



IPL Summer School 2021

The Fundamentals of Digital Science for Chemists

Dr. John SAMUEL
Dr. Oscar CARRILLO

The Fundamentals of Digital Science for Chemists

1. Internet of things	<p>Objective: This part gives an introduction to different themes related to Internet of things required for chemists</p> <p>It will cover the following topics:</p> <ul style="list-style-type: none">• History of Internet of Things (IoT)• Definition of IoT• Industry 4.0• IoT architectures• Fog/Edge/Cloud computing
2. Introduction to Data Science	<p>Objective: This part is an introduction to different themes related to data science required for chemists</p> <p>We will take a look at different concepts related to data science</p> <ul style="list-style-type: none">• History of Data Science and computing• Computer Architecture and Systems• Major phases of data analysis• Algorithms for data acquisition and process control
3. Data acquisition protocols and technologies for IoT	<p>Objective: This part presents data acquisition protocols and technologies for IoT</p> <p>We will take a look at the key concepts of IoT</p> <ul style="list-style-type: none">• IoT Technologies• Data acquisition protocols like SPI, I2C• Sensors• Actuators
4. Fundamentals of Programming	<p>Objective: This part gives a general overview of programming in Python with the goal of using it for data analysis</p> <p>The student will be able to get an overview of</p> <ul style="list-style-type: none">• Fundamentals of Python programming• Manipulation of files, especially reading, writing and modifying text files and CSV/TSV and JSON files• Interaction with the user• Data Analysis (basic) using built-in Python methods

<p>5. Data Analysis and visualization</p>	<p>Objective: This part gives the fundamentals of data analysis and visualization</p> <p>It will cover the following topics</p> <ul style="list-style-type: none"> • Clustering algorithms • Classification algorithms • Linear regression models • Recommender systems • Visualization techniques
<p>6. Practical session on Microcontrollers</p>	<p>Objective: This part gives a hands-on experience on the microcontrollers</p> <p>The student will be able to perform the following</p> <ul style="list-style-type: none"> • Coding, compiling and flashing a firmware for microcontroller • Interacting with sensors and actuators using SPI and I2C protocols • Reading digital and analog measures
<p>7. Network protocols for IoT</p>	<p>Objective: This part gives an introduction to the network protocols for data communication</p> <p>We will cover the following topics</p> <ul style="list-style-type: none"> • Network protocols like LPWAN and WPAN • Message exchange protocols like MQTT
<p>8. Data Mining</p>	<p>Objective: This part gives an opportunity to the students to use data mining tools</p> <p>We will look at the following topics:</p> <ul style="list-style-type: none"> • Introduction of Python libraries like numpy, matplotlib and pandas • Manipulating CSV and JSON files using the above libraries • Data analysis • Data visualization techniques for different types of data • Clustering, classification and linear regressing using the library Scikit-learn.
<p>9. Scaling up IoT</p>	<p>Objective: This part introduces ways to scale up the IoT architectures</p> <p>The students will discover</p> <ul style="list-style-type: none"> • The challenges while scaling up IoT • IoT Lab infrastructure

<p>10. Machine Learning</p>	<p>Objective: This part gives an introduction to machine learning techniques</p> <p>We will cover the following topics</p> <ul style="list-style-type: none"> • Supervised, unsupervised and semi-supervised learning • Neural network models including single and multilayered perceptron • Analysis of sensor data • Image analysis • Prediction • Recognition of handwriting
<p>11. Practical session on IoT-Lab</p>	<p>Objective: This part introduces ways to use message and network protocols for IoT lab</p> <p>The students will work on</p> <ul style="list-style-type: none"> • LoRa WAN • MQTT
<p>12. Big Data</p>	<p>Objective: This part will introduce the key concepts of Big Data</p> <p>Following are the topics covered in this module:</p> <ul style="list-style-type: none"> • 5V of Big Data • Data storage of voluminous data, especially non-relational databases • Artificial Intelligence • Open databases and extraction of information
<p>Evaluation</p>	<p>Final exam of two hours based on all the topics covered in this module.</p>