Methods for Numerical Computing

# Introduction

The purpose of this course is to teach basic programming techniques required for scientific computing and engineering. These skills can be applied to the development of computational modelling applications. The researcher spends a significant amount of time analysing the results of both laboratory and computational experiments. Very often such analyses will require the researcher to develop routines applying different numerical methods to the data sets.

There are many different tools and libraries for developing computational models and for data analysis. These libraries and tools encapsulate many of the basic techniques reviewed in this course. However, very often, it is useful to have a good understanding of the basic underlying numerical methods. The following topics are considered.

1. Finding the root of an equation
2. Numerical integration
3. Numerical differentiation
4. Interpolation
5. Solution of differential equations
   1. Euler method
   2. The Runge-Kutta method
   3. The shooting method
6. Optimisation
   1. Comparing the Steepest Descent Simulated Annealing Methods
   2. Genetic Algorithms
7. A Study of Wave Propagation
   1. Characteristics of Wave Phenomena
   2. Beats and Interference
   3. The Vibrating String
   4. The Vibrating Membrane
   5. The Shallow Water Wave Equation
   6. The Van der Pol Oscillator
   7. The WKB Method
   8. Partial Wave Analysis for Quantum Mechanical Scattering

For each of these sections the following programming techniques are considered

1. Finding the root of an equation

Basic programming techniques

1. Numerical integration

Conditional and repeating programming structures

1. Numerical differentiation

Programming units, functions

1. Interpolation
2. Solution of differential equations

Basic file input and output

1. Optimisation

Putting it all together programming case studies

1. A Study of Wave Propagation

Further programming case studies with an emphasis on visualisation

# Finding the Root of an Equation

# Numerical Integration

# Numerical Differentiation

# Interpolation

# Solution of Differential Equations

## Eulers-Method

## The Runge-Kutta Solver

## The Shooting Method

# Optimisation

## Comparing the Steepest Descent Simulated Annealing Methods

A case study looking at the optimisation of interactions of atomic interactions modelled using the Lennard-Jones 6-12 potential

## Genetic Algorithms

# A Study of Wave Propagation

## Characteristics of Wave Phenomena

## Beats and Interference

## The Vibrating String

The Lax-Wendroff Solver solving partial differential equations and introduction to numerical stability.

## The Vibrating Membrane

## The Shallow Water Wave Equation

## The Van der Pol Oscillator

Entrainment and limit cycles

## The WKB Method

## Partial Wave Analysis for Quantum Mechanical Scattering