



One Week Workshop on Super Computing Organized under National Supercomputing Mission (HRD Group)

Organized by

Centre for Development of Advanced Computing, Pune (India) IIT Kharagpur.

Venue: IIT Kharagpur	Duration: From Date to To Date
Part I	Introduction, SLURM: Overview of HPC , Introduction to PARAM
	Shakti , Introduction to Slurm , Job submission Procedure for CPU
	and GPU nodes.(Day1-Day2 agenda)
Part II	Parallel Concepts, Intel tools: Shared Memory and distributed
	Memory parallelism, matrix multiplication and Parallelization, Intel
	tools and code Optimization Training, Intel AI Portfolio and Python
	Demonstration (Day3 –Day4 agenda).
Part III	GPU: Introduction to Image Processing, Parallelism in Image
	Processing using NVidia GPU, CUDAtoolkit and OpenACC, NVidia
	DL/ML (Day5–agenda).

** This is an online workshop so there will be no HANDS-ON sessions for the users. Only presenters will demonstrate and answer the questions. **

Day 1-Day 2: 23/Nov/2020 – 24/Nov/2020

D A Y 1	Time (Hrs.)	Lecture/Hands-on Session
	10:00 - 10:30	Overview of HPC
	10:30 - 11:00	General Idea of PARAM Shakti
	11:15 – 13:00	Introduction to SLURM, slurm Batch script and Job Submission procedure . Sample batch scripts for Serial Job, Parallel Job, Hybrid Job (MPI+ OpenMP) and details about the different Flags of the each script.
		Lunch Break - 1.00 hr.
D	14:00 – 15:45	Lab Session: Job submission using sample batch scripts for Serial Job, Parallel Job, Hybrid Job (MPI+ OpenMP) for different Application (i.e GROMACS, LAMMPS) utilizing CPU Cores and CUDA cores.
A Y		Break
2	16:00 – 17:00	Lab Session: Job submission using sample batch scripts for Serial Job, Parallel Job, Hybrid Job (MPI+ OpenMP) for different Application (i.e OpenFoam, NAMD) utilizing CPU Cores and CUDA cores.





Day 3: 25/Nov/2020

D A Y 3	Time (Hrs.)	Lecture/Hands-on Session
	10:00 - 11:00	Shared Memory Parallelism with OpenMP.
	11:15 – 12:00	Distributed Memory Parallelism with MPI (Point to Point Communication)
	12:00 - 13:00	Distributed Memory Parallelism with MPI (collective Communication)
		Lunch Break - 1 hr.
	14:00 - 14:30	Parallelization of Matrix – Matrix Multiplication
	14:30 - 15:30	Lab Session: Shared Memory Parallelism with OpenMP
	Break	
	15:45 – 17:00	Lab Session: Distributed Memory Parallelism with MPI

Day 4: 26/Nov/2020

D A Y	Time (Hrs.)	Lecture/Hands-on Session
	10:00 - 13:00	Intel tools and code Optimization Training
4		Intel [®] Parallel Studio XE 2019
		 Intel[®] compiler for C++/Fortran and hands-on
		 Vectorization+ Intel[®] Advisor hands-on
		Intel [®] MPI Library
		 Intel[®] VTune[™] Amplifier and demo
	^{II} Lunch Break - 1 hr.	
	14:00 - 15:45	Intel AI Portfolio and Python Demonstration
		 Intel[®] Distribution for Python and demo
		 Intel[®] Data Analytics Acceleration Library and PyDAAL demo
		Break
	16:00 - 17:00	Intel AI Portfolio and Python Demonstration
		 Deep learning frameworks optimized by Intel
		 Intel OpenVINO[™] toolkit





Day 5: 27/Nov/2020

D A Y	Time (Hrs.)	Lecture/Hands-on Session
	10:00 - 13:00	Nvidia (CUDA and OpenACC)
5	Lunch Break - 1 hr.	
	14:00 – 15:45	 Introduction and Parallelism aspects of Image Processing using GPGPU Nvidia (DL/ML) What is GPU computing and why now? Deep Learning GPU Hardware
	Break	
	16:00 – 17:00	 Domain based high level intro: IVA, Health Care NVIDIA GPU clouds Inferencing (TensorRT) Domain based high level intro: NVIDIA RAPIDS, RAPIDS and NGC