Advanced Course in Bio-Informatics (ACB-2005)

Organized by C-DAC, Hyderabad/Pune, IICT-Hyderabad and JNTU-Hyderabad
Venue: Biology, IICT-Hyderabad **Date :** September 26, 2005 - October 04, 2005

High Performance Computing Module for ACB 2005
Organized by*:* NPSF, C-DAC, Pune **HPC Module Coordinator***: Dr. VCV. Rao*

Day 1: September 26, 2005 (Monday)

Time (Hrs)	Activity
0900 ~ 0915	**An Overview of Parallel Computing Module:** An overview of HPC Module; Summary of Class–Room Lectures; An overview of Hands-on Sessions on PARAM Padma, Summary of Assignments, Examination pattern (Class-Room Lectures /Hands-on Session) for ACB 2005
0915 ~1000	**Introduction (part-I):** Introduction, What is Parallel Computing? The Scope of Parallel Computing, Concept of Scalability, Notations and Conventions
1000 ~1100	**Explicit Parallelism: Message Passing Programming (MPI) - Part I:** Introduction, MPI Basics, MPI Messages, Features, MPI Point-to-Point Communication library calls, Simple MPI programs
Tea and Refreshments Break: 1100 Hrs ~1115 Hrs	
1115~1200	**Introduction (Part-II):** Application requirements, Issues in Parallel Computing, Performance of Parallel Programs Parallel Programming Overview, Basic Communication Operations, Scalability
1200~1245	**Hands-on Session on PARAM Padma:** Compile and Execution of Sequential Parallel programs on PARAM Padma, Simple MPI Parallel programs using MPI point-to-point Communications
1245~1300	**Assignment I:** Questions on Assignment 1 for Day 01/02 Class-Room lectures and writing parallel programs using MPI on PARAM Padma
Lunch Break: 1300 Hrs~1400 Hrs; Tea and Refreshments Break:1600 Hrs ~1630 Hrs	
1400~1800	**Hands-on Session on PARAM Padma:** *Understanding Basic library calls semantics, Compilation and Execution of Simple MPI Parallel Programs (FORTRAN or C language); MPI Parallel programs using MPI point-to-point library calls on PARAM Padma*

Day 2: September 27, 2005 (Tuesday)

Time (Hrs)	Activity
0900 ~1000	**An overview of Parallel Computing and PARAM Padma:** An overview of SIMD, and MIMD Machines, An overview of Cluster Computing and Challenges, Performance Issues on Clusters An overview of PARAM Padma – PARAMNet System Interconnect, Compute Node features, Parallel Programming Environment and tools, Basic Communication Library operations
1000 ~1100	**Performance – Using Compiler Techniques for Sequential /Parallel Codes:** Basic Compiler Techniques: What an Optimizing Compiler does to get maximum performance of your code? Compiler role in loop optimization techniques; Single processor optimization techniques
Tea and Refreshments Break: 1100 Hrs ~1115 Hrs	
1115~1230	**Parallel Programming Paradigms, Programming Models & Parallel Algorithms design -** An overview of Parallel Algorithmic Paradigms, Programming Models; Implicit /Explicit Parallelism Types of Parallelism, Decomposition techniques; Static and Dynamic load balancing techniques; Overheads in algorithm design, Performance Issues
Lunch Break:1300 Hrs ~ 1400 Hrs; Tea and Refreshments Break:1600 Hrs ~1630 Hrs	
1400~1800	**Hands-on Session on PARAM Padma:** *Performance of FORTRAN/c programs using compiler optimization features and using code restructuring techniques, MPI Parallel programs using MPI Collective Communications Library Calls and Simple Programs on Dense Matrix Computations.*

Day 3: September 28, 2005 (Wednesday)

Time (Hrs)	Activity
0900~1000	**Explicit Parallelism: Message Passing Programming (MPI) – Part II:** Message Envelope in MPI. MPI Collective Communication library calls, MPI Collective Computation and Computation Library Calls, Timing MPI Programs, MPI Implementation, Examples
1000~1100	**Explicit Parallelism: Shared Memory Programming (OpenMP):** (An Overview of Shared Memory Programming Model, OpenMP Constructs, Parallel for Loops, Critical Sections; Performance Improvements, Support of Data Parallelism, Example Programs)
Tea and Refreshments Break: 1100 Hrs ~1115 Hrs	

High Performance Computing Module for ACB 2005

The Supercomputing People

Day 3: September 28, 2005 (Wednesday)

Time (Hrs)	Activity
1115~1145	**Explicit Parallelism: Data Parallel Programming (f90/f95/HPF):** The Data-Parallel Model; The Fortran 90 /95 Approach (Parallel Array Operations); High Performance Fortran (Data Mapping in HPF, Support for Data Parallelism); Fortran 95 Enhancements - Performance Issues
1145~1200	**Assignments I and Assignment 2:** Solutions to Assignment 1; Questions on Assignment 2 for Day 02/03 Class-Room lectures and parallel programs using MPI/OpenMP on PARAM Padma
1200~1245	**Principles of Parallel Algorithms and Design - Load Balancing Issues :** Principles of Algorithms design - Decomposition techniques; Static and Dynamic load balancing features; Overheads in algorithm design and performance Issues
1245~1300	**Hands-on Session on PARAM Padma:** Parallel Programs using OpenMP, Parallel on vector-vector, matrix-vector and matrix-matrix multiplication algorithms
Lunch Break: 1300 Hrs ~1400 Hrs; Tea and Refreshments Break:1600 Hrs ~1630 Hrs	
1400~1800	**Hands-on Session:** Simple OpenMP and /MPI Parallel programs, Performance of programs for matrix computations using math libraries BLAS; Parallel MPI Fortran 77/C/f90 programs on vector-vector, matrix-vector and matrix-matrix multiplication algorithms

Day 4: September 29, 2005 (Thursday)

Time (Hrs)	Activity
0900-1000	**Explicit Parallelism: Message Passing Programming (MPI) - Advanced Features – Part -III:** MPI advanced point-to-point communication; MPI Communication modes; MPI Collective Communications; MPI Derived Data types; Grouping data for Communication, Communication and Topologies; Cost of Message Passing Operations, MPI-2 Features
1000 ~ 1100	**Explicit Parallelism: Advanced Feature of OpenMP:** Examples OpenMP Programs, Advanced Features of OpenMP –Critical Sections, Functional Parallelism, Reductions & Data Parallelism
Tea and Refreshments Break: 1100 Hrs ~1115 Hrs	
1115~1200	**Performance Metrics, Scalability and Speed Up Analysis:** Types of Performance requirements, Performance and Workload Speed Metrics; Parallelism and interaction overheads; Overhead Quantification and measurement methods; Scalability and Speed-up Analysis
1200~1245	**Shared Memory Programming: PThreads**: What is Thread model; Designing Threaded Programs; Examples of Threaded Programs; Understanding Pthreads implementation; Pthread functions for Synchronization, Debugging tools; Pthread - Performance issues
Lunch Break 1300 Hrs ~1400 Hrs; Tea Break: 1630 Hrs ~1645 Hrs	
1400 ~1800	**Hands-on Session on PARAM Padma:** *MPI and OpenMP Parallel programs; Parallel programs on matrix-matrix multiplication algorithms; Solution of matrix system of linear equations by Direct/Iterative Methods; parallel programs using combination of MPI and OpenMP*

Day 5: September 30, 2005, (Friday)

Time (Hrs)	Activity
0900-1000	**An overview of Application and System Benchmarks:** Benchmarks Classification; Micro Benchmarks (LINPACK, TOP-500 Benchmark, LMBENCH, STREAM, P-COMS); Macro Benchmarks (NAS, PARKBENCH, SPEC, TCP Benchmarks) & Performance Issues
1000~1100	**Explicit Parallelism: Combination of MPI/OpenMP** Combining MPI and OpenMP; Profiling; Performance of MPI/OpenMP programs; Examples of MPI/OpenMP Programs
Tea and Refreshments Break: 1100 Hrs ~1115 Hrs	
1115-1200	**An overview of PARAM Padma:** Features of PARAM Padma Cluster, PARAMNet-Interconnect and Compute nodes features, Programming Environment, Performance of Benchmarks
1200 ~1215	**Assignments 2 and Assignment 3**: Solutions to Assignment 2 Questions; Questions on Assignment 3 for Day 04/Day 05 Class-Room lectures and parallel programs using MPI/OpenMP
1215~1300	**Hands-on Session on PARAM Padma:** Parallel Programs using OpenMP/MPI, Parallel on vector-vector, matrix-vector and matrix-matrix multiplication algorithms; Assignments
Lunch Break:1300 Hrs ~1400 Hrs; Tea and Refreshments Break:1600 Hrs ~1630 Hrs	
1400~1800	**Hands-on Session on PARAM Padma:** *Demonstration of MPI parallel programs using parallel visualization tools; Demonstration of MPI parallel programs to measure communication overheads (P-COMS) on PARAM Padma, Demonstration of Performance benchmarks on PARAM Padma, Example programs using combination of MPI and OpenMP*

October 1 & 2, 2005 (Saturday & Sunday): Holiday

High Performance Computing Module for ACB 2005

Day 6: October 03, 2005 (Monday)

Time (Hrs)	Activity
0900~1000	**Performance Visualization tools**: Performance Visualization tools for Parallel Programs; MPI's Profiling Interface; Upshot – Performance Analysis Tool; Parallel Debuggers on PARAM Padma
1000~1100	**An overview of Performance of Scientific Applications**: Performance Scalability issues of Applications, Domain Decomposition Methods and load balancing issues, Memory Optimization, Performance of tuned Mathematical libraries on Shared and Distributed Memory Machines.
1100 Hrs ~1115 Hrs Tea break	
1115-1200	**Feedback** Session on HPC module **& Discussion on** Solutions to Assignment 3 Questions.
Lunch Break: 1300 Hrs ~1400 Hrs; Tea and Refreshments Break:1600 Hrs ~1630 Hrs	
1400 ~1800	**Hands-on Session on PARAM Padma:** *MPI parallel programs* using parallel visualization tools; *MPI parallel programs* to measure communication overheads using P-COMS. *Parallel programs* using different OpenMP *programs on Dense Matrix Computations*

Day 7: October 04, 2005 (Tuesday)

Time (Hrs)	Activity
0900~1100	**Examination for Hands-on Session on PARAM Padma:** Writing, Demonstration and explanation of parallel programs on PARAM Padma
1100 Hrs ~1115 Hrs Tea break	
1130~1230	**Computational Challenges-Parallel Molecular Dynamics Applications:** Introduction, Classical MD simulation, Force Computations, Issues in Parallelization, Partitioning Algorithms: Atom Decomposition, Domain Decomposition, Force Decomposition Methods; Overview of AMBER
Lunch Break: 1300 Hrs ~1400 Hrs	
1400-1600	**Examination for Classroom Lectures (Theory) - Open Book System**