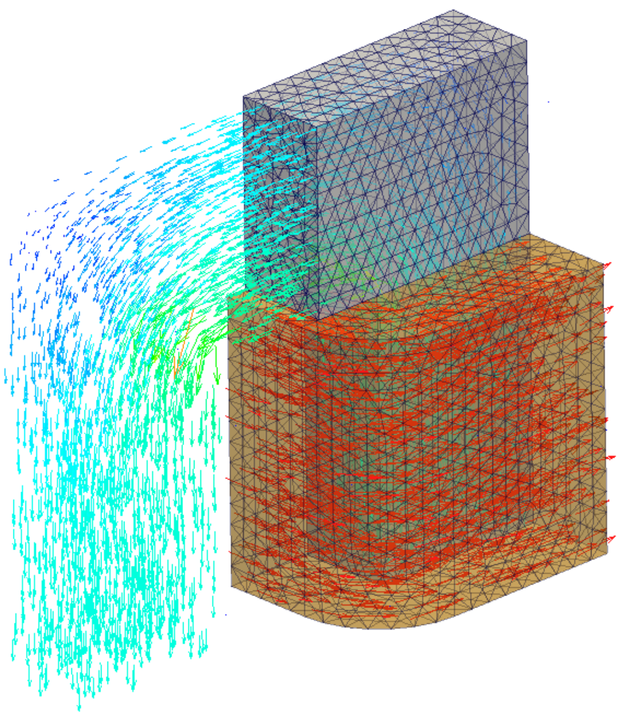
FACULTÉ DES SCIENCES ET TECHNOLOGIES
Département Mathématiques

Université de Lille

MASTER 2 Science, Technology, Health
MASTER 2 Sciences, Technologies, Santé

Mention Mathematics and applications

Advanced Scientific Computing



ACADEMIC YEAR 2024 – 2025

https://sciences-technologies.univ-lille.fr/les-departements-de-formation/mathematiques/

PRESENTATION

DESCRIPTION

This Master degree in Mathematics and applications, specialized in scientific computing, from Lille offers a top rate international interdisciplinary training year in high performance computing for numerical simulations. It is proposed for postgraduate students who wish to specialize in modelling, numerical simulation and supercomputing.

ACADEMIC STAFF

The academic staff in charge of the master is composed of distinguished Researchers and Professors from 5 laboratories and research institutions (CNRS, INRIA…) located at Villeneuve d'Ascq – Cité scientifique campus. We also welcome seminars 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 the MesoNet supercomputer from the regional data center located at University of Lille as well as to the Slices.fr/Grid'5000 computational grid of several thousands of processing cores located at 9 geographically distributed sites.

CAREER PROSPECTS

- Fully qualified engineers or research and development engineers in various sectors such as automotive 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 Hauts-de-France 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
There are opportunities for Excellence grants (see p. 5).

COURSE MODULES 2024 - 2025

SEMESTER 3

Basics tools and soft skills	**Prerequisites**	**2 courses to be chosen among the following 3 :** - Computer systems, algorithms and computation - Introduction to numerical methods - Modelling	9 ECTS
		English (self training)	
	Seminar	Seminar and workshop BAIP	3 ECTS
High profile skills	**Mathematical tools for simulation**	Finite element methods, finite volume methods, project in PDE	9 ECTS
	Supercomputing	Supercomputing, project	9 ECTS

SEMESTER 4

Scientific computing applications	**2 practise courses in scientific computing to be chosen in the following fields (only 2 practise courses will be offered each year)**	Machine learning and optimization for scientific computing	6 ECTS
		Scientific computing for electrical engineering	6 ECTS
		Scientific computing for mechanics	6 ECTS
		Scientific computing for parallel numerical linear algebra	6 ECTS
		Scientific computing for material sciences	6 ECTS

Internship	**Internship in company or research laboratory**	4 to 6 months	18 ECTS

CONTACTS

PROFESSORS IN CHARGE :

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ADMISSION

ADMISSION CRITERIA

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

APPLICATION

Information on the application procedure is available on the University of Lille website:
https://www.univ-lille.fr/etudes/candidater/

LANGUAGE PROFICIENCY

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

EXCELLENCE GRANTS

9.000€ per year will be allotted to the most deserving applicants. Master 2 fellowships are funded by LABEX CEMPI (http://math.univ-lille1.fr/~cempi/).

The deadline to apply for grants is attached to **February 15th.**

COURSE DETAILS

2024 – 2025

- **S3 : Computer Systems and Algorithms (4 ECTS) – 40h CTD**

Description

The main goal of this lecture is to provide to the students the knowledge and skills of the C language. As this language is the main langage used to implement operating systems, this will enable the student to see the link between algorithmic (programming) and the computer they're using (more precisely a single processor in the context of this lecture). As a consequence, the student will also get used to UNIX operating systems.

Program

Quick survey on the UNIX operating system and command line operations.

Programming in C (basics, separated compilation – including using a makefile, structures, pointers and dynamic allocation).

Short overview on how the filesystem / processor are dealt with on UNIX.

Acquired skills

Basic knowledge on UNIX operating system, makefile and programming in C, and Understanding how a processor is working.

Exam and grades

An exam mark (Exam/ 20) and one or more practical project(s) for a second mark (PP / 20), applying the formula MARK = (Exam + PP) / 2.

- **S3 : Introduction to numerical methods (4 ECTS) – 40h CTD**

Description

Acquire the theoretical and practical backgrounds for the numerical approximation of ODEs and PDEs using standard numerical methods.

Program

1) Resolution of linear systems: direct methods, iterative methods

2) Finite difference method for usual linear PDEs: introduction to PDEs, principle of the finite difference method, application to Poisson and heat equations in 1D.

3) Finite element method for elliptic linear PDEs: variational formulation and Lax-Milgram theorem, variational approximation and convergence study, algorithmic implementation in 1D of Lagrange P1 finite elements.

Acquired skills

Numerical analysis of ODEs and PDEs, functional analysis basic tools, practical implementation using Python.

Exam and grades

Two exam marks (Exam 1 / 20 and Exam 2 / 20) applying the formula MARK = (Exam 1 + Exam 2) / 2

- **S3 : Modelling (4 ECTS) – 40h CTD**

Description

The student must be able to extract mathematical models from physical phenomena. Starting from the basic Newton model, how to generalize it to continuous media leading to the Navier-Stokes equations. Same problem with the Schrödinger or Maxwell equations.

Program

Algebra and vector analysis, kinematics of the continuous medium (velocity, material derivative, acceleration, ...), dynamics of the continuous medium (conservation principles (mass, momentum, kinetic moment, energy, Cauchy stress tensor and its properties), simple laws of behavior of fluid and solid, Stokes and Navier-Stokes equations.

Acquired skills

Continuous medium mechanic modelling, modelling of "simple" fluids or solids.

Exam and grades

Written exam (theoretical questions, and kinematics and dynamics exercises).

- **S3 : Seminar (2 ECTS) – 14h TD**

Description

A series of 5 seminars, given by professionals and/or researchers, will be offered to the student during the first semester. The goal is to let him/her get started with 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.

Acquired skills

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.

Exam and grades

The student will be asked to write a report on one seminar.

- **S3 : Mathematical tools for simulation (9 ECTS) – 40h courses and 20h exercises**

PART 1 : Finite Element Methods

Description

This course is concerned with the theoretical and practical aspects of the numerical approximation of elliptic/parabolic PDEs using Finite Element Methods.

Program

Mathematical pre-requisites: Hilbertian analysis and convex optimization; Sobolev spaces (trace theorem, duality, Poincaré inequalities)

Content:

Variational formulation of elliptic PDEs: strong/weak solutions; derivation of a variational formulation; well-posedness (coercive case; Lax-Milgram); equivalence with the strong form; treatment of different types of data (variable coefficients, homogeneous/non-homogeneous cases) and boundary conditions (pure Dirichlet, pure Neumann, mixed-type, Robin-type)

Variational approximation of elliptic problems: internal approximation; matricial viewpoint; Céa's lemma; general convergence theorem

Finite elements: definition of a FE (unisolvence, shape functions); reduction/reconstruction/interpolation operators; stiffness/mass matrices

Lagrange FE in 1D: algebraic realization (quadrature formulas, static condensation); convergence theorems (interpolation, duality techniques)

Lagrange FE in 2D/3D: barycentric coordinates; algebraic realization (assembly procedure, cubature formulas); convergence theorems (interpolation, mesh regularity)

Approximation of parabolic problems: diagonalization of the heat operator; Euler/FE time/space schemes (explicit and implicit versions); convergence theorems; CFL condition; mass lumping; implementation

Implementation of 1D Lagrange FE in Matlab/Octave

Project in C/C++ (2D, use of Gmsh)

Acquired skills

Numerical analysis of PDE's, practical implementation of Finite Element Methods using C++.

PART 2 : Finite Volume Methods

Description

Acquire the theoretical and practical backgrounds for the numerical approximation of (systems of) PDEs (of hyperbolic, elliptic, or parabolic types) using Finite Volume Methods.

Program

Content :

Modelling of transport and propagation phenomena: derivation of scalar conservations laws and of wave equations.

Modelling of diffusion, transport and propagation phenomena: derivation of scalar conservations laws

Finite Volume methods for conservation laws : Lax-Friedrichs, Lax-Wendroff, Godunov and Roe schemes, implementation and numerical analysis.

Finite volume methods for elliptic and parabolic problems: implementation and numerical analysis.

Acquired skills

Numerical analysis of PDE's, practical implementation of Finite Volume methods using Python, C++.

PART 3 : Project

Description

Acquire the theoretical and practical backgrounds for the numerical approximation of (systems of) PDEs (of hyperbolic, elliptic, or parabolic types).

Program

This unit consists in a project using both Finite Volume and Finite Element methods.

Acquired skills

Ability to understand a model based on Partisal Differential Equations and to derive and implement numerical methods for PDE's using C++. Ability to assess the efficiency and correctness of these implementations.

Exam and grades
MARK = (Exam MARK + 2 Project MARK) /3
Project MARK = (2 Report MARK + defense MARK) /3

- **S3 : Supercomputing (9 ECTS) – 40h courses and 20h exercises**

Description

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

Program

- Overview of parallel distributed machines (shared-memory machines, distributed-memory machines, coprocessors and GPU accelerators, large-scale environments – A case study: Grid'5000).
- Parallel distributed algorithm design and programming
  - Paradigms of parallel and distributed programming (task parallelism, data parallelism, shared memory paradigm, message passing paradigm).
  - Parallel distributed programming environments and tools (OpenMP, MPI, Cuda).
- Fundamental problems of parallel distributed programming (task / data partitioning, load balancing, scheduling, fault tolerance, performance evaluation).
- Getting started with parallel machine administration through Grid'5000 (resource reservation, application deployment, monitoring, fault tolerance, etc.).
- Towards the exascale era: challenges and alternatives of massively parallel and heterogeneous programming.

Acquired skills

The student will learn how to design and implement parallel and/or distributed computing applications (using MPI, OpenMP, 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).

Exam and grades

An exam mark (Exam/ 20) and a practical project mark (PP / 20), applying the formula MARK = (Exam + PP) / 2.

- **S4 : Machine learning and optimization for scientific computing (6 ECTS) – 30h courses and 25h exercises**

Description

The student will learn the concepts of parallel optimization assisted by statistical learning. He/She will be introduced to the methods of optimization, including meta-heuristics and Bayesian optimization, their coupling to machine learning and their parallelization. Engineering simulation will be considered as a field of application and experimentation.

Program

- General introduction
- Statistical learning models (reminder on statistics, Metamodels - Gaussian Processes, Neural Networks)
- Statistical learning–assisted Optimization
  - Optimization methods (Gradient descent, meta-heuristics)
  - Bayesian optimization (acquisition functions, constraints handling, some basic examples, parallelization)
  - Neural Networks-assisted Meta-heuristics (evolution control mechanisms, constraints handling, some basic examples, parallelization)
- Applications of ML-assisted optimization to some problems in various fields including design engineering, image processing, etc.

Acquired skills

The student will learn to design and implement optimization methods assisted by statistical learning. He/She will also learn how to apply, test and validate them in the context of simulation engineering. He/She will also discover the existing statistical learning tools and their linkage with optimization software platforms.

Exam and grades

An exam mark (Exam/ 20) and a practical project mark (PP / 20), applying the formula MARK = (Exam + PP) / 2.

- **S4 : Scientific computing for electrical engineering (6 ECTS) – 30h courses and 25h exercises**

Description

This teaching unit is structured around three themes related to electrical engineering:

- Study of continuous and discrete models describing electromagnetic phenomena.
- Propagation of uncertainties in numerical models
- Model order reduction and error estimator applied to electromagnetic phenomena

This course enables 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/her own numerical model during a project.

Program

- Introduction of Tonti's diagram
- Formulations in potential
- Introduction of Whitney's complex
- Discretization laws of behaviour
- Equation's systems to solve

Uncertainties propagation (8h)

- 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

Model order reduction (8h)

- Linear problem: presentation of a-priori and a-posteriori methods
- Nonlinear problem: interpolation of nonlinear terms
- Presentation of Greedy learning algorithm

Error estimator (8h)

- Definition of error discretization
- Introduction to reliability and efficiency
- Presentation of residual and equilibrated estimators

Computing Exercise (22h)

- Implementation of program to compute magnetic fields through the finite element method
- Computation of error estimators
- Mini project

Acquired skills

In this course, the necessary course complements will be given to understand and program such methods. During the project, the student will then be led to program his/her own numerical model.

Exam and grades

The final mark consists of two exam marks (Exam1/20 and Exam2/20) and a practical project mark (PP/20), applying the formula MARK = (Exam1 + Exam2 + PP) /3.

- **<u>S4 : Scientific computing for mechanics (6 ECTS) – 30h courses and 25h exercises</u>**

Description

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

2) Examples of numerical simulations of problems arising from Fluids Mechanic and applications arising will be given as illustrations or as student project.

Program

PART 1

During this course we will be interested in the specificities of the simulation of turbulent flows. After a short introduction to the statistical tools necessary to study these flows, the student will see different numerical methods relying on this statistical description.
The course will give an introduction to various classical methods as Direct Numerical Simulation (DNS), Reynods-Averaged Navier Stokes (RANS) , Large Eddy Simulation (LES), Detached Eddy Simulation (DES), hybrid LES-RANS and unsteady RANS.
During the lectures the theory will be discussed and during the practice sessions on computer simple fortran and python codes will be used in order to gain detailed insight in various numerical and modeling aspects.
The aspects related to the parallelization of the codes will also be addressed within the framework of the implementation of a DNS or LES code in order to make the best use of the capacities of the supercomputers.

PART 2

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 projets are proposed : Burgers equations, use of 2D Chebychev Collocation Navier-Stokes code applied to the lid-driven cavity flow problem or to dipole-wall impact,...

Acquired skills

The aim of this course is to approach numerical methods from a problem solving perspective, and to solve problems arising from applications of Fluids Mechanic and 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 Fluids Mechanic.

Exam and grades

An exam mark (Exam/ 20) and a practical project mark (PP / 20), applying the formula MARK = (Exam + PP) / 2.

- **<u>S4 : Scientific computing for parallel numerical linear algebra (6 ECTS) – 30h courses and 25h exercises</u>**

Description

The students will learn and master a classical method in data science, and apply it to a financial problem. They will also learn how to strongly reduce the computation time on modern HPC architectures : multicore CPUs and GPUs.

Program

This lecture presents parallel numerical methods illustrated on the following financial problem: determine the principal tendencies of a group of market shares during a time period.

The principal component analysis (PCA) will be presented and computed to solve the above problem.

Computations will involve the standard numerical algebra librairies BLAS/LAPACK, and will be deployed on a CPU-GPU cluster. Different approaches on CPU will be investigated: pure MPI (multiprocess) programming, MPI+Thread programming, with serial or multithreaded BLAS. The GPU performance impact will also be studied.

A large amount of time will be dedicated to programming and making experiments: in the end, the students will implement a complete software for analyzing market shares evolution.

Acquired skills

Knowledge of the PCA and eigenvalues computation methods, knowledge of basic numerical algorithms, application of multicore, distributed, and GPU computing to a real case problem.

Exam and grades

An exam mark (Exam/ 20) and a practical project mark (PP / 20), applying the formula MARK = (3PP + Exam) / 4.

- **<u>S4 : Scientific computing for material sciences (6 ECTS) – 30h courses and 25h exercises</u>**

Description

Computational methods are extensively used in various domains in physics and chemistry.

In particular, modeling at the molecular scale enables to describe processes that can very fundamental or global. Simulations can be carried out on systems studied experimentally but also under extreme conditions that are difficult to handle in laboratories. The goal of the unit is to give an overview of popular computational methods that are used in materials science.

Program

Numerical optimization, molecular dynamics, Monte carlo, machine learning in molecular modeling.

Acquired skills

Knowledge in simulation approaches and their specificities. Acquire the theoretical and practical basis of molecular modeling. Being able to differentiate the methods and their domains of application

Exam and grades

Report and oral presentation