



$$\int_a^b f(x) dx \approx \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right],$$
$$\int_a^b f(x) dx \approx \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right].$$
$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$
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```
while abs(x_old-x) > 10^-3 && x ~= 0
    x_old = x;
    x = x - (x^3 - 0.512*x^2 + 2.443*10^-4)/(3*x^2 - 1.024*x);
    iter = iter + 1;
    fprintf('Iteration %d: x=%20f, err=%20f\n', iter, x, x_true-x);
    pause;
end
```

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    pause;
end
```

PHYS4017 Numerical Methods

Course Information Guide 2023-24

1 Course Details

Lecturers:	Dr. J. Taylor	Schedule:	18 lectures, Tues 10am, Thurs 10am; labs – Mon pm
SCQF Credits:	10	ECTS Credits:	5
Assessment:	Examination (75%) Coursework (25%)	Co-requisites:	None
Level:	Honours	Prerequisites:	Physics 2
Typically Offered:	Semester 1		

2 Course Aims

This course is an elective for third year Physics, Theoretical Physics and Designated Degree programmes and is available as an elective to most single honours students in fourth and fifth years (excluding Chemical Physics) in the School of Physics & Astronomy. It aims to provide students with an opportunity to develop their knowledge and understanding of the key principles and applications of numerical methods, and their relevance to current developments in physics. In particular, it will provide a working knowledge of:

- Interpolation and extrapolation;
- Numerical integration;
- Random numbers;
- Root finding;
- Minimising and maximising functions and data analysis;
- Fast Fourier transform;
- Integration of ordinary differential equations;
- Partial differential equations.

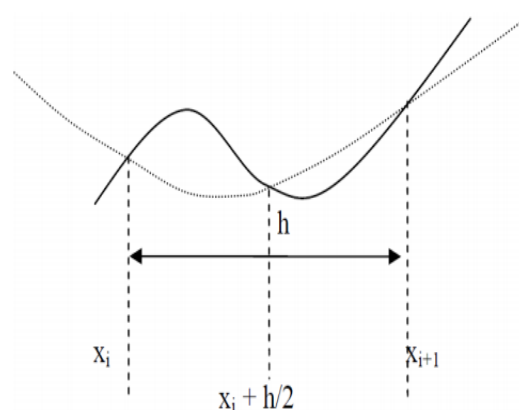


Figure 1: Illustrating Simpson's rule

3 Intended Learning Outcomes

By the end of the course students will be able to:

- Demonstrate knowledge and a broad understanding of numerical methods;
- Describe qualitatively and quantitatively process, relationships and techniques relevant to the topics included in the course outline, and apply these techniques to solve general classes of problems;
- Write down and, where appropriate, either prove or explain the underlying basis of physical laws relevant to the course topics, discussing their applications and appreciating their relation to the topics of other courses taken.

4 Course Outline

Interpolation and extrapolation: Polynomial interpolation. Splines. Smoothing data.

Numerical integration: Simple methods for equally spaced nodes; e.g. Simpson's rule and the effect of step size. Gaussian quadrature. Examples from Physics of integrals that cannot be determined analytically.

Random numbers: Generation of random numbers with normal, Poisson and other distributions. Simulation of data with a random error. Monte-Carlo methods for integration and simulations.

Root finding: Bracketing and bisection methods. Secant method etc. Solution of non-linear systems of equations. Examples from Physics of equations without an algebraic solution; e.g. from quantum mechanics, solving the bound states of one, two and three dimensional square wells and, from waves, the solution of the normal modes of strings with awkward boundary conditions.

Minimising and maximising functions and data analysis: Brief description of common techniques used for the minimising of a function with more than one parameter. Fitting data by minimising chi-squared. The special case of linear parametrisations. Error matrix and the calculation of the errors for the fitted parameters.

Fast Fourier transform: The FFT. FFT of real functions, sine and cosine transforms. Data sampling, aliasing etc. The FFT in signal processing.

Integration of ordinary differential equations: Simple methods - e.g. Euler. Step size errors. Runge-Kutta methods. Adaptive step size. Stiff equations. Numerical solution of differential equations in the Python programming language. Boundary value problems including two point boundary values. Examples of the numerical solution of differential equations from Physics and elsewhere; e.g. from dynamics, the solution of the motion of a spinning top and of a freely rotating body in three dimensions; from waves, the normal modes of a hanging rope with and without a mass at the end.

Partial differential equations: Types of PDEs; elliptic, parabolic and hyperbolic with examples from physics. Finite difference methods. Relaxation methods for boundary value problems.

5 Further Information

Further information can be found on the course Moodle page and also using the links below:

- [Course specification](#)
- [Reading list](#)

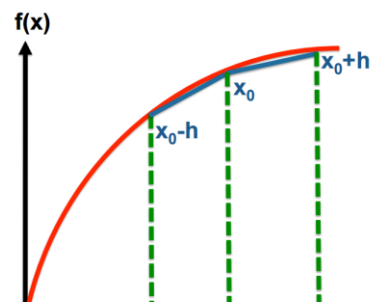


Figure 2: Illustrating the central difference method