

Project presentation

Programming Concepts in Scientific Programming
EPFL, Master class

November 19, 2018

Rules

1. Project realized in groups of **two** students
2. Delivery on c4science (Sources and report): Deadline **Friday 14th December 2018, 14h**
3. CMake build system
4. Inline documentation of your code (Doxygen)
5. Test suite
6. Make a small report **per group** (4 pages) can be though as an extended README:
 - ▶ how to compile the program
 - ▶ typical program execution (the flow) and usage
 - ▶ List of features
 - ▶ List of tests
 - ▶ TODOs and perspectives
7. Make one oral presentation **per student**
 - ▶ the structure of the program
 - ▶ list of features
 - ▶ limitations and problems

What is important in the evaluation:

- ▶ The code
 1. must be compiling
 2. should be clean (coding convention)
 3. should have inline comments (and Doxygen)
 4. must have validating tests
 5. The git log entries/comments must be understandable
- ▶ The report should describe:
 1. the implementation in a concise way
 2. the validating tests
 3. the limitations and problems

Project 1: Linear systems

Implementation of direct and iterative methods for the solution of linear systems

- ▶ Mandatory: Direct methods: LU and Cholesky
- ▶ Mandatory: Iterative methods: Conjugate Gradient, Jacobi, Gauss-Seidel, Richardson
- ▶ Optional: Preconditioners, implementation of the Preconditioned Gradient and Preconditioned Conjugate Gradient methods

Project 2: Eigenvalue problems

Implementation of numerical methods for eigenvalue computation.

- ▶ Mandatory: Power and Inverse power method.
- ▶ Mandatory: Implementation of Power and Inverse power methods with shift
- ▶ Optional: Implementation of the QR method

Project 3 and 4: Ordinary Differential Equations

- ▶ The first project focuses on scalar **ODE**, with generic non-linear function:

$$y'(t, x) = f(t, x)$$

- ▶ The second focuses on vectorial ODEs, only using a linear function:

$$y'(t, x) = f(t, x) = A * x + g(t)$$

Description:

- ▶ The implementation of explicit methods, such as **Forward Euler** and the multistep **Adams Bashforth** (up to 4 steps) is mandatory for both projects.
- ▶ The implementation of the implicit **Backward Euler method** is mandatory for the scalar ODE project.
- ▶ Optional: implementation of **Runge-Kutta methods** and/or **Backward Differentiation Formulas** (BDF schemes) and/or multistep **Adams-Moulton**.

Project 5: Non-linear systems

Implementation of numerical methods for the solution of nonlinear equations.

- ▶ Mandatory: consider a scalar nonlinear problem and implement the bisection, aiten, chord, newton and fixed point methods.
- ▶ Optional: extension to systems of nonlinear equations solved by the Newton and/or modified Newton method.
- ▶ Sources: [here](#) for the Newton's, chord and bisection method, and [here](#) for the fixed point method.

Project 6: Data approximation

This project deals with interpolation and data fitting.

- ▶ Mandatory: implement numerical methods such as polynomial approximation and piece-wise polynomial approximation for the solution of interpolation problems.
- ▶ Mandatory: For the data fitting, the least squares method has to be implemented.
- ▶ Mandatory: input data by reading file
- ▶ Optional: Fourier approximation of periodic data.
- ▶ Sources: see Chapter 3 of the book Scientific Computing with MATLAB and Octave (Quarteroni, Saleri) for the description of the methods. It can be downloaded [here](#).

Project 7: Numerical Integration

Implementation of methods for the numerical computation of integrals in one or two dimensions.

- ▶ Mandatory: A simple geometrical domain can be considered (square, rectangle) and the first step consist in generating grids which can be structured.
- ▶ Optional: extension to more complex shaped domain.
- ▶ The numerical integration has to be carried out by the implementation of the following methods: Midpoint/Trapezoidal/Cavalieri-Simpson.
- ▶ Sources: see Section 4.2 of the book Scientific Computing with MATLAB and Octave (Quarteroni, Saleri) for the description of the methods. It can be downloaded [here](#).

Project 8: Image/sound processing

This project deals with the treatment of images or sound

- ▶ Mandatory: Computation of intensity **histograms**
- ▶ Mandatory: Implementation of the **discrete Fourier transform** with the **Fast Fourier Transform** algorithm for 1D or 2D. (Find the algorithm at [here](#))
- ▶ Mandatory: Contour extraction of an image or noise removal
- ▶ Optional: filtering image/sound (By using the Fourier transform)

Project 9: Monte Carlo

This project deals with the statistical study of non-linear operators

- ▶ Mandatory: Implement random number generators following a **probability distribution** for the **normal** and the **uniform** distributions
- ▶ Mandatory: Computing numerically the **expectation value** of a user defined function
- ▶ Mandatory: Visualization of **statistical moments**
- ▶ Mandatory: Verification of the **central limit theorem**