



Intensive Course on Parallel Programming with MPI/OpenMP for Scientific Computing (27 - 31 August 2012)

Over the years, the trend of multi-core chips has revolutionised the high performance computing (HPC) scenario and immensely benefited the computational science streams. Computational biology, bio-informatics, computational chemistry, high-fidelity CFD analysis and climate science are all prime examples of beneficiaries of such a revolution. CSIR scientists have deep research engagement all these fields of scientific endeavour.

Now-a-days most desktops and laptops come with dual or quad-core processors and it is common to see high end HPC systems with several thousands of cores. Moving from TeraFLOP systems to PetaFLOP systems, computer hardware manufacturers are already pushing the frontiers for exaFLOP systems. More than just the sheer compute power, modern day data centres provide a HPC environment i.e., *raw computing power, storage and data management, visualization, ease of remote computing with minimal front end systems, access to facilities on the go, availability of vast pool of software tools etc.* Recognising the importance of such HPC facilities in realizing CSIR's vision of pursuing the emerging fourth paradigm of data intensive computational scientific research, CSIR is actively pursuing setting up of its supercomputing facilities in a pyramidal architecture.

CSIR C-MMACS is one of the premier HPC centres of India and currently hosts some of the most powerful systems in

the country which include a 27TF Altix Ice cluster and a 288-core shared memory Altix 4700 system. These will be augmented with a 300TF system in September. The optimal use of these systems demands a good command of parallel programming, especially the paradigms of Message Passing Interface (MPI) and OpenMP.

To exploit the on-chip parallelism in HPC systems fully, the software must be parallel and should scale efficiently with the number of cores. The importance of availability of skilled manpower in parallel programming cannot therefore be overemphasised. It is with this vision that the present course has been conceptualised.

The course covers a wide range of topics:

Computer Architecture, Introduction to Parallel Computing, CSIR C-MMACS Computing system, Numerical Methods (Algebraic Equations, Quadrature, Interpolation, ODE/PDE) MPI and OpenMP, Debugging, Intel Tools (Compiler, Optimiser, V-Tune Amplifier and Performance Analyser) and Parallel I/O. Case studies from a few disciplines: climate modelling, computational chemistry, genomics, data mining and CFD are also included.

Course Schedule

Dates: 27-31 August 2012

Venue: CSIR C-MMACS

Faculty CSIR – P.S. Swathi (PSS), R. P. Thangavelu (RPT), U.N. Sinha (UNS), T.N. Venkatesh (TNV), Pavanakumar Mohanamurthy (PM), G. K. Patra(GKP), V. K. Suman (VKS), Ashapura Marndi (AM), N. Prabhu (NP) , Sourav Pal (SP) , P. Seshu (PS)
 CDAC– N. Mangala (NM) and Vineeth Simon (VS)
 Strand Life Sciences– Vijay Chandru (VC)
 Intel – R. K. Lagu (RKL) and Rama Kishan Malladi (RKM)
 SGI – Manjunath Doddam (MD)

Programme

27/8/2012	
09:30 - 10:00	Registration, Overview, Inaugural Session
10:00 - 11:00	Inaugural technical talk: Computer Architecture (NM)
11.00 - 11:15	Tea
11:15 - 12:15	Introduction to Parallel Computing (NM)
12:15 - 01:30	C-MMACS Computing system ; Job submission ; Policy; (RPT and GKP)
01:30 - 02:15	Lunch
02:15 - 03:15	MPI Part I (VS)
03:15 - 03:30	Tea
03:30 - 05:00	Numerical Methods –I Algebraic Equations, Quadrature, Interpolation ,ODE/PDE (PS)
05:00 - 05:30	Totalview Debugger (PSS)
05:30 - 06:30	Hands-on (Job submission, Basic MPI with examples, Total view Debugger – Resource people VS, RPT, GKP, PM, VKS, AM, NP, MD, PSS)



SILVER JUBILEE CELEBRATIONS (1988 – 2013)

28/8/2012

09:30 - 10:30	MPI –II (VS)
10:30 - 11:00	Tea
11:00 - 12:15	Intel Tools - I (Compiler and VTune amplifier) (RKM)
12:15 - 01:30	Numerical Methods – II (Iterative Methods for linear systems) (PM and VKS)
01:30 - 02:15	Lunch
02:15 - 03:15	Intel Tools – II (Trace analyser and MKL) (RKM)
03:15 - 03:30	Tea
03:30 - 04:30	Valgrind Debugger (PM)
04:30 - 05:00	Open MP (RKM)
05:00 - 06:30	Hands-on (MPI, Num Methods – I and II, Intel Tools, Valgrind)

29/8/2012

09:30 - 10:30	Data Mining – I (RKL)
10:30 - 11:00	Tea
11:00 - 12:15	Data Mining – II (RKL)
12:15 - 01:30	Spectral Methods for PDES (TNV)
01:30 - 02:15	Lunch
02:15 - 03:15	MPI – III (PM and GKP)
03:15 - 03:30	Tea
03:30 - 04:30	DNA sequencing application (UNS)
04:30 - 06:30	Hands-on (Data Mining , MPI, Spectral)

30/8/2012 (Applications)

09:30 - 10:30	Ab initio Computational Chemistry: Challenges and scope of parallelization–I (SP)
10:30 - 11:00	Tea
11:00 - 12:00	Ab initio Computational Chemistry:Challenges and scope of parallelization- II (SP)
12:00 - 01:30	Unstructured/ Irregular computation in CFD (PM and VKS)
01:30 - 02:15	Lunch
02:15 - 03:15	Data Intensive Science: A case study of Genomics (VC)
03:30 - 06:30	Hands-on

31/8/2012

09:30 - 10:30	Parallel I/O HDF-5 (PM and VKS)
10:30 - 11:00	Tea
11:00 - 12:15	PDES and Flexible Modelling System (PSS)
12:15 - 01:30	Hands-on
01:30 - 02:15	Lunch
02:15 - 03:15	Hands-on
03:15 - 03:30	Tea
03:30 - 04:30	Concluding session

CSIR CENTER FOR MATHEMATICAL
MODELLING AND COMPUTER
SIMULATION (CSIR C-MMACS)



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Course co-ordinators

P.S.Swathi

Pavanakumar Mohanamurthy

