Computational Physics (6810): Activities 7

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Activities 6 Follow-ups

Activities 7 Preview

Follow-up: First look at OpenMP (Activities 6)

- Your computer (laptop, desktop) divides its time doing different things (adding, multiplying, storing and retrieving data, . . .).
- But there are multiple processors, called “cores”, that can run different things simultaneously, or, parts of one program can run on more than one core at once.
- If quad core (for example), than in principle we can make our code run (almost) four times as fast. [Not perfect scaling $\Longrightarrow$ overhead]

How to do this in practice? $\Longrightarrow$ OpenMP [is one way]

- Identify loop(s) that can be split among processors
- Should variables be accessible by all processors (`shared`) or are distinct for each processor working on it (`private`)?
- See Activities 6 notes for an example with both private and shared variables

Other follow-ups to Activities 6

- Counting parentheses: keep a running total, adding one for each left paren and subtracting one for each right paren. Must be zero at the end and never negative. Try these:

```
1./(a + pow(b*(cos x),2.)
(2*($1)/(($2))-0.5))
(x+1.)/(sqrt(pow(x,3)) + 2.)
```

- What is encapsulation and why is it good?
  - What does it mean that the class introduces an “interface”?
  - How does class encapsulation help to reuse code?
  - How does it help with reliability? (Consider testing and then using on an unknown problem.)
  - How does it help with testing by using a different method?
- Threads versus cores. If 2 threads/core and 4 (physical) cores, can we get an 8-time speed-up? How can it be greater than 4?
- Intel compilers (see `simpson_cosint_openmp.cpp` comments). Use `module` command on Department Linux (not a free compiler!) and then `icpc` instead of `g++`.

Solving differential equations step-by-step

- Builds on numerical derivatives

$$\frac{dx}{dt} = f(x,t) \quad \text{e.g.,} \ \frac{dx}{dt} = -ax \ \text{ or } \ \frac{dx}{dt} = -bt \text{ or } \ldots$$

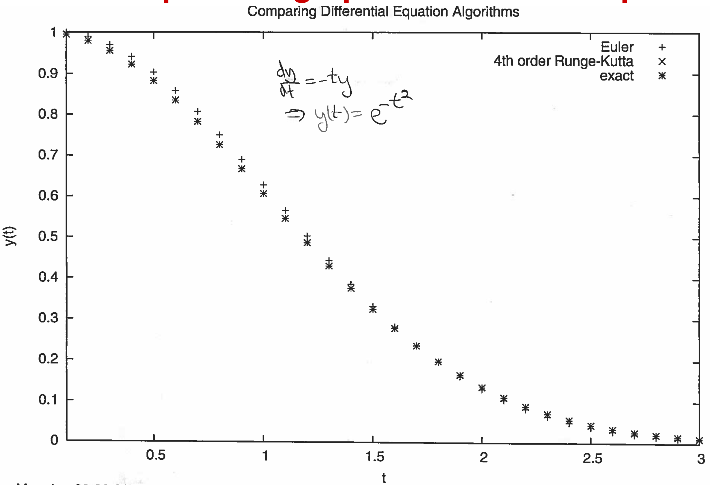
  - instruction on how to change x from one t value to a nearby one (i.e., $t + \Delta t = t + h$)
- Goal: Given $x(t = t_0)$, find $x(t = t_f)$
- Plan: the diff. eq. tells us how to take one step at a time
  $\Longrightarrow$ find $x(t_0 + h)$, then $x(t_0 + 2h)$, then $x(t_0 + 3h)$ until $x(t_f)$

$$x(t_0 + h) = x(t_0) + h \left.\frac{dx}{dt}\right|_{t=t_0} + \mathcal{O}(h^2) \ \text{ from Taylor expansion}$$

$$= x(t_0) + hf(x(t_0), t_0) + \mathcal{O}(h^2)$$

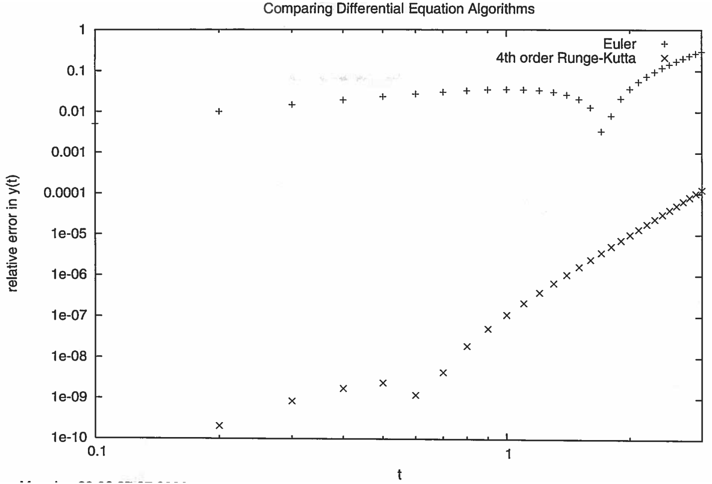
- How to do better?
  - Explore errors, other strategies, how to pick h, etc.
  - Some tricky parts: look for implementation errors if you get unexpected results

Differential equations graphs and their interpretation



- The differential equation *does not* have $y(t=0)$ on the right side.
- The approximate solution crosses the exact sometimes. What happens to the error?

Differential equations graphs and their interpretation



- You should not interpret the slope as the diff. eq. error? Why not?
- How should you look for the global approximation error here?
- What is the local vs. global error? What are the dips from?

Activities 7 Preview: Implementation of coupled equations

- $y[0]$ is not y at time $t = 0$: it is the zeroth component of a vector
- Consider Newton's Second Law:

$$\frac{d^2x}{dt^2} = \frac{F(x, v, t)}{M} ,$$

re-express as vector differential equation:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f} \quad \text{where} \quad \mathbf{y} = \begin{pmatrix} y^{(0)} \\ y^{(1)} \end{pmatrix} \quad \text{and} \quad \mathbf{f} = \begin{pmatrix} y^{(1)}(t) \\ \frac{1}{M}F(\mathbf{y}, t) \end{pmatrix}$$

if we make the definitions

$$y^{(0)}(t) \equiv x(t) \qquad \text{and} \qquad y^{(1)}(t) \equiv v = \frac{dx}{dt} = \frac{dy^{(0)}}{dt} .$$

- In the code, at each t

$$y^{(0)}(t) \longrightarrow \texttt{y[0]} \quad \text{and} \quad y^{(1)}(t) \longrightarrow \texttt{y[1]}$$

- Euler increment from t to $t + h$:

```
y[i] += h * f (t, y, i, params_ptr);
```

Activities 7 Preview: Other things to look for

- What step size h to use? See the Activities 7 notes for a discussion of how to make it *adaptive* (changes as you go to keep the error fixed)
- Period vs. amplitude: for a harmonic oscillator they are independent. But not for other potentials!
  - Energy diagrams like those used for central potentials can help you understand the observed relation
- When doing damping: make sure phase space plots are reproduced (see handout)
  - With increasing time, does the phase space trajectory go clockwise, counter-clockwise, or both?