# Laurea Magistrale Interateneo UniTS –UniUD - Physics Academic year 2017/18 INFORMATION AND COMMUNICATION TECHNOLOGY ABILITIES (ABILITA' INFORMATICHE E TELEMATICHE) (update: October 11, 2017)

To the students of the "Laurea Magistrale" in Physics, with priority to those of the **II year of the training tracks of: Condensed Matter Physics, Theoretical Physics, Environmental Physics**, who have this activity planned in their "plan of studies" (3 credits).

Students are invited to choose **at least 4 among the 10 activities proposed** in the following (5 IN EACH SEMESTER). Then, they have to contact a supervisor, agree and **work on a project** (of about 60 hours of workload). At the end, the supervisor will judge the work and certificate that the student has obtained/not obtained the 3 credits. Prof. Pastore is in charge of the registration on the Esse3 system. Other activities can be also accepted. Contact in advance prof. Pastore and the referent person of the training track.

IMPORTANT: Since these activities will consist in practical lab sessions (Lab. POROPAT), students must subscribe to the selected activity at least 1 week in advance using Doodle: https://beta.doodle.com/poll/5da448yw4a6divwg

# <mark>l semester</mark>

### 1. Bash scripting for dummies (Thursday, 9 November 2017; 9:00-12:00)

(Giorgio Pastore - pastore@ts.infn.it)

Main tools, available in Unix-like environments, to increase programmer's productivity. Bash as a programming language and a selection of shell tools.

### 2. Why is my code taking so long?!? A practical introduction to optimization (Thursday, 23 November 2017 ; 9:00-12:00) (Paolo Giannozzi - paolo.giannozzi@uniud.it)

This mini-course will provide an overview of the main factors affecting the performances, in terms of speed, of codes on modern computer architectures, in particular for floating-point-dominated computations. A few general rules and practical recipes that may lead to significant speed enhancements will be described. In particular, the importance of choosing the correct algorithm and optimized mathematical libraries will be stressed. Although the focus is on modern Fortran (90/95/2003), these rules and recipes are typically valid independently upon the specific language used.

# Abstract data types for physicists (and examples of implementation in high level languages) (Thursday, 7 December 2017 ; 9:00-12:00)

# (Giorgio Pastore - pastore@ts.infn.it)

Abstract data types provide a logic organization of data. They can usefully exploited for simplifying and to provide a concise description of algorithms. Almost every programmer meets the simplest abstract data types like arrays or records through their concrete implementations present in the most popular programming languages. Additional data types are routinely used in computer science and also physicists may find interesting to know about them. Stacks, queues, linked lists, trees, hash tables will be introduced and discussed with practical examples from the perspective of a physicists.

# 4. Introduction to parallel computing using MPI (Thursday, 11 January 2018 ; 9:00-12:00) (Paolo Giannozzi - paolo.giannozzi@uniud.it)

This mini-course will provide an overview of programming for modern parallel machines. The two main software paradigms for parallel computing: OpenMP and MPI, will be introduced, with focus on the latter. The main factors affecting MPI parallelization: load balancing, communication speed, latency, as well as pitfalls to be avoided, will be described.

5. Open source tools for scientific visualization: examples with Gnuplot, Jmol, VMD... (Thursday, 18 January 2018 ; 9:00-12:00) (Maria Peressi - peressi@ts.infn.it, Virginia Carnevali - cavirgi@gmail.com)

Scientific visualization allows fast and effective analysis and interpretations. An image is able to convey the results of a simulation in a more effective and immediate way than a numerical tabulation and to communicate it efficiently. We will explore some well know tools, such as Gnuplot for 2D e 3D plots, fits, animation...; Jmol and VMD for molecular structure visualization.

**Il semester** (dates are tentative; to be confirmed)

#### 6. Fast Fourier Transforms (Thursday, 8 March 2018 ; 9:00-12:00)

#### (Pierluigi Monaco - monaco@oats.inaf.it)

Fast Fourier Transforms are one of the most used techniques in physics, because they allow to solve equations like the Poisson equation, or compute spatial derivatives of a field on a grid, with high accuracy and a scaling like N log N. After illustrating the technique and the organization of data in memory, I will introduce the fftw package (<u>http://www.fftw.org/</u>). The usage of this package will be illustrated through the example of the differentiation of an analytic function defined on the plane.

# 7. Introduction to symbolic calculation and Mathematica (Thursday, 15 March 2018 ; 9:00-12:00) <u>(Edoardo Milotti - milotti@ts.infn.it)</u>

In this first lesson I shall briefly introduce symbolic calculus and and its implementations, with special attention to Mathematica, a widely used commercial software. Over the years, Mathematica has become increasingly wide-ranging and at present it has more than 3000 built-in instructions spread over a dozen application areas. This short introduction shall only cover the most basic features of this software tool, with the aid of a few simple examples.

### 8. Selected application examples of Mathematica to scientific problems (Thursday, 22 March 2018 ; 9:00-12:00) (Edoardo Milotti - milotti@ts.infn.it)

In addition to symbolic manipulation, Mathematica can also be used for numerics. In this lesson I shall consider some scientific applications to be selected by the students during the first lesson. Here is a list of possible case studies: A. statistical analysis and display of scientific datasets; B. analytical and numerical solution of differential equations with applications to dynamical systems; C. Markov Chain Monte Carlo with Mathematica; D. image processing with Mathematica.

#### 9. and 10. Introduction to ROOT (Thursday, 5 and 12 April 2018; 9:00-12:00)

(Stefano Piano - stefano.piano@ts.infn.it, Lea Ramona - ramona.lea@ts.infn.it) ROOT is a software framework for data analysis and I/O. Its prominent features are an advanced graphical user interface, an interpreter for the C++ programming language, a powerful library of mathematical functions and a persistency mechanism for C++ objects. These introductory lectures illustrate the main features of ROOT, which are relevant for the typical problems of a Master Thesis data analysis in experimental physics: input and plotting of data from measurements and fitting of analytical functions.

11. Scientific visualization with Mathematica (to be scheduled) (Matteo Carlesso - carlesso.mat@gmail.com)