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 $$\Rightarrow$$ overhead]

How to do this in practice? $$\Rightarrow$$ 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:
  
  \[
  \frac{1}{a + \text{pow}(b \times (\cos x), 2.)} \\
  (2 \times (\$1)/(\$2) - 0.5)) \\
  (x + 1.)/(\text{sqrt}(\text{pow}(x, 3)) + 2.)
  \]

- 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
  \[
  \frac{dx}{dt} = f(x, t) \quad \text{e.g.,} \quad \frac{dx}{dt} = -ax \quad \text{or} \quad \frac{dx}{dt} = -bt \quad \text{or} \ldots
  \]
- 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
  \[ \implies \text{find } x(t_0 + h), \text{ then } x(t_0 + 2h), \text{ then } x(t_0 + 3h) \text{ until } x(t_f) \]
  \[
  x(t_0 + h) = x(t_0) + h \frac{dx}{dt} \bigg|_{t=t_0} + \mathcal{O}(h^2) \text{ from Taylor expansion}
  \]
  \[
  = x(t_0) + h f(x(t_0), t_0) + \mathcal{O}(h^2)
  \]
- 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
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?
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:
  \[ \frac{dy}{dt} = f \quad \text{where} \quad y = \begin{pmatrix} y^{(0)} \\ y^{(1)} \end{pmatrix} \quad \text{and} \quad f = \begin{pmatrix} y^{(1)}(t) \\ \frac{1}{M}F(y, t) \end{pmatrix} \]
  if we make the definitions
  \[ y^{(0)}(t) \equiv x(t) \quad \text{and} \quad y^{(1)}(t) \equiv v = \frac{dx}{dt} = \frac{dy^{(0)}}{dt}. \]
- In the code, at each $t$
  \[ y^{(0)}(t) \rightarrow y[0] \quad \text{and} \quad y^{(1)}(t) \rightarrow y[1] \]
- Euler increment from $t$ to $t + h$:
  \[ y[i] += h \ast f (t, y, i, \text{params_ptr}); \]
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?