Class One
Computational Physics
Kigali Institute of Science and Technology

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Welcome to **Computational Physics**! Here are some details about the class:

1. There will usually be a short homework assignment due every week at the beginning of class on Thursday.
2. The first assignment will be due December 22.
3. I have shipped from the U.S. around ten textbooks that you can use.

Why learn computational physics?

1. Computers are necessary to do physics calculations that are too hard or long for people to do.
2. Knowing how to use computers to solve complicated problems is a *very* valuable skill in physics and elsewhere.
3. Teaching a computer to solve problems is a good way to deepen your understanding of physics and math.
4. Learning to write programs is excellent intellectual training.

Course Goals: I want you to learn how

1. to construct and analyze algorithms.
2. to implement algorithms in Matlab.
3. to use good programming practices.
4. to use Matlab's built-in functions.
5. to translate physics problems into computational problems

The main topic today is **Finding Roots** of a function. The statement of the problem is: given $f(x) = 0$, solve for x. Seems easy, right? If $f(x) = 7x^2 + -4x + -10$, then the problem is not too hard. We just use the quadratic formula.

But if $f(x) = 40x^5 - 33x^4 - 18x^3 + 4x^2 - 2x + 13$, then the problem is difficult. There does not exist an algebraic formula for finding the roots of polynomials fifth order and higher. This is an example of a fairly simple problem for which we have no choice but to find a solution numerically. Today we will learn two techniques for solving problems like this.

Bisection Method: Suppose I am thinking of a number, not necessarily an integer, between 0 and 100. What efficient strategy might you use to guess the number? The bisection method uses this strategy to find the root of a function.

Let's illustrate this with a simple example: $f(x) = -x^2 + 3600$. We don't need a computer to solve this, of course. But this example will be good to work through so that we can follow all the step. We will work through this example in class.

Let ϵ_i be the error, or uncertainty, at step i in this process. We then see that:

$$\epsilon_{i+1} = \frac{\epsilon_i}{2} . \tag{1}$$

The error is halved every step. We say that the convergence is *linear*, since the error at the next step is a linear function of the current error.

Algorithms that converge linearly are slow. Think how long it would take to guess a number between 0 and 100 if you needed and accuracy of six decimal points.

Netwon's Method Let $M(d)$ be the money on your cell phone as a function of the day d. Suppose it is currently day y and you have 4000 Frs and you use are currently using 800 Fr a day. On what day to you expect to run out of money?

We will work through this example in class. Thinking about how you solve this problem is the key step in Newton's method. The idea is, start with a guess x_0 near where you think the root is. Calculate the line tangent to $f(x)$ at x_0. Use this to estimate the root. This process leads to the following formula:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} . \tag{2}$$

Let's work through the first couple steps of applying Newton's method for $f(x) = -x^2 + 3600$. Let's choose $x = 40$ as our first guess. We will work through this in class.

We see that Newton's method is quite fast. It gets close to the correct answer much faster than the bisection method. This makes sense. In Newton's method we are using our knowledge of $f(x)$ to make smarter guesses. Specifically, we use the slope of $f(x)$ to make guesses for where $f(x) = 0$.

One can show, using a Taylor expansion, that successive errors for Newton's method are given by

$$\epsilon_{i+1} = -\epsilon_i^2 \frac{f''(x_i)}{2f'(x)} . \tag{3}$$

Thus, the convergence of Newton's method is *quadratic*. The error at the next step is a quadratic function of the error at the current step. Thus, ϵ_i gets small quickly.

Taylor Series: Finally, a reminder about Taylor series. A differentiable function $f(x)$ is approximated near $x = a$ by

$$f(x) \approx f(a) + (x-a)f'(a) + (x-a)^2 \frac{f''(a)}{2!} + (x-a)^3 \frac{f^{(3)}(a)}{3!} + \cdots . \tag{4}$$

This is one of the most useful and amazing formulas in all of mathematics.

Summary:

1. Bisection method for finding roots
2. Newton's method for finding roots
3. Linear vs. quadratic convergence