* NVIDIA T4 GPU on PCIe
  - Omnipath/EDR Infiniband adapters with necessary cables
  - IPMI / Remote management features
  - Redundant Power Supplies
- 6) GPU Compute Nodes (GeForce RTX2080 Ti) 3 servers with 4 GPU cards each
  - Dual Intel Xeon 6240 processors, 18 Core, 2.6 Ghz
  - Minimum 384 GB 2933 Mhz, Balanced memory configuration

- 2\* 1.92 TB SSD on RAID 1
- Dual Gigabit LAN ports
- 4 \* Nvidia RTX2080 Ti GPU Card on PCIe
- Omnipath/EDR Infiniband adapters with necessary cables
- IPMI / Remote management features
- Redundant Power Supplies
- 7) High End CPU Node: 1 node only as a part of the cluster
  - Dual Processor with a total number of 96 cores per node with a minimum base clock frequency of 2.2 GHz and a minimum rated of 6 TF per node
  - Minimum 768 2933 Mhz, Balanced memory configuration
  - 960GB SSD
  - Dual Gigabit LAN ports
  - Omnipath/EDR Infiniband adapters with necessary cables
  - IPMI / Remote management features
  - Redundant Power Supplies
- 8) Network/Interconnect:
  - Omnipath/EDR switch with 1:1 non-blocking architecture with sufficient ports for the proposed cluster with 25% additional capacity for future expansion.
  - A separate 1G network should be provided for management and administration of the cluster.
  - Also, all network cables and drivers should be listed and supplied.
  - 4 42U Rack with PDUs and other Accessories must be quoted.
- Parallel Studio: Please quote Intel Parallel Studio XE Cluster Edition for Linux Floating Academic 2 Seats for 3 Years (ESD) – To be installed with the cluster and tested for performance.
- 10) In case of AMD based solutions, AOCC need to be quoted and installed and the bidder need to support with regular updates and patches (As and when released by AMD).
- 11) Other Software:
  - a) CentOS operating system, latest version.
  - b) Open Source Cluster Management tools such as xCAT, Rocks, Ganglia

- c) Application packages provided by IISC should be installed and demonstrated on the HPC Cluster. A complete list of the software packages is provided below. Unless the listed software packages are installed properly and tested to satisfaction for performance and efficiency, the payment will not be done.
- d) CUDA tools should be installed and CUDA enabled applications provided by IISC should be installed and demonstrated.
- e) The following software packages needs to be installed and tested. Vendor may be requested to also test software not mentioned in the list. For more information on the software packages, please send an email to Dr. Anand Srivastava (anand@iisc.ac.in) with specific questions.

Molecular Dynamic Simulation Packages: GROMACS (patched with plumed) - with mpi, LAMMPS - with mpi, NAMD - with mpi and VMD, AMBER, VOTCA (with gromacs), MDAnalysis GAUSSIAN (licence can be obtained from institute) (academic license is available for all).

CryoEM Related Packages: RELION, Cryosparc, SCipion, EMAN, Simple, Xmipp, cisTEM, Chimera and SPHIRE cryo-EM software suite

Generic day-to-day Softwares: Python3/3.5 - with numba, numpy, scipy, matplotlib, Matlab BLAS and LAPACK (licence can be obtained from institute), R, opencv-python, opencv contrib-python, pandas 17) Anaconda package manager, OpenCL and PyopenCL, FreeSurfer ANTs, BrainSuite

Compilers: OpenMPI, Intel & Intel MPI, GNU compilers, Mpicc, Cmake, keras, tensorflow-gpu, CUDNN

Biomolecule Analysis Software: Rosetta , Modeller-IMP, FastQC ,Trim Galore, Cutadapt, Bowtie2,TopHat, Samtools, Htseq-count, Cufflinks, IGVTools, Depth, EMBOSS, AutoDock, ClustalX, Packpred, OpenMPI, CCP4, Phenix,FoldX

#### **General Specification:**

- a. All the equipment must be compatible with Indian electrical standards/codes
- b. The bidder must carry out Racking, stacking, installation, commissioning and cabling of all supplied hardware components and software.
- c. The HPC cluster solution must be housed in suitable chassis. Dense computing platform with extensibility option is preferred.

- d. The bidder should provide manufacturing authorization form (certificate from OEM for quoting the requirement)
- e. Also, bidder must provide at least three reference sites 50 TF or above (CPU only) where they have carried out the installations in the last 3 years. The purchase committee will independently obtain inputs from referees before making the final decision on the bid. PO copies and installation reports must be submitted along with the Technical Bid.
- f. The lowest commercial bid and/or the most agreeable technical bid should have the option for further negotiations.

#### **Eligibility Criteria:**

- a. The bidder/OEM should have set up at least 3 or more HPCs in the last 3 years with at least one cluster with 512 cores and Omnipath/Infiniband interconnect.. Purchase order copies of previous installations are required.
- b. The bidder should be in HPC business for at least 10 years. Support documents should be submitted.
- c. The bidder should have an annual turnover of Rs. 50 Crores or above in the last 3 Financial Years. Audited Balance sheets should be submitted.
- d. The bidder should have a sales and service office in Bangalore.
- e. The OEM should have a registered office in India with service centre facilities in Bangalore. Details of HPC engineers of bidder and OEM should be provided.
- f. The OEM should give an undertaking that warranty will be directly provided by the OEM. Also the OEM should give an undertaking to provide necessary Technical support in case the bidder fails to provide such a service to IISC.
- g. Bidder/OEM with poor service track record at IISC will not be considered.
- h. Bidder/OEM has to quote exactly as per mentioned specifications for entire solution, partial offers will not be accepted.

### The quotation should be in two parts:

Part I (Technical bid) and Part II (Commercial bid)

Part I should be put in a sealed cover and superscripted "Technical Bid". Part II should be put in a separate sealed cover and superscripted "Commercial Bid". Technical bid should be exactly same as commercial bid except that prices are not shown in technical bid. Technical bid should have item wise compliance report of all specifications. The above covers should be put in another cover. This cover should be sealed and subscripted "Bid for Biological Science Division High Performance Computational cluster". <u>The Bids in a sealed cover should be addressed to Project Investigator, DBT-IISc Partnership Program Office</u>,

## Biological Sciences, Indian Institute of Science, Bangalore-560 012, Phone: (80) 2293 3371.

The Technical bid should not have any details about pricing. The commercial bid should have pricing for each of the configuration quoted in the technical bid. The last day for submitting the bid is <u>October 21, 2019</u>. The offer should be valid for a period of at least 60 days from the last date for submission of quotes. Prices quoted should be inclusive of all taxes / duties. The prices quoted should be inclusive of delivery of the items to the site and installation at site and should include both rupee and US dollar quotes. Both technical and commercial bid will be negotiable for the lowest costing commercial bid and most desirable technical bid. While evaluating the technical bid, weightage will be given for extendibility, performance and adherence to specifications and references from past customers. The purchase committee may want to contact past customers and the vendors are requested to provide references that can be contacted for the same.

Payment will be made after satisfactory supply and installation. The system supplied may be tested/certified by us through an identified person/committee. Three year on-site warranty should be provided for the hardware. The warranty period will commence from the date of acceptance of the equipment.

### **Important Dates:**

Date of release of the enquiry : Pre-bid clarification : Date of submission of Quote :

1<sup>st</sup> October, 2019 15<sup>th</sup> and 16<sup>th</sup> October, 2019 (12 Noon to 3 PM) 21st October, 2019, 4:30 PM. DBT-IISc office in Biological Science Building (Contact Ms. Vijavalaxmi @ 080-2293-3371)

Best regards, Anand Srivastava Assistant Professor, Molecular Biophysics Unit Indian Institute of Science-Bangalore Bangalore 560012

Anand .