Homework Assignments

All homework assignments (reports + programs) have to be submitted by e-mail before the deadlines (have physics 811 in the subject line). A carbon copy of the report has to be in the instructor's mailbox (department of physics) or given in class before the due day and time.

All submitted programs have to have a good description and be self-explanatory as possible

Example

```
/* ---------------------------------------------------------------
  John Doe              Physics 811          September 25, 2008
  Assignment # hw 05
  Integration by trapezoid rule of f(x) on [a,b]
  Method: trapezoid rule
  ---------------------------------------------------------------
  Input:
    f - Function to integrate
    a - Lower limit of integration
    b - Upper limit of integration
    n - number of intervals
  Output:
    r - Result of integration
  Compiler: Dev C++
  Comments:
  -------------------------------------------------------------*/
```

Homework 0.1: Warming up – no grades (Due on Thursday, September 10, 2009 by 13:30)

1 In classes that you took earlier you met problems that were difficult, or impossible to solve analytically. Suggest three problems that are interesting ones to solve with a computer. Describe physics and equations needed to solve these problems. Explain why you need computational physics in these cases.

2 Install a C/C++ compiler or Fortran, or Java on your computer (if you don't have one). Remember that later you may select a different compiler. See the list of available compilers on the web page. http://www.odu.edu/~agodunov/computing/lib_soft.html

Homework 0.2: More warming up – no grades (Due on Thursday, September 17, 2009 by 13:30)

3 Write a program to solve the quadratic equation $ax^2 + bx + c = 0$ by using the quadratic formula to obtain roots. Your program should also be capable to handle complex roots.

4 Write a program that calculates a series of Fibonacci numbers and checks which ones are prime numbers. Test your program on the first 25 Fibonacci numbers.

5 Write a program that calculates the values of the Legendre polynomials using the recurrence relation $(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0$ where $P_0(x) = 1$ and $P_1(x) = x$ Test your program on available analytic solutions for specific values of n or x . What is the largest n when you can still use the recurrence relation? (a very helpful reference: "Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables" by Abramowitz, M. and Stegun, I.A.)

Homework 1.0: Nonlinear equations (Due on Thursday, September 24, 2009 by 13:30)

For this homework you may use programs from the course web page However it is strongly advised to write (at least to try) your own programs.

1 Solve the following equations by the closed domain methods (bisectional method and the false position method), and open domain methods (the Newton's method and/or the method of secants).

$f(x) = x + \cos(x) = 0$ on [-10.0, +10.0]

$f(x) = \exp(x) - x\sin\left(\frac{\pi x}{2}\right) = 0$ on [-5.0, -2.5] (try also [-5.0, +5.0])

$f(x) = x^3 - 2x^2 - 2x + 1 = 0$ on [0.0, +2.0]

2 Find all real roots of the following equations using the brute force method (with closed or open domain methods inside)

$x^4 - 6x^3 + 12x^2 - 36x - 18 = 0$ on [-10.0, +10.0]

$f(x) = \exp(x) - x\sin\left(\frac{\pi x}{2}\right) = 0$ on [-10.0, +10.0].

3 Solve the following systems of two nonlinear equations using Newton's method

$$\begin{cases} \cosh(x) - y = 0 \\ x^2 + y^2 = 2 \end{cases}$$

$$\begin{cases} x^2 + y^2 = 2x + y \\ 0.25x^2 + y^2 = 1 \end{cases}$$

4 Consider a one-dimension quantized system, namely a finite square well with U(x)=-U_0 for |x|<a, and U(x)=0 for |x|>a. Solutions can be found from the following nonlinear equations

for even states $\sqrt{U_0 - |E|}\, tg\sqrt{2m(U_0 - |E|)\, a^2/\hbar^2} = \sqrt{|E|}$

for odd states $\sqrt{U_0 - |E|}\, ctg\sqrt{2m(U_0 - |E|)\, a^2/\hbar^2} = -\sqrt{|E|}$

In textbooks these equations are solved graphically. Find numerically solutions for a few lowest bound states using closed or open domain methods for some U_0, m, a that you need to define.

Homework 2.0: Numerical differentiation (Due on October 1, 2009 by 13:30)

5 Write a program that implements Newton difference polynomials of orders 1, 2, and 3 on equally spaced data (2, 3, or 4 data points accordingly) to evaluate first and second derivatives. Consider the number of points as an input parameter. You may need to do some analytic work first to derive equations.

6 Study the quality of numerical differentiation using following functions in n uniform points in [0.0,4.0] interval.

$f(x) = \sin(x)$

$f(x) = \exp(x)$

Compare the errors and ratios of the errors for the two sets of n (let's say n and 2n). Find the difference between results for 3 and 4 point polynomials used for numerical differentiation.

7 Using Taylor series approach derive following equations for numerical differentiation f(x) at point x_i

$$f_x = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2\Delta x} - \frac{1}{3} f_{xxx}(\zeta)\Delta x^2$$

$$f_x = \frac{-11f_i + 18f_{i+1} - 9f_{i+2} + 2f_{i+3}}{6\Delta x} - \frac{1}{4} f_{xxxx}(\zeta)\Delta x^3$$

$$f_x = \frac{f_{i-2} - 8f_{i-1} + 8_{i+1} - f_{i+2}}{12\Delta x} + \frac{1}{30} f_{xxxx}(\zeta)\Delta x^4$$

$$f_{xx} = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} - \frac{1}{12} f_{xxxx}(\zeta)\Delta x^2$$

$$f_{xx} = \frac{-f_{i-2} + 16f_{i-1} - 30f_i + 16f_{i+1} - f_{i+2}}{12\Delta x^2} + \frac{1}{90} f_{xxxxxx}(\zeta)\Delta x^4$$

Homework 3.0: Ordinary differential equations: 1D particle motion (Due on October 9, 2009 by 13:30)

One-dimension motion of a particle satisfy a differential equation of the form

$$m\frac{d^2x}{dt^2} + f\left(\frac{dx}{dt}, x, t\right) = 0$$

where m is the particle's mass, and the function f may depend on time as well as particle's velocity and position.

1 List as many as you can physics problems that can be described by the equation above. Specify forces (equations) acting on an object.

2 Write a program that numerically solves an initial value problem for the equation above using the 4-th order Runge-Kutta method.

3 Study (numerically) a simple harmonic motion of a particle mass m=1.0 on a spring with k=1.0.

$$m\frac{d^2x}{dt^2} + kx = 0$$

Check conservation of energy of the system. Find (numerically) the period of oscillations. Compare your numerical results to analytic solutions.

4 Consider the vertical motion of a particle with air resistance.

$$m\frac{d^2y}{dt^2} = -mg - 0.5C\rho A\frac{dy}{dt}\left|\frac{dy}{dt}\right|$$

Where C is a drag coefficient (dimensionless constant), ρ is the air density, A is the projectile cross section (area).

Suppose an object (select any) is thrown vertically upward with an initial velocity. How does the time of ascent compare to the time of descent if air resistance is taken into account? The initial velocity should be fast enough (but realistic) to observe effects of air resistance.

Find numerically the terminal speed for a skydiver (use textbooks or the Web to find proper values of the coefficients A and C). Compare your results with known solutions.

Homework 4.0: Numerical integration (Due on October 26, 2009 by 13:30)

1. Derive the Newton-Cotes formulas for polynomial of degree n=4 (and, optional, for n=5 too)
2. Write a program that calculate an integral with a given integrand f(x) in the region [a, b] by one of the Newton-Cotes rules with n>1 (Simpson's 1/3 rule, or Simpson's 3/8, Milne or higher). (examples from the lecture notes, or from the C++/Fortran library page may help).
3. Evaluate following integrals

$$\int_0^{\pi/2} \cos(x)dx$$

$$\int_0^1 \frac{4}{x^2+1}dx$$

$$\int_0^{2\pi} \sqrt{x}\cos(12x)dx$$

$$\int_0^{\infty} \frac{\sqrt{x}}{x^2+1}dx$$

   using your program, and as many other approximations as you want.
   Getting experience with quanc8.cpp or quanc8.f is highly recommended (you may find both programs on the course web page).
4. Evaluate numerically 2-D integrals

$$\int_0^1\int_0^1 (x+y)^2 dxdy$$

$$\int_0^1\int_0^{\sin(x)} \frac{x^2}{y^2+2}dxdy$$

5. Extra credit. Write a program that calculates an integral from f(x) in the region [a, b] using Gauss quadratures for 12 points or 24 points (the lecture notes have an example for 8 points). Coefficients for Gauss quadratures (up to 96 points) can be found in Abramowitz and Stegun "Handbook of Mathematical Functions", or on the web. Calculate the integrals in the part 3, and study the efficiency and accuracy of the Gauss method for these integrals.

Homework 5.0: Systems of linear equations & eigenvalue problem (Due on December 3, 2009 by 13:30)

Solve either problems 1,2 or 3,4.

1. Write a program that solves a system of linear equations using Gauss elimination (with scaling and partial pivoting). As a starting point you may use the programs Gauss_2.f90 from the course program library.
2. Apply the program to solve following system

$$\begin{bmatrix} 1 & 3 & 2 & -1 \\ 4 & 2 & 5 & 1 \\ 3 & -3 & 2 & 4 \\ -1 & 2 & -3 & 5 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 9 \\ 27 \\ 19 \\ 14 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 2 & -2 & 2 & 1 \\ 2 & -4 & 1 & 3 \\ -1 & 3 & -4 & 2 \\ 2 & 4 & -3 & -2 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 7 \\ 10 \\ -14 \\ 1 \end{bmatrix}$$

3. Write a program that computes all eigenvalues of a real symmetric matrix using Jacobi method. As a starting point you may use the program Jacobi.f90 from the course library.
4. Apply the program to computer eigenvalues (and eigenvectors if you can) for the following matrix

$$\begin{bmatrix} 18 & 6 & 4 \\ 6 & 10 & 3 \\ 4 & 3 & 12 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 2 & 3 \\ 2 & 2 & -2 \\ 3 & -2 & 1 \end{bmatrix}$$