MASTER 2 Sciences, Technologies, Santé

Mention High Performance Computing, Simulation

Parcours Scientific Computing

ACADEMIC YEAR 2017 - 2018

PRESENTATION

DESCRIPTION
This Master degree in High Performance Computing, Simulation, specialized in scientific computing, from Lille 1 offers a top rate international interdisciplinary training year in applied scientific computing. It is available to postgraduate students who wish to specialize in modelling, numerical simulation and supercomputing.

ACADEMIC STAFF
The academic staff in charge is composed of distinguished Researchers and Professors from 8 laboratories and research institutions (CNRS,INRIA…) located on Lille 1 campus and we also welcome lecturers from Business and Industry.

COMPUTING FACILITIES
The students will have at their disposal computing resources dedicated to high-performance scientific computing. They will have access to a hybrid cluster with a power of 45 TFlops including GPU devices and Xeon Phi coprocessors and the access to Grid'5000 nation-wide computational grid of several thousands of processing cores located at 11 geographically distributed sites.

CARRIER PROSPECTS
- Fully qualified engineers or research and development engineers in various sectors such as car industry, aeronautics, space research, nuclear energy, environment, fossil and renewable energy.
- A doctoral thesis in a research laboratory or in the industry.

STUDYING IN LILLE
The Nord-Pas de Calais region is well known for being lively, dynamic and for having a strong international interest. With almost 1 million inhabitants and 5 European capital cities within 300 kms, Lille has a privileged position at the heart of North Western Europe. It offers direct links to Great Britain, the Benelux, Germany and Central Europe countries. The campus in Villeneuve d'Ascq is entirely self-contained and can be reached directly from Lille center by the underground in ten minutes.

FINANCIAL ASPECTS
The French government will subsidize the Master Program (equivalent to 12 000€). The student is only required to pay a token administrative fee (around 450€) and his/her leaving expenses in Lille.
COURSE MODULES 2017 - 2018

Semester 3

2 courses to be chosen among the following 3 :

- Refresher course in numerical methods (5 ECTS)
- Refresher course in modelling (5 ECTS)
- Refresher course in algorithms and computation (5 ECTS)

Required courses

- Mathematical tools for simulation (7 ECTS)
- Supercomputing (7 ECTS)
- International enterprise project management, employment law and social security law (4 ECTS)
- Seminar (2 ECTS)

Semester 4

2 practise courses in scientific computing to be chosen in the following fields

- Scientific computing for mechanics (5 ECTS)
- Scientific computing for electromagnetic field computation (5 ECTS)
- Scientific computing for bioinformatics (5 ECTS)
- From modelling to numerical simulation (5 ECTS)
- Scientific computing for computer science (5 ECTS)
- Scientific computing for optimization (5 ECTS)
- Scientific computing for non linear optics and photonic (5 ECTS)
- Scientific computing for material science (5 ECTS)

Internship in company or research laboratory (4 to 6 months) (20 ECTS)
PROFESSORS IN CHARGE:

CLAIRE CHAINAIS
Laboratoire Paul Painlevé UMR CNRS 8254
Université des sciences et technologies de Lille
Cité scientifique - Bâtiment M2
59655 VILLENEUVE D’ASCQ CEDX (France)
Mail: Claire.chainais@math.univ-lille1.fr

NOUREDINE MELAB
Laboratoire d’Informatique Fondamentale de Lille UMR 8022
Université des sciences et technologies de Lille
Cité scientifique - Bâtiment M3
59655 VILLENEUVE D’ASCQ CEDX (France)
Mail: Nouredine.melab@lifl.fr

SECRETARY:

AURORE SMETS
Université des sciences et technologies de Lille
Cité scientifique - Bâtiment M2 - Bureau 010
59655 VILLENEUVE D’ASCQ CEDX (France)
Mail: math-masters2@univ-lille1.fr
Tel: +33 (0) 3.20.43.42.33
ADMISSION

ADMISSION CRITERIA
The program is open to students who have 240 ECTS credits (or equivalent) in a scientific university study program or who have obtained a Bachelor Degree with Honors in these areas.

APPLICATION
Applicants that are enrolled in their final year of their academic program should submit an official letter in English (or in French) from their university confirming that the student is expected to finalize his/her course at the end of the current academic year, and submit up-to-date authenticated transcript with the results of the previous years. An academic board will select the students. People from Industry or unemployed but having obtained equivalent proficiency through professional experience can apply to this program. Their application will be examined by the academic board with a specific procedure.
Deadline for application: before the 31st of March for foreign students and before the 23rd of June for French students.
The application form has to be sent to:
Université Lille 1 Sciences et Technologies
UFR de Mathématiques - Bâtiment M2
Secrétariat Pédagogique - Aurore SMETS
Cité scientifique
59655 - VILLENEUVE D’ASCQ Cedex
Mail: math-masters2@univ-lille1.fr
The applicant can download the application form at: http://mathematiques.univ-lille1.fr/

DOUBLE PROCEDURE FOR STUDENTS HOLDING A FOREIGN DIPLOMA
The application procedure is twofold: you have to send both your application form and (only if it is necessary) the certificate for your validation of years studies. These are two separate administrative procedures that have to be completed in parallel. Instructions can be found online: http://www.univ-lille1.fr/.

LANGUAGE PROFICIENCY
Students should submit proof of their level in English and/or French via a computer-based TOEFL, IELTS grade or proof of having studied at least one academic year in an English language program.

EXCELLENCE GRANTS
10,000€ per year will be allotted to the most deserving applicants. Master 2 fellowships are funded by the French region Nord - Pas-de-Calais and by LABEX CEMPI (http://math.univ-lille1.fr/~cempi/).
The deadline to apply for grants is attached to February 15th.
COURSE DETAILS

2017 - 2018
S3-UE1 : Refresher Course in Numerical Methods (5 ECTS) - 25h courses and 25h exercises

Description

This lecture will be devoted to the study of several tools and fundamental numerical methods for mathematical engineering. The main purpose is to give the essential background in mathematics, to make the student able to follow the following compulsory lectures of the master. After this lecture, the students will be able to choose and to develop and numerical methods for the resolution of large linear system or for ordinary differential equations. They will also gain knowledge of usual numerical methods for partial differential equations approximation.

Detailed program

1) Resolution methods for linear systems.
   • Direct methods : LU and variants.
   • Iterative methods : Methods of gradient.
2) Numerical resolution schemes for ordinary differential equations.
   • Explicit Euler, Implicit Euler.
   • Runge-Kutta methods.
3) Finite difference methods for usual linear DPE.
   • Principle of the finite difference method.
   • Application to usual linear DPE: Poisson and heat equations.
4) Finite element method for elliptic linear DPE.
   • Variational formulation, variational approximation.
   • Lagrange P1 Finite elements : Algorithmic implantation.

S3-UE2 : Refresher Course in Algorithms and Computation (5 ECTS) - 25h courses and 25h exercises

Description

Securing a sufficient knowledge in computer science so that the student can follow the Supercomputing and the Mathematical Tools lectures. At the end of this course, the student must know the classical techniques in computer science (architecture, classical programming, compilation techniques, object oriented programming). He/she must be aware of the existence of various data representations.

Detailed program

• Notions of computer architecture and of performances (representation of numbers)
• Sequential computing
• Data structures
• Algorithmics
• Programming languages (C and FORTRAN)
• Compilation and code optimisation
• Notion of processus
S3-UE3 : Refresher Course in Modeling (5 ECTS) - 25h courses and 25h exercises

Description

This course has for ambition to complete in an effective and optimal way the student's knowledge in Physics. It will take into account the interdisciplinary aspect of the students while allowing for a robust understanding of the fundamental laws of the physics. The student must be able, at this level, to find the mathematical models from the physical phenomena. He must know how to interpret and master the standard models of physics: Newton, Laplace, Navier-Stokes, Schrödinger, or Maxwell equations.

Detailed program :

- Waves, propagation phenomena.
- Vectorial Analysis.
- Modelling: diffusion and transport phenomena
- Fluid mechanics.
- Electromagnetism or introduction to quantum mechanics (depending on the students background).

S3-UE4 : Seminar (2 ECTS) - 20h courses

Description

A series of 6 seminars, given by professionals and/or researchers, will be offered to the student during the first semester. The goal is to initiate him/her to the presentation of research works, a technology, and so on. The student will also learn to discuss topics related to technology watch, to research careers, to the organization of research, to the intellectual property, etc.

The student will learn to follow and understand a scientific, technological or other talk with taking notes. He/She will also be initiated to the drafting of a report from his/her notes.

S3-UE5 : Mathematical Tools for the Simulation (7 ECTS) - 35h courses and 35h exercises

Description

The « Mathematical Tools for the simulation » aims to give high level mathematical lectures concerning the numerical methods for different kind of Partial Differential Equations: isotropic and anisotropic elliptic equations, parabolic equations, scalar hyperbolic equations. These various methods will all be applied on high performance computers.

At the end of this teaching, the student will have a global seeing of all required numerical techniques to solve problems coming from physics applications. He will have the ability to evaluate the advantages and disadvantages of the methods to solve a specific problem.
Detailed program

1) Isotropic and anisotropic elliptic equations
   - Modeling: fluid flow in porous media, ...
   - Notion of solutions and complements on variational formulations
   - Approximation by finite element methods in 2D and 3D, implementation
   - High order methods
   - Approximation by finite volume methods, implementation in 2D

2) Diffusive and dispersive problems
   - Modeling: heat equation, Schrödinger equation, ...
   - Different choices for time discretization
   - Stability analysis
   - Finite element and finite volume methods, implementation

3) Scalar hyperbolic equations
   - Modeling: transport phenomena and waves propagations
   - Different kinds of solutions, existence and uniqueness results
   - Riemann problem
   - Finite volume methods
   - Lax-Friedrichs, Lax-Wendroff, Godunov and Roe schemes

S3-UE6: Supercomputing (7 ECTS) - 35h courses and 35h exercises

Description

The student will be provided with the skills of parallel and distributed computing. He/She will learn about parallel distributed architectures and parallel distributed programming paradigms, environments and tools. He/She will be also introduced with some notions of administration of parallel machines.

The student will learn how to design and implement parallel and/or distributed computing applications (using MPI, OpenMP, Pthreads and Cuda). The course will also allow the student to discover the required tools for the deployment and execution of those applications, and the evaluation of their performances on parallel/distributed small and large scale machines (networks of workstations, clusters of multi-core/GPU processors, and computational grids).

Detailed program

1) Overview of parallel distributed machines (networks of workstations, clusters of processors, multi-core/GPU processors, hierarchical environments).
2) Principles of parallel algorithm design (data and task decomposition techniques, task mapping for load balancing, analytical performance modelling of parallel programs)
3) Message passing programming using MPI (the message passing paradigm, point-to-point and collective communications, derived types, multi-threaded MPI, building parallel programs, ...)
4) Shared memory programming (SM programming using PThreads, and SM programming using OpenMP)
5) GPU programming using Cuda (the basics, thread model, memory model, performance issues and solutions)
6) Distributed computing: from computational grids to clouds (concept of computational grid, Grid5000 platform, programming computational grids/clouds)
7) Notions of administration of parallel machines (reservation of resources, deployment of applications, supervision, fault detection and tolerance, etc.).
S4-UE7 : International enterprise project management, Employment law and social security law (4 ECTS) - 20h courses and 20h exercises

Description

- **International enterprise project management (24 h)**
  The need for flexibility and responsiveness is a key challenge for today organisations and companies in a global world. How can complex organisations react timely in front of a moving environment, with changing competitors and customers? How can each element or individual in this organisation react with the same discipline? The International Enterprise Project Management approach is one answer to this challenge. Using industry-standard templates and methodologies, the course will provide students with operational tools and organisation principles that are needed to manage cross-functional projects, especially in the Business Process Re-engineering area.
  The course will allow students to understand & apply the project management methodology & discipline, which is key to success in most compartments of companies and organisations. The course is illustrated by real-life projects in which the instructor is involved personally at IBM.

- **Employment law and social security law (12 h)**
  This class aims at providing students with an overview of French employment law and social security law. In employment law, a distinction must be made between individual and collective relationships. Regarding individual relationships the employment contract (unlimited term and fixed-term) is scrutinized together with the circumstances in which a dismissal procedure must be carried out. Turning to collective relationships, the different types of personnel representatives will be studied together with their respective functions. Negotiation of collective agreements will be scrutinized as well as the working hours: legal working hours and overtime. Litigation before the industrial tribunals will be examined in detail: the functions and organization of industrial tribunals, and preparation and presentation of cases before the tribunals. In social security law, French social security contributions will be covered, as well as social security inspections and associated litigation.

Detailed program

1) **International enterprise project management (24 h)**

- What is a project? What is an IEPM?
- Project phases / Critical Success Factors
- Teams and Roles / Communication Management
- Proposal project / Workplan / Business plan /
- Work Breakdown Structure / Estimating / Planning
- Risk Management /Contracting
- Project Execution / Launching the project rollout
- Cross management / Controlling / Managing organisation changes
- Communication plan / Control book
- Managing project changes / Reviews / Project Close out
- Managing Troubled projects
- Intellectual Capital Management
2) Employment law and social security law (12 h)

- Employment law
  - Individual relationships:
    Employment contract (hiring, collective bargaining agreement, specific clauses of the employment contract, different types of employment contract: fixed-term contracts, unlimited term contracts, fulltime contracts, part-time contracts).
    Employment relations: disciplinary procedures, professional evaluations, vacation pay indemnity, Dismissals: individual/collective; for personal or economic reasons, final settlement agreement.
    Litigation before the industrial tribunals and court of appeal.

  - Collective relationships:
    Elections of personnel representatives (personnel delegates, work committee, health and safety committee, trade unions).
    Collective agreements.
    Working hours, Compulsory and voluntary profit share plans.

- Social security law
  Social security contributions.
  Social security inspections.
  Litigation before the social security tribunals and court of appeal.
S4-UE 1 : Scientific Computing for Mechanics (5 ECTS) - 25h courses and 25h exercises

Description

The aim of the course is to understand how to apply traditional and advanced numerical methods to different problems in Fluid and Solid Mechanics. Which numerical method will be more suitable to apply to a specific problem?

Examples of numerical simulations of problems arising from Fluid and Solid Mechanics up to fluid-structure interaction applications arising in Civil Engineering will be given as illustrations or as student project.

The aim of this course is to approach numerical methods from a problem solving perspective, and to solve problems arising from academia or industry applications from Fluid and Solid Mechanics up to fluid-structure interaction applications. The goal of this course is to enhance problem solving skills for students, and to allow students to join research laboratories in academia or in industry. Indeed, students can join research and development teams that share interest in developing numerical software, or specific numerical tools in software in order to solve real life problems for different applications in Fluid and Solid Mechanics up to fluid-structure interaction applications arising in Civil Engineering.

Detailed program

- **Part 1 (10h)**
  - Introduction to Continuum Mechanics in fluid and Solid.
  An Introduction of equilibrium and conservation equations in Mechanics for fluid and structure materials will be developed for the students to understand the link between mathematical equations and mechanical phenomena.

  - **Numerical Simulation for problems in Mechanics**
  Different Numerical formulations, Lagrangian, Eulerian and ALE (Arbitrary Lagrangian Eulerian) used for fluid and structure mechanics will be presented.

  - **Workshop for simulation fluid and solid problems**
  Students will be presented to simulation software used for industrial applications. The goal of the workshop is to setup problems, (mesh, loading) for fluid and structure applications.

- **Part 2 (20h)**
  - Introduction to direct numerical simulation (DNS) of Navier Stokes equations for turbulent flows in simple geometries (periodic domain, channel, boundary layer)
  - Introduction to subgrid scale modelling (LES) for turbulent incompressible flows.
  - Learn how to use a parallel code for the simulation of incompressible homogeneous isotropic turbulence, implementation of a subgrid scale and validation of Large Eddy Simulation (LES) by comparison with equivalent DNS.

- **Part 3 (20h)**
  The traditional discretisation methods such as finite differences, finite volumes and finite elements offer spatial errors decaying algebraically with the mesh refinement. Moreover, these methods suffer from numerical defects like dissipation and dispersion errors that affect the prediction capabilities of the simulation software packages. Higher order method, like Legendre Spectral elements bring their exponential rate of convergence combining high-order accuracy with the geometrical flexibility of finite elements. In computational fluid dynamics, direct numerical simulation traditional(DNS) and large eddy simulation (LES) of turbulent flow demand a careful numerical treatment, as sharp boundary layers may
develop and increase the overall stiffness of the numerical problem. For simple geometry like cavity flow, the numerical tool consists of a Chebychev collocation spectral. Both high order methods are reviewed, together with velocity-pressure decoupling techniques (including Uzawa, projection or influence matrix methods) which are the bottleneck for an efficient and accurate simulation of the incompressible flow. Several illustrations are given in term of DNS or LES of laminar to turbulent incompressible flow. Several projects are proposed: Burgers equations, use of 2D Chebychev Collocation Navier-Stokes code applied to the lid-driven cavity flow problem or to dipolewall impact,…

S4-UE2 : Scientific Computing for Electromagnetic Field Computation (5 ECTS) - 25h courses and 25h exercises

Description

This teaching unit can be split into three knowledge:
Propagation uncertainties in numerical models
Studies models continuous and discrete describing electromagnetic phenomena
Modeling of ferromagnetic materials

This course enable students to understand the numerical methods used in models describing the electromagnetic phenomena in low frequency. During the course, specific lectures required to understand and to program such methods are given. The student has to program his own numerical model during a project.

Detailed program

- Studies of continuous and discrete models describing electromagnetic phenomena (10h)
  Continuous domain
  Introduction to tonti’s diagramm
  Formulations in potential
  Discret domain
  Introduction of Whitney’s complex
  Discretization laws of behaviour
  Equation’s systems to solve

- Uncertainties propagation (10h)
  Basics in Probability theory
  General presentation of methods of propagation of uncertainties
  Introduction to Monte Carlo Simulation Method
  Introduction to Spectral approach to take into account uncertainties
  Programming in a Finite Element Code in electromagnetism
    - Ferromagnetic materials Modelisation (4h)
      Basics in magnetism
      Hysteresis phenomenon in ferromagnetic materials
      Modelling of the behaviour law
    - Computing Exercise (24h)
      Implementation of program to compute magnetic fields through the finite element method
      Account for uncertain behavior laws
**S4-UE3 : Scientific Computing for Bioinformatics (5 ECTS) - 25h courses and 25h exercises**

**Description**

Molecular biology is currently undergoing a revolution due to new sequencing technologies. This results in the availability of a large body of genomic data, such as complete genomes, transcripts, metagenomes, ... Achieving accurate analyses in those terabytes of data requires a good combination of efficient algorithms with suitable architectures. The lecture will present some key problems in biological sequence analysis together with high performance computing solutions that have been developed in this context.

**Detailed program**

- The world of bioinformatics data
- Sequence algorithms: alignment, pattern matching, indexing structures
- Parallel solutions and implementation: multicore, GPU, reconfigurable architectures, ...
- Success stories and open problems.

**S4-UE4 : From Modeling to Numerical Simulation (5 ECTS) - 25h courses and 25h exercises**

**Description**

The aim of the course is to study mathematical questions arising in other sciences:
- modelling, hierarchy of models,
- mathematical analysis, existence and uniqueness of solutions,
- development of numerical methods, analysis
- implementation, simulation

In practice, the difficulties will come from the complexity of physical problems: coupling, nonlinearity, ...

The choice of the problems studied in this course may vary from one year to the next. Student following this module will acquire the skills of an applied mathematician: modeling, mathematical analysis, choice of numerical methods. The non linear coupling and the multi-scale characteristics of these problems provide difficulties for the numerical simulation. Some solutions will be presented in order to overcome these difficulties.

**Detailed program**

- Sample topics that may be addressed:
  - Bose-Einstein condensates: stationary and time-dependent Gross-Pitaevskii equation, systems of equation for multi-species BEC, imaginary time and gradient Sobolev methods, splitting techniques and spectral methods.
S4-UE5 : Scientific Computing for Computer Science (5 ECTS) - 25h courses and 25h exercises

Description

Applying the notions studied in Supercomputing and in Mathematical Tools for Simulation to a real problem from computer science. Providing to the student a sufficient knowledge to permit him/her to interact with the domain specialist in his/her future jobs.

Given a grid implementation problem of an algorithm belonging to the computer science domain studied in this UE, the student will be able to identify the issues to overcome, to estimate the performance improvements to expect and to carry out the implementation.

Detailed program

The problem to be studied may vary every year.
The following applications are considered:

- Exact real solving of zerodimensional polynomial systems, root isolation, interval arithmetic, system simplification. Applications to the topological analysis of algebraic curves, computer assisted conception and bifurcations analysis in dynamical systems.
- Multi-criteria optimisation.

S4-UE6 : Scientific Computing for Non Linear Optics and Photonics (5 ECTS) - 25h courses and 25h exercises

Description

Initiation to analytical methods and presentation of recent developments of mathematical tools necessary in modelling photonic and nonlinear optical phenomena.

Methods for numerical integration of equations appearing in nonlinear optics will be introduced.

This course enables students to understand the basis of the nonlinear optics. The student has to master the modelling of the linear and/or nonlinear optical problems. He also must be able to perform a linear stability analysis and to characterize the critical situations. Finally, he has to develop numerical codes devoted to scientific computing according to specific physical problems he encountered.

Detailed program

Acquisitions of detailed knowledge of the theories, the mechanisms and the recent developments of the Radiation-Matter interaction. From Maxwell equations, we derive fundamental models of non linear optics. The originality of this course is to show that, under reasonable assumptions, it is possible to reduce these equations to universal models. We shall study more specifically an application in photonics (photonic crystal fibers for their numerous technological applications) that leads to linear and/or non-linear universal Schrödinger equation. The second part is devoted to the presentation of advanced numerical methods allowing finding, in particular, nonlinear solutions that can not be obtained analytically. This enables us to highlight the crucial role of scientific computing in the resolution of modern physical problems.
S4-UE7 : Scientific Computing for Optimization (5 ECTS) - 25h courses and 25h exercises

Description

Initiation to optimization. Modeling and solving complex discrete and continuous optimization problems. From continuous to discrete optimization for difficult optimization problems (non convex, non linear, NP-hard). This course enables students to understand some advanced tools of continuous and discrete optimization. The student has to master the modelling and solving tools of difficult optimization problems (graph theory, mathematical programming). Finally, he has to design and implement optimization algorithms to solve complex optimization problems.

Detailed progam

- Continuous non-linear programming
- Discrete non-linear programming
- Graph theory
- Global optimization
- Multi-objective optimization
- Discrete optimization
  - Exact algorithms: branch and bound, dynamic programming
  - Metaheuristics: evolutionary algorithms, local search, ...
- Parallel distributed optimization (using Cuda, MPI and PThreads)

S4-UE8 : Scientific Computing for Material Science (5 ECTS) - 25h courses and 25h exercises

Detailed progam

- Introduction to material modelling at the atomic scale (why, what, how...)
- Part 1 : Molecular static
  Force field, quantum mechanics, energy calculations, minimization algorithms-steepest descent, Newton, conjugate gradient
- Part 2 : Molecular dynamic
  Force field integrator, motion equations, thermostat - barostat
- TP : Practical applications
  Crystal structure calculations, periodic boundary conditions, elastic properties, point defect diffusion, stress field in complex crystal