Workshop: Advanced computational skills across scientific domains

14-18 October 2024
Classroom: Edificio I-G - P2G4A
Schedule: 11:30 -13:30 (10 h total)

Module 1: Mastering Shared-Memory Parallelism with OpenMP

- Understanding OpenMP Essentials
- Overview of OpenMP directives and constructs
- Identifying opportunities for parallelization in shared-memory systems
- Hands-On Thread Programming
- Practical exercises implementing OpenMP directives in C/C++/Fortran
- Thread synchronization techniques and best practices
- Real-World Applications
- Case studies illustrating successful applications of OpenMP in various industries
- Discussion on challenges and solutions when scaling with shared-memory parallelism

Module 2: Message-Passing Mastery with MPI

- Basics of Message-Passing Interface (MPI)
- In-depth understanding of MPI principles and communication concepts
- Practical considerations for data distribution and synchronization
- Creating Scalable Parallel Applications
- Hands-on sessions developing parallel applications using MPI
- Strategies for load balancing and minimizing communication overhead
- Case Studies and Best Practices
- Exploration of real-world MPI applications in scientific research and industry
- Best practices for optimizing MPI-based parallelization in diverse scenarios

Module 3: GPGPU and Vector Programming

- Overview of General-Purpose GPU (GPGPU) Programming
- Introduction to CUDA, OpenCL and OpenACC for GPGPU programming
- Understanding the architecture of GPUs and their role in parallel computation Basics of Vector Programming for Optimal Performance
- Techniques for leveraging vectorization in code
- Hands-on exercises for writing vectorized code in high-level languages
- Applications and Challenges
- Exploration of real-world applications bene ting from GPGPU and vector programming
- Discussion on challenges and considerations when implementing these techniques

This course is designed for graduate students and advanced undergraduates in their Junior and Senior years. Students majoring in science, technology, engineering and mathematics with a focus towards computational science will gain the most from this course. The course covers most of the contents in a hands-on manner with a lot of live demonstrations and examples. At the completion of the course the student will be exposed to the working of the internals of a modern parallel computer. The student will also be familiar with different parallel programming paradigms and the methodology to code in them. The course prepares the student to carry out his or her research in computational science in a more effective manner.