



UCAM
UNIVERSIDAD CATÓLICA
DE MURCIA

BIG DATA FUNDAMENTALS & APPLICATIONS IN BIOINFORMATICS



Duration

3 weeks, 60 contact hours.

Objectives

- To explore techniques and tools for interpreting and analyzing large volumes of data.
- To study and analyze different hardware architectures in Big Data environments.
- To analyze and understand different strategies for cleaning, modeling and analyzing data from the Big Data perspective.
- To learn security and privacy techniques applied to Big Data.
- To learn about real problems where the problem of large volumes of data is present, especially in Bioinformatics.

Business Partners

VISUALTIS



Fee

€2,500 /student

Services provided:

- 1 Professor/tutor for free
- Accommodation (triple or double room upon availability)
- Breakfast and lunch (excluded weekends)
- Group airport transfer service
- Bus ticket
- UCAM welcome pack
- Teaching materials
- Murcia city center tour

Contact

International Admissions Office
(+34) 968 278 786
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Schedule

WEEK 1

Session 1: Introduction to Big Data (Dr. Andrés Muñoz)

- What is Big Data?
- Datification
- The value of data
- Big Data examples and success stories
- Big Data challenges
- Data Visualization in Big Data

Session 2: Big Data technologies (Dr. Andrés Muñoz)

- Hadoop
- Map-Reduce
- Spark
- Latest technologies

Session 3: Hands-on Session on Big Data technologies (Dr. Andrés Muñoz)

- Lab session with small exercises on Hadoop

Session 4: Addressing the Challenge of Securizing Big Data / Interface and Costs of Big Data (Dr. Fernando Pereñíguez / Dr. Joaquín Lasheras)

- Security and Big Data
- Why security is necessary in Big Data?
- Security Risks in the Big Data Era
- The necessary basic security services
- Overview of existing solutions
- Interfaces in Big Data
- Need for a good visualization
- Good practices in visualization
- Tools
- Cost in Big data
- The value of the data
- Who is it addressed to?
- Providers

Session 5: Company Visit I (Dr. Andrés Muñoz / / Dr. Joaquín Lasheras)

WEEK 2

Session 1: The landscape of HPC platforms for the Big data challenge. (Dr. José Luis Abellán)

- Introduction to computing platforms
- Current landscape of supercomputers
- Future trends in developing computer architectures

Session 2: Graphics supercomputer for big data era. (Dr. José María Cecilia)

- Introduction to Graphics Processing Units
- General purpose on Graphics Processing Units
- Application examples

Session 3: Towards data processing in Big Data (Dra. Raquel Martínez)

- Introduction to Intelligent Data Analysis
- What is data preprocessing?
- Important tasks in data preprocessing
- Techniques from data preprocessing
- Examples of application

Session 4: Lexical analysis and sentiment analysis (Dr. Francisco Arcas)

Session 5: Company Visit II (Dr. Andrés Muñoz / / Dr. Joaquín Lasheras)

WEEK 3

Session 1: Introduction to Big Data in Structural Bioinformatics and Drug Discovery (Dr. Horacio Pérez Sánchez)

- What is Structural Bioinformatics?
- What is Computational Chemistry?
- Need of HPC in Structural Bioinformatics and Computational Chemistry
- Success cases
- Technology Transfer
- State of the art and future perspectives

Session 2: Hands on session: Big Data in Structural Bioinformatics and Drug Discovery (I). (Helena den Haan)

- Virtual Screening of Chemical databases: general background
- Structure based approaches in Virtual screening

- Ligand Based methodologies in virtual screening
- Hands on work: DIA-DB, ChemMapper, ZincPharmer

Session 3: Introduction to Big Data in Quantum Chemistry (Dr. José Pedro Cerón Carrasco)

- Quantum Chemistry: a general background
- Computational codes for simulating molecules
- What can we learn from quantum descriptors?
- Required resources and produced files
- Working examples

Session 4: Hands on session: Big Data in Structural Bioinformatics and Drug Discovery (II). (Dr. Ricardo Rodríguez Schmidt)

- Introduction to 'Blind Docking'
- Blind Docking Server: an online tool for Blind Docking
- Working examples

Session 5: Company Visit III (Dr. Andrés Muñoz / / Dr. Horacio Pérez)

Teaching Staff

Andrés Muñoz

Senior lecturer in the Technical School at the Catholic University of Murcia (UCAM), Spain. He obtained his PhD in Computer Science in 2011 at the University of Murcia.

Ricardo Rodríguez Schmidt

He is a member of the Structural Bioinformatics and High Performance Computing at the Catholic University of Murcia (UCAM), Spain. He obtained his PhD in Computational Chemistry in 2012 at the University of Murcia.

Helena den Haan Alonso

She has a BS in Biology and a MS in Bioinformatics obtained in 2011 at the University of Murcia. Currently she is an Industrial PhD student in collaboration with the pharma company Villapharma.

José L. Abellán

He received the B.S., M.S. and Ph.D. degrees in Computer Science and Engineering from the University of Murcia, Murcia, Spain, in 2007, 2008 and 2012, respectively. From 2012 to 2014, he was a post-doctoral researcher at Boston University, Boston, MA, USA.

José M. Cecilia

He received his B.S. degree in Computer Science from the University of Murcia (Spain, 2005), his M.S. degree in Computer Science from the University of Cranfield (United Kingdom, 2007), and his Ph.D. degree in Computer Science from the University of Murcia (Spain, 2011).

Raquel Martínez España

She is an Assistant Professor of the Computer Science Department, Catholic University of Murcia, Murcia, Spain. She received her B.S M.S. and Ph.D. degrees in Computer Science and Engineering from the University of Murcia, Murcia, Spain, in 2009, 2010 and 2014, respectively.

José Pedro Cerón-Carrasco

He earned his Ph.D. at the University of Murcia in Spain (2009). He joined the University of Namur in Belgium (2009), the University of Nantes in France (2011), and the University of Murcia in Spain (2013) during his postdoctoral training supported by Fundación Séneca and the European FP7 Marie Curie program.

Fernando Pereñíguez-García

He received B.E, M.E and Ph.D. degrees in Computer Sciences from University of Murcia in 2007, 2008 and 2011, respectively.

Joaquín Lasheras

He is an Associate Professor in the Technical School at the Catholic University of Murcia (UCAM), Spain. He had previously obtained his BSc and MSc degrees (computer science) in 2003 and 2005 respectively at the University of Murcia. He obtained his PhD in 2011 at the same university.

Francisco Arcas

He is an Assistant Professor of the Computer Science Department, Catholic University of Murcia, Murcia, Spain. He received her B.S, M.S. and Ph.D. degrees in Computer Science and Engineering from the University of Murcia, Murcia, Spain, in 1991, 1993 and 2008, respectively.

Horacio Pérez Sánchez

He earned his Ph.D. at the University of Murcia in Spain (2006). He joined the Forschungszentrum Karlsruhe in Germany (2007), Karlsruhe Institute of Technology (2009), during his postdoctoral training supported by German Ministry of Science and FP7 Marie Curie programme.