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Advanced Computational Science
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Serie 6 Ausgabe: March 31, 2009 Abgabe: April 6, 2009

Guidelines

▷ Submission: Submit a written or typed report with your answers and graphics.

▷ Code: Send your source code (and makefile) to the TA of your session. Use "[ACS] Homework5" in the subject of your email.

▷ Credit: Your report should list all the contributors.

▷ Bugs: Print-outs of your source code are *not* required in your report, unless you have bugs. Help us give you partial marks.

▷ Deadline: Assignments have to be handed in at the beginning of the next exercise session.

Exercise 1 (20 points) Finite Difference Schemes (paper and pencil)

The estimation of the derivative of a function is one of the most common tasks in computational science and one of the most important ones. The schemes we choose to do it will determine our accuracy, the CPU cost, and affect numerical stability.

If we work on data points that are uniformly distributed, e.g. in one dimension,

$$\begin{aligned} x_i &= x_{i-1} + \Delta x \\ f_i &= f(x_i) \end{aligned}$$

we can derive families of schemes to evaluate the derivatives $d^n f/dx^n$. One such technique is Finite Differences.

1. (5 points) Using the Taylor series of f about x_i

$$f(x + \Delta x) = f(x_i) + \frac{df}{dx}(x_i)\Delta x + \frac{1}{2}\frac{d^2 f}{dx^2}(x_i)\Delta x^2 + \frac{1}{6}\frac{d^3 f}{dx^3}(x_i)\Delta x^3 \dots ,$$

   derive the schemes for $df/dx(x_i)$ and $d^2 f/dx^2(x_i)$ which are second order accurate and symmetric about x_i.

2. (15 points) Starting from these two schemes, use Richardson extrapolation to derive fourth order accurate schemes for $df/dx(x_i)$ and $d^2 f/dx^2(x_i)$.

Exercise 2 (20 points) Multistep time integration

We consider the Ordinary Differential Equation

$$\frac{dx}{dt} = f(x, t)$$

with the initial condition $x(t = 0) = x_0$.

We design a numerical time integration that uses information from previous time steps

$$x_{i+1} = x_i + \beta_0 f_i + \beta_1 f_{i-1} + \mathcal{O}(\Delta t^3)$$

1. (10 points) Using Taylor series, solve for β_0 and β_1.
2. (10 points) Implement your scheme and apply it to the Predator-Prey models of Assignment 5.