Numerical Methods for Engineering Applications
S8 - EN1800KA – 2015/2016

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A. COURSE TEAM

Name	Organization	Position
Léo Cunha Caldeira Mesquita	CentraleSupélec, Laboratoire EM2C, CNRS	PhD student
Nicolas Dumont	CentraleSupélec, Laboratoire EM2C, CNRS	PhD student
Ronan Vicquelin	CentraleSupélec, Laboratoire EM2C, CNRS	Maître de Conférence
Aymeric Vié	CentraleSupélec, Laboratoire EM2C, CNRS	Maître de Conférence

B. OBJECTIVES

Numerical simulations of physical phenomena have become inevitable. Indeed, on the one hand, benefiting from computational resources in the 21st century is common practice. On the other hand, due to the increasing complexity and transdisciplinary of practical engineering systems, no analytical solutions are available and the cost of experimental investigations becomes prohibitive. Therefore, engineers in charge of the design of such systems have no choice but to rely on numerical simulations.

The course objectives are:

. Understanding of standard numerical methods
. Applications of these methods in problem-solving workshop
. Critical analysis of simulations results

Combining their skills in computer science, heat transfer, fluid mechanics, mathematical analysis and numerical methods, the students will write their own programs from a blank page and answer a couple of practical engineering problems such as:

- Find the optimal residence time in a BioReactor.
- Identify the value and location of the maximum temperature of a heated structure.
- Risk of pollutant dispersion or flame flash-back.
- Prediction of recirculation length backwards a facing step
- …

On completion of the course, the students should spontaneously solve a simple problem with a small script to implement a numerical resolution; Formalize a physical problem into equations and identify their mathematical nature; Discretize a set of differential equations; Analyze the accuracy and stability of a numerical method; Derive an adapted numerical method in terms of accuracy and efficiency to solve the problem; Ensure the validity of the results though hypotheses checking and numerical errors characterization; Have a critical interpretation of the physical results; Solve problems found in engineering applications.

C. ORGANISATION

For students following the course as a S8 elective, it is organized the following way:

- 8 lectures,
- 14 problem-solving workshop.
- 4 projects to be realized during the course period

For students following the ECP+R program, the course is organized as follows:

- 5 lectures,
- 6 problem-solving workshop.
- 3 projects to be realized during the course period

Lectures will give the fundamental notions of the course while workshop sessions will aim at a direct application of the course contents.

The mandatory tool for the course is a personal computer with a working installation of Python.

The program is detailed in the following pages, including the time line, course contents, and problems of interest during workshops. Homework is required to acquire and understand all the necessary skill as well as to finalize the projects.

D. DETAILED PROGRAM

Lecture 1: Finite Differences

A1	**Wednesday, 30th March, 2016**	**11h30**
Introduction	Importance of numerical methods in today's engineering and research. Program, objectives, organization, course team and work methodology.	90 mn
Lecture	Introduction to numerical methods. Hierarchical methodology to numerically solve engineering problems. Examples of PDE. Classification of PDE. Numerical approximation with finite differences.	
Pause		15 mn
B1-1		**14h00**
	Introduction to Python • Syntax, program execution and use of modules • Plotting results in 1D/2D/3D • Test of quadrature formula and root-finding algorithms	90 mn
Pause		15 min
B1-2		**15h45**
	Problems • Derivation of arbitrary order finite difference approximations • Verification the approximations' order using Python code • Explicit Euler method applied to an Ordinary Differential Equation	
End of the lecture		**17h15**

Key elements	• Writing python's code and using appropriate libraries • Being able to derive arbitrary order finite difference formulae • Quantifying errors and validating a finite difference method

Lecture 2: Ordinary Differential Equations (ODEs)

A2	**Wednesday, 6th April, 2016**	**14h00**
Lecture	Notion of modified wave number for finite difference schemes. Time-marching method to solve Ordinary Differential Equations. Forward Euler method. Local and Global convergence order. Numerical stability analysis. Explicit vs Implicit methods. Backward Euler method. Trapezoidal method. Linearization of implicit methods. Stiffness	90 mn
Pause		15 mn
B2		**15h45**
	Problems • Harmonic oscillator • Non-linear ODEs • Characterization of errors	90 mn
End of the lecture		**17h15**

Homework	• Project #1 to be finalized within one week	

Key elements	• Applying classical methods to solve ODEs • Evaluating the global and local errors • Characterizing the accuracy and stability of a specific method • Handling the stiffness of a system

Lecture 3: Elliptic PDE (1)

A3	**Wednesday, 13th April, 2016**	**11h30**
Lecture	Runge-Kutta (RK2, RK3, RK4) and multi-step methods (Adams, BDF) for ODEs. Examples of elliptic PDE. Direct vs iterative methods. Jacobi and Gauss-Seidel methods. Ghost cells for boundary conditions.	90 mn
Pause		15 mn
B3-1		**14h00**
	Problems • Jacobi and Gauss-Seidel methods applied to a Poisson equation • Laplace equation with different boundary conditions	90 mn
Pause		15 min
B3-2		**15h45**
	Project #2	
End of the lecture		**17h15**

Homework	• Project #2 to be finalized within 3 weeks	

Key elements	• Using high order methods for ODEs • Using direct and iterative solvers for elliptic problems • Choosing the appropriate methods for boundary conditions

Lecture 4: Elliptic PDE (2)

A4	**Wednesday, 4th May, 2016 (ECP+R : Monday, 2nd May, 2016)**	**14h00 (8H00)**
Lecture	Effect over over-relaxation with the SOR method. Conjugate gradient method. Notions on preconditioning, multi-grid and Krylov methods.	60 mn
Pause		15 mn
B4		**15h15**
	ECP+R : Wednesday, 4th may, 2016	**11H30**
	Problems • Application of SOR and conjugate gradients • Multi-block structured meshes and block iterations • Project #2	120 mn
End of the lecture		**17h15**

Homework	• Project #2 to be finalized for the next lecture	

Key elements	• Using efficient iterative methods (SOR, conjugate gradient) • Being able to handle different boundary conditions • Building a multi-block algorithm

Specific planning for ECP+R students

A4	**Monday, 2nd may, 2016**	**8h00**
B4	**Wednesday, 4th may, 2016**	**11h30**

Lecture 5: Explicit methods for Parabolic and Hyperbolic PDEs

A5	**Wednesday, 11th May, 2016**	**14h00**
Lecture	Examples of Parabolic/Hyperbolic PDEs. Stability analysis with semi-discrete form, Von Neumann analysis, modified wavenumber. CFL criterion in convection problems. Fourier criterion in diffusion problems.	90 mn
Pause		15 mn
B5		**15h45**
	Problems • Unsteady heat equation • Advection equation	90 mn
End of the lecture		**17h15**

Homework	• Project #3 to be finalized for lecture 7	

Key elements	• Using finite differences to solve parabolic and hyperbolic problems • Analyzing the stability of a finite difference scheme for hyperbolic and parabolic equations

Lecture 6 : Characterization of numerical errors

A6	**Friday, 13th May, 2016**	**14h00**
Lecture	Notions of dispersion and dissipation of numerical schemes. Modified PDE and interlink with the behavior of the numerical solution. Centered schemes, Lax-Wendroff and Lax-Friedrich schemes. Order of convergence, Lax theorem.	90 mn
Pause		15 mn
B6		**15h45**
	Problems • Analysis of different numerical schemes (order, stability, consistency) • Impact of the CFL number on dispersion and dissipation • Use of Fast Fourier Transform	90 mn
End of the lecture		**17h15**

Key elements	• Analyzing the consistency, stability and convergence of different numerical methods • Implications of the dispersive and dissipative nature of numerical schemes. • Using adapted tools to properly quantify dispersion and dissipation errors.

Lecture 7 : Implicit methods for multi-dimensional parabolic PDEs

A7	**Wednesday, 25th May, 2016**	**14h00**
Lecture	Highlight role of Fourier number in stiffness of parabolic PDEs. Implicit methods for stiff and/or multi-dimensional problems. Thomas algorithm. Crank-Nicolson method. Matrix factoring and ADI methods.	90 mn
Pause		15 mn
B7		**15h45**
	Problems • 1D unsteady heat equation with implicit method • 2D unsteady heat equation: Comparison between explicit and implicit methods. Crank-Nicolson vs ADI. • Steady solutions : comparison between unsteady parabolic solver and elliptic solver.	90 mn
End of the lecture		**17h15**

Key elements	• Using implicit methods to avoid time step limitation of explicit methods • Applying it to multi-dimensional stiff problems • Computing a steady solution through an accelerated transient solution.

Lecture 8: Methodology in numerical computations

B8-1	**Friday, 27th May, 2016**	**14h00**
	Problems • Finalize ADI implementation to 2D unsteady heat equation • Application of hierarchical solving methodology to a study case	90 mn
Pause		15 mn
B8-2		**15h45**
		90 mn
End of the lecture		**17h15**

Key elements	• Controlling the different interacting elements leading to the numerical resolution of an engineering problem: Problem setup, mathematical model, numerical resolution, mesh convergence, post-processing, hypotheses verification, validation, physical analysis. • Critical analysis of numerical results

Lecture 9: Incompressible Flow equations

A9	**Wednesday, 1st June, 2016**	**14h00**
Lecture	Unsteady incompressible Navier-Stokes equations for the velocity and pressure fields. Role of pressure in the incompressible limit. Pressure/velocity coupling. Explicit formulation.	90 mn
Pause		15 mn
B9		**15h45**
	Problems • *Flow in a driven cavity with explicit method*	90 mn
End of the lecture		**17h15**

Key elements	• Identifying the structure of the NS equations • Understanding the role of the pressure which fulfils a Poisson equation to enhance the continuity equation. • Implement an explicit collocated method for NS in a cavity flow

Lecture 10: Semi-implicit method for incompressible flows

B10 -1	**Friday, 3rd June, 2016**	**14h00**
	Semi-implicit for diffusion operator, predictor-corrector. Problems • *Flow in a driven cavity with semi-implicit method*	90 mn
Pause		15 mn
B10-2		**15h45**
	Problems • *Flow in a driven cavity with semi-implicit method*	90 mn
End of the lecture		**17h15**

Key elements	• Being able to implement a semi-implicit method for cavity flow • Using previously presented algorithms (ADI, Conjugate gradient, …)

Lecture 11: Final project

B10 -1	**Wednesday, 8th June, 2016**	**14h00**
	Final project on incompressible flows	90 mn
Pause		15 mn
B10-2		**15h45**
	Methodology rules applied to the final project	90 mn
End of the lecture		**17h15**

Key elements	• Synthetizing all the numerical methods presented in the course • Using them appropriately to solve a full CFD problem with incompressible Navier-Stokes equations

E. EXAMINATION

The course examination is done through 4 projects to realize during the course:

- 2 small projects to be handed out within a week
- 2 comprehensive projects as mid-term and final examinations.

All deliverables are to be handed out as slides.

F. Online resources

Claroline

Prerequisite

The prerequisites of the courses correspond to the common core of the 1^{st} year at CentraleSupelec:

- Differential and integral calculus;
- Vector and matrix analysis;
- Programming in Python
- Heat and mass transfer

Notions in fluid mechanics are not required but are appreciated.