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|  | **Madhava HPC Cluster**  **Name of the equipment:**  Madhava HPC Cluster  **Make & Model:**  Lenovo ThinkSystem (SR-650 and SR-630)  **I-Stem Registration ID:**  3245582  **Category of Instrument**  High Performance Computing  **Application:** Used to perform complex calculations and simulations that require immense computational power.  **Description of Instrument**  Computing Cluster for parallel computing in Science and Engineering |

**Booking Details**

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| **Book through I-STEM:**  <https://www.istem.gov.in/>  **Slot Booking Link**  [I-STEM Slot Booking link for Internal User](https://www.istem.gov.in/equipment-info/45582/High-Performance-Computing-Cluster) | **Booking available for**  Internal  **Requisition form for**  [Internals](https://drive.google.com/file/d/1LIoXQdh72steMKVQchsVP-vQGb5dSuZX/view?usp=sharing) |

**Contact Details**

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| **Faculty In-charge:**  Dr Raghu C  **Email ID:**  [raghuc@nitc.ac.in](mailto:raghuc@nitc.ac.in)  **Phone number:**  +91-9495066073 | **Technical Staff:**  R R Krishna (TA) [rrkrishna@nitc.ac.in](mailto:rrkrishna@nitc.ac.in)  Sajil N P (TA)  [sajilnp@nitc.ac.in](mailto:sajilnp@nitc.ac.in) | **Department**  CCMS (Centre for Computational Modelling and Simulation)  **Office Email ID**  [ccmsadmin@nitc.ac.in](mailto:ccmsadmin@nitc.ac.in)  **Location**  Old Library Building, Central Campus, NIT Calicut  **Lab Phone No**  0495-2285600 |

**Features and Specifications**

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| **Component** | **Model** | **Processors / GPU** | **Memory** | **Storage** |
| 1 Master Node | Lenovo ThinkSystem SR-650 | 2 × Intel Xeon Gold 5218 16C 2.3GHz Processor | 192 GB |  |
| 31 Compute Nodes | Lenovo ThinkSystem SR-630 | 2 × Intel Xeon Gold 6248 20C 2.5GHz Processor | 192 GB |  |
| 2 GPU Nodes | Lenovo ThinkSystem SR-650 | 2 × Intel Xeon Gold 6248 20C 2.5GHz Processor  2 × NVIDIA Tesla V100 PCIe 32GB GPU | 192 GB |  |
| 2 Storage Nodes | Lenovo ThinkSystem SR-630 | 2 × Xeon Silver 4208 8C 2.1GHz Processor |  |  |
| Storage Array | ThinkSystem DE6000H, DE6000S |  |  | 260TB |

**Installed Software**

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| **Quantum Mechanical Simulation Software** | **VASP** (Vienna Ab initio Simulation Package)  **Quantum ESPRESSO**  **Gaussian**  **MOLPRO**  **SIESTA** |
| ****Molecular Dynamics Simulation Software**** | **LAMMPS** (Large-scale Atomic/Molecular Massively Parallel Simulator)  **GROMACS** (GROningen MAchine for Chemical Simulations) |
| ****Computational Fluid Dynamics (CFD) Software**** | **OpenFOAM**  **REEF3D**  **DIVEMesh** |
| **Data Science and Statistical Computing** | **Anaconda** (Distribution for Python and R)  **R** (Programming language for statistical computing) |

**User Charges Rs. (GST Extra)**

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| **Internal** | **External Academic**  **Institutes** | **National R&D Lab** | **Industry** |
| No Charges | Available only for Internal Users | | |