

Chapter 1:

1.1 Radioactive Decay

- Many nuclei are unstable (like ^{235}U which has a small probability for decaying into two nuclei of approximately half its size)
 - $(dN_U/dt) = -N_U/\tau$ is the behavior governed by differential equations where $N_U(t)$ is the number of uranium nuclei that are present in a sample at time t
 - τ is the “time constant” for decay
 - $N_U = N_U(0)e^{-t/\tau}$ where $N_U(0)$ is the number of nuclei present at $t = 0$

1.2 A Numerical Approach

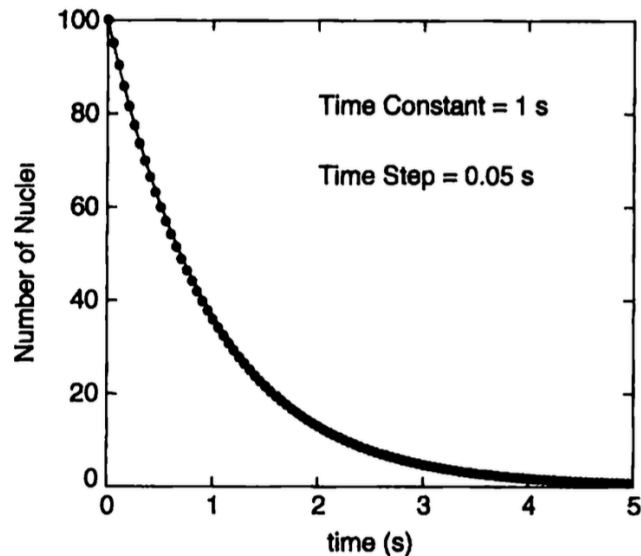
- N_U should be obtained as a function of t
 - Taylor expansion:
 - Given that Δt is small, then we can determine:
$$N_U(\Delta t) = N_U(0) + \frac{dN_U}{dt} \Delta t + \frac{1}{2} \frac{d^2 N_U}{dt^2} (\Delta t)^2 + \dots,$$
- The derivative of N_U evaluated at time t can be written as:
$$\frac{dN_U}{dt} \equiv \lim_{\Delta t \rightarrow 0} \frac{N_U(t + \Delta t) - N_U(t)}{\Delta t} \approx \frac{N_U(t + \Delta t) - N_U(t)}{\Delta t},$$

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- The equation above is an approximation
 - The error terms were dropped in deriving this new equation
 - We will use pseudocode along with actual code in order to see how the translation from pseudocode to an actual code can be done
 - It is important to understand code that we write as well as code written by others

1.3 Structures of Coding

- Code structure consists of (1) declaring necessary variables, (2) initializing all variables and parameters, (3) doing the calculations, and (4) storing the results
 - The code should start with a few comment statements that identify the program and tell what it is supposed to do
- Although the code will display results as numbers in a file for how N_U varies with time, we still need to understand the result
 - Best done by examining the results in graphical form (VERY ESSENTIAL)
 - Graphs should look something like the one below:



1.4 Testing Your Program

- A working program considers not only no errors in syntax or spelling but also that the output is correct
- Guidelines to debugging
 - Does the output look reasonable?
 - Is it consistent with your intuition and instincts?
 - Does your program look reasonable?
 - Check each step of every calculation leading up to the final result
 - Check that the program gives the same answer for different values such as “step sizes”
 - The final answer should be independent of the values of parameters such as the time-step variable

1.5 Numerical Considerations

- Issues with numerical errors is central to the computational solutions of any problem
- You need to choose the best algorithm for a particular problem
 - How to estimate the numerical errors associated with the algorithm is very important
- With a radioactive decay program, errors were introduced by the approximation used to estimate the solution of the differential equation
 - Also produced by finite numerical precision in any programming language
 - Round-off errors
 - Time was treated as a discrete variable
 - Converted the differential equation into a difference equation
 - Allows us to compute estimates for N_U at the discrete times $n \cdot \Delta t$ where n is an integer

- Always check that the calculated result converges to a fixed value as the step size is made smaller
 - Make sure that your step size is a reasonable value

1.6 Programming Guidelines and Philosophy

- Program structure: use subroutines to organize the major tasks and make the program more readable and understandable
 - The main program for the decay problem was basically an outline for the program
 - Subroutines or functions should be used when they are no more than a few lines of code or are required repeatedly
- Use descriptive names: choosing names of variables and subroutines according to the problem will make it easier to follow
 - Built in comment statements also make the code more understandable
 - Explain the program logic and describe the variables
- Sacrifice everything for clarity: compact code may occasionally run faster but it is a less reliable indication of computational efficiency
 - Compact code will always have a cost in terms of clarity and readability