Computational Physics (6810): Session 1

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Course logistics

Verification and validation

Representation of floating point numbers

Overview of 6810 Computational Physics

- Each session: brief overview/recap then work through "session guide" (e.g. *6810: 1094 Activities 1*) with a partner
  - Night before class: read session *notes* ($\approx$ 10 pages)
  - Pick up new or returned activities guides
  - Each student has own computer (but talk to each other!)
  - Fill in answers and hand in at end (unless told otherwise)
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- Course info (Goggle "6810 OSU" to get to web pages)
  - Look at main web page (readings and downloads), info page (references and other course info), gameplan page
  - Instructors: Dick Furnstahl, Bryan Smith
  - Office hours: hope to use Sm1094 (stay tuned!)
  - Grade based on effort and (scaled) accomplishment
    - session sheets graded $\checkmark$, $+$, $-$; always upgradable
    - homework assignments (follow-ups to class); usually $\approx$ 4
    - independent project (more later!)
  - Carmen (Canvas) course page for scores

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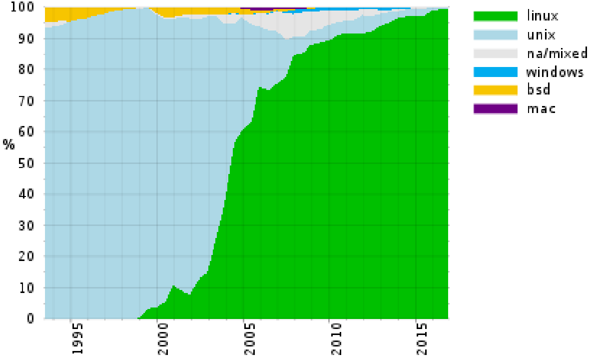
- *Questions?*

Pedagogical philosophy

- See Session 1 notes and 6810 gameplan webpage for details
- Approach: “Throw you in the water to learn how to swim”
- Like physics research: YOU have to figure things out (which means you will be confused much of the time)
- Spiral approach: keep returning to learn things incrementally
- “Just enough” detail is given (plus clues)
- Quicker to modify programs (trick is to get you to read code!)
  - identify mistakes (“bugs”) that need to be fixed
  - changes that must be made to accomplish task
- Try to predict but *always* postdict. Question authority!
- Ask about *anything* (connected to physics/computing :)

Why GNU/Linux, command-line, C++, Python, . . . ?

- Physics approach: look inside black box
- Large-scale computation uses Fortran 2008 or C++
- Python as *scripting* language (although gaining for HPC)
- Easy to segue to IDE's later (e.g., Eclipse)
- 99% of Top 500 Supercomputers (and most clusters) use Linux



Session 1 Plan: Basics we'll need this semester

- Get started with Unix command line environment on Linux or Windows/Cygwin
- Successfully download compile, run, and modify a "Hello, World!" C++ program (and some other simple programs)
- Try out *make* and use g++ warnings
- Understand how underflow, overflow, and machine precision limits can be determined "experimentally"
- Try out a program that uses a special function from the Gnu Scientific Library (GSL)
- Try out Python
- Activate BuckeyeBox account. We'll use it to hand in homework.
- Setting up your own machine: details to follow (but ask).

Verification and validation $\Longrightarrow$ Checks

- Definitions: Validation ensures that "you built the right thing". Verification ensures that "you built it right".
- Basic questions to *always* ask: "How do you know a program is working correctly? And to the accuracy it should?
- Getting an answer (no error messages) is not enough!
- Think about how to check your answer (be creative!)
  - units
  - analytic ("model") solution to compare (usually simpler case)
  - solve by another method
  - special or limiting cases
  - scaling laws [$T = 2\pi\sqrt{L/g} \Longrightarrow T$ should double if $L \to 4L$]
- Programming [see Session 1 notes and Hjorth-Jensen 1–2]
  - Use compiler to find errors (turn on all warnings)
  - Good habits $\Longrightarrow$ reliability, portability, extensibility
  - E.g., pseudocodes, comments, formatting, variable name choice, . . .

Computational math $\neq$ regular math

- Two main issues:
  - approximate representation of floating point ("with decimal points") numbers $\Longrightarrow$ only finite # of *machine numbers*
  - binary (base 2) representation
- Think about base 10 first ("Do the simple case first")
  - normalized scientific notation,
    e.g., $35.2163 \Longrightarrow 0.352163 \times 10^2$
  - general: $x = \pm r \times 10^n$ with $1/10 \leq r < 1$

  - store sign, mantissa, exponent
  - suppose we store sign, 6-digit mantissa, 1-digit exponent

$$-\frac{4}{3} = -1.333\overline{3} \approx (-1) \times (0.133333) \times 10^1$$
$$= (-1) \times (0.133333) \times 10^{[6-5]}$$

  with "bias" so we get $+$ or $-$ exponents without storing sign
- Only a finite # of numbers $\Longrightarrow$ largest, smallest

Computational math $\neq$ regular math

- Continue with decimal example: sign, 6-digit mantissa, 1-digit exponent with bias
- Largest: $0.999999 \times 10^{[9-5]} = 9999.99$ (so ≥ 10000 will *overflow*)
- Smallest $0.100000 \times 10^{[0-5]} = 0.000001$ (so 10^{-7} will *underflow*)
- Most numbers not represented exactly (cf. machine numbers)
  - $z_c = z(1+\epsilon)$ where $-\epsilon_m < \epsilon < \epsilon_m$
  - for our decimal example, $\epsilon_m \approx 10^{-6}$
  - ϵ_m is "machine precision" $\Longrightarrow$ worst case of gap
- Consequences of finite precision: no limits! (no $\epsilon \to 0$)
  - $x = 3500 = 0.35 \times 10^{[9-5]}$ and $y = 0.0021 = 0.21 \times 10^{[2-5]}$ both represented accurately
  - but $x + y = x$ (!) $\Longrightarrow$ round-off error!
  - subtraction of similar numbers is even worse
- What about derivatives, integrals, etc.?

Decimal vs. binary

- Recall how numbers are represented in decimal (base 10):

10^3	10^2	10^1	10^0		10^{-1}	10^{-2}	10^{-3}
3	1	2	4	.	1	2	3

- Analog in binary (base 2):

2^3	2^2	2^1	2^0		2^{-1}	2^{-2}	2^{-3}
1	0	1	1	.	0	1	1

- Finite decimals may not be binary machine numbers!
  - machine numbers: $5 \to 101$, $1/4 \to 0.01$
  - but what about $1/5$ or $1/3$? [answers: $0.\overline{0011}$ and $0.\overline{01}$]
  - binary long division:

$$\frac{1}{3} \longrightarrow \frac{1}{11} =$$

- What are the largest, smallest binary numbers? What is ϵ_m? (warning: IEEE standard for binary representation differs!)