Algorithms and High Performance Computing

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Realism and Performance





https://dual.sphysics.org/



Multi-GPU DSPH Analysis Project Video N. Gutierrez, S. Gelvez, J. Chacon, I. Gitler and C.Barrios

The Challenge









Science and Advanced Technology for All



Citizens, All

Experts- ScientistsExperts Scientists – Computer and Informatics(Biologists, Architects, Pysiciens)Informatic, Math Applied

Technology - Infrastructure

What is Scientific Computing?







HPC and Scientific Computing



Major Applications of HPC and Scientific Computing



The Scientific Computing Process



About the Course

A Theoretical/Practical Course for Physics students with these general goals (after survey):

- Learn how to program scientific computing codes in different computing systems and achieve
 - High performance Computing and Accuracy
 - Functionality
 - Interaction with Computer Scientists
 - Scalability and Portability
 - Special Trends in Scientific Computing
- Introduce some Technical subjects
 - Understand Algorithms
 - Scientific programming using C/C++
 - Debugging and Performance Evaluation of Codes
 - Parallel programming, tools and techniques
 - Principles and patterns of parallel algorithms
 - Platforms, Frameworks and Architectures (Including quantum computing)

Content (Not in Order)



Fundamentals to Algorithms

- Quiclky Survey and Introduction
- Programming Scientific Algorithms with C/C++: An Introduction
 - Good Practices
 - Compiling, Efficient Execution and Optimisation (or vice-versa)
 - Debugging, Profiling and Tracing

Systems, Platforms and Frameworks

- Computer Architectures for Research (and Scientific Development)
 - Scientific Computing Infrastructures
 - Github/Gilab, Linux and more...
- Large Scale Computing and Interaction
 - Hand On with SC3UIS and SCALAC platforms

• Parallel Scientific Computing

- Concurrency and Parallelism
- Parallel Programming Paradigms
 - Shared Memory with OpenMP
 - Distributed Memory with MPI
 - Hybrid Memory with OpenACC (and some of CUDA)
- Exploiting Quantum Parallelism: An Introduction using MyQLM and Others
- A Survey for Libriaries and Solvers to Different Areas
 - SCALAPACK, Quantum Expresso, NamD, and others.

Evaluation

- Collaborative Work in Teams
 - 1) 20% Analysis and Algorithm Approach 20% Implementation and Solution
 - 2) 20% Performance Analysis and Evaluation
 - 3) 20% Digital Poster* 20% Work at Class Assessments (From Today)

Bonus: Participation in Free virtual Seminars proposed by the professor

- Team conformation for research/domain common interests
- (All information of the Course in Detail will be published this week in <u>www.sc3.uis.edu.co</u>)

*The evaluation points 2) and 3) will be in the Digital Posters and in a github/gitlab repository)

Course Highlights

- 3 hours Theoretical Practical Sessions (Tuesdays)
 - Session starts at 7:10am (First, the Theoretical Approach)
 - 10 minutes break
 - The session continues after the break (Second part, the Practical Approach)
 - (If the team or the Individual finish the practical part before 10:00 a.m. it is possible to leave the classroom or class zoom session)
 - Please Punctuality!
- Consultation sessions
 - Please, send an email to schedule the rendez-vous (in real or virtual) to the email <u>cbarrios@uis.edu.co</u>
- Course site: http://wiki.sc3.uis.edu.co (To be Update this week)

About Teaching and Instruction



• Carlos Jaime Barrios Hernández, PhD. cbarrios@uis.edu.co@carlosjaimebh

- Director of High Performance and Scientific Computing Centre SC3UIS (www.sc3.uis.edu.co) and CAGE Research Group Director
- Associate Professor EISI/UIS (http://cormoran.uis.edu.co)
 - Systems Engineering UIS, Bucaramanga, Colombia (2002), Master in Mat. Applied, Systems and Informatics UJF-Grenoble I, Grenoble, France (2005), Computer Science and Informatics Doctor, UNSA, Nice-Sophia Antipolis, France (2009), PostDoctoral Research, I3S/CNRS, Sophia Antipolis, Francia (2010).
 - Researcher in Advanced, High Performance and Scientific Computing (LIG, I3S/CNRS, INRIA (France), GPPD/UFRGS (Brazil), SC3UIS (Colombia)) and International Instructor in HPC and SC (ICTP/UNESCO (Italy), SCCAMP).
 - Chair of the Advanced Computing System for Latin America and Caribbean (SCALAC)
 - NVIDIA Deep Learning Institute Instructor

• SC3 and CAGE Team (More Information in www.sc3.uis.edu.co)

Contact: EISI Block : LP 226, PTG-EDI I 205 and SC3 Space 4to Floor CENTIC Please, Send an email before for rendez-vous

Important Notes

- All Available materials in English (International Technical/Scientific English)
- Bibliography and other resources are available in the site of the course. This material is used for the assessments and Project
- Attention to Students : (Please, Send an email before for rendez-vous)
- By default, the communication is via email from cormoran utility or email direct (cbarrios@uis.edu.co) or to the instructor guest.
- Autolearning and Curiosity Awarded

Questions?

