#### FOCUS COMPSCI 006G Genome Revolution

**Owen Astrachan** 

http://www.cs.duke.edu/courses/cps006g/fall04

http://www.cs.duke.edu/~ola

### Where are we going?

- What is computer science?
- What is biology?
- What is computational biology?
- What is bioinformatics?
- What tools do scientists need?
- What is a scientist?

### What is **Bioinformatics**?

- Synonym?: computational biology <a href="http://www.pasteur.fr">www.pasteur.fr</a>
- The application of computational techniques to the management and analysis of biological information. <a href="http://www.informatics.jax.org">www.informatics.jax.org</a>
- Bioinformatics is a rapidly developing branch of biology and is highly interdisciplinary, using techniques and concepts from informatics, statistics, mathematics, chemistry, biochemistry, physics, and linguistics. It has many practical applications in different areas of biology and medicine. <a href="http://www.pasteur.fr">www.pasteur.fr</a>

#### What is **Bioinformatics**?

- Bioinformatics applies principles of information sciences and technologies to make the vast, diverse, and complex life sciences data more understandable and useful. Computational biology uses mathematical and computational approaches to address theoretical and experimental questions in biology. Although bioinformatics and computational biology are distinct, there is also significant overlap and activity at their interface. www.bisti.nih.gov/CompuBioDef.pdf
- Because of the great success of genome-sequencing projects, the quantity of DNA sequence data that are now available greatly exceeds the tools that are available to process those data. Consequently the analysis of those data presents one of today's great scientific challenges.

http://www.life.umd.edu/labs/delwiche/bsci348s/BioCompCareers.html

### What is Computer Science?

• Computer science is no more about computers than astronomy is about telescopes.



Edsger Dijkstra

• Computer science is not as old as physics; it lags by a couple of hundred years. However, this does not mean that there is significantly less on the computer scientist's plate than on the physicist's: younger it may be, but it has had a far more intense upbringing!



**Richard Feyneman** 

http://www.wordiq.com

#### **Scientists and Engineers**

• Scientists build to learn, engineers learn to build

- Fred Brooks



### **Computer Science and Programming**

- Computer Science is more than programming
  - > The discipline is called *informatics* in many countries
  - Elements of both science and engineering
  - Elements of mathematics, physics, cognitive science, music, art, and many other fields
- Computer Science is a young discipline
  - Fiftieth anniversary in 1997, but closer to forty years of research and development
  - First graduate program at CMU (then Carnegie Tech) in 1965
- To some programming is an art, to others a science, to others an engineering discipline

#### What is Computer Science?

What is it that distinguishes it from the separate subjects with which it is related? What is the linking thread which gathers these disparate branches into a single discipline? My answer to these questions is simple --- *it is* the art of programming a computer. It is the art of designing efficient and elegant methods of getting a computer to solve problems, theoretical or practical, small or large, simple or complex.

C.A.R. (Tony)Hoare

### **Algorithms as Cornerstone of CS**

- Step-by-step process that solves a problem
  - > more precise than a recipe
  - ventually stops with an answer
  - general process rather than specific to a computer or to a programming language
- Searching: for phone number of G. Samsa, whose number is 929-9338, or for the person whose number is 489-6569
  - > Are these searches different?
- If the phone book has 8 million numbers in it (why are there only 7.9 million phone numbers with area code 212?)
  - How many queries to find phone number of G. Samsa?
  - How many queries to find person with number 929-9338
  - What about IP addresses?

### Search, Efficiency, Complexity

- Think of a number between 1 and 1,000
  - respond high, low, correct, how many guesses needed?
- Look up a word in a dictionary
  - Finding the page/word, how many words do you look at?
- Looking up a phone number in the Manhattan, NY directory
  How many names are examined?
- How many times can 1,024 be cut in half?
  > 2<sup>10</sup> = 1,024, 2<sup>20</sup> = 1,048,576

### **Sorting Experiment: why do we sort?**

- Groups of four people are given a bag containing strips of paper
  - > on each piece of paper is an 8-15 letter English word
  - create a sorted list of all the words in the bag
  - there are 100 words in a bag
- What issues arise in developing an algorithm for this sort?
  >
- Can you write a description of an algorithm for others to follow?
  - > Do you need a 1-800 support line for your algorithm?
  - > Are you confident your algorithm works?

#### **Themes and Concepts of CS**

- Theory
  - properties of algorithms, how fast, how much memory
  - average case, worst case: sorting cards, words, exams
  - *provable* properties, in a mathematical sense
- Language
  - programming languages: C++, Java, C, Perl, Fortran, Lisp, Scheme, Visual BASIC, ...
  - Assembly language, machine language,
  - Natural language such as English
- Architecture
  - > Main memory, cache memory, disk, USB, SCSI, ...
  - pipeline, multi-processor

### Theory, Language, Architecture

- We can prove that in the worst case quicksort is bad
  - > doesn't matter what machine it's executed on
  - > doesn't matter what language it's coded in
  - unlikely in practice, but worst case always possible
- Solutions? Develop an algorithm as fast as quicksort in the average case, but has good worst case performance
  - quicksort invented in 1960
  - introsort (for introspective sort) invented in 1996
- Sometimes live with worst case being bad
  - bad for sorting isn't bad for other algorithms, needs to be quantified using notation studied as part of the theory of algorithms

### **Abstraction, Complexity, Models**

- What is an integer?
  - In mathematics we can define integers easily, infinite set of numbers and operations on the numbers (e.g.,+, -, \*, /) {...-3, -2, -1, 0, 1, 2, 3, ...}
  - In programming, finite memory of computer imposes a limit on the magnitude of integers.
    - Possible to program with effectively infinite integers (as large as computation and memory permit) at the expense of efficiency
    - At some point addition is implemented with hardware, but that's not a concern to those writing software (or is it?)
    - C++ doesn't require specific size for integers, Java does
- Floating-point numbers have an IEEE standard, it's more expensive to do arithmetic with 3.14159 than with 2

# Alan Turing (1912--1954)

- Instrumental in breaking codes during WW II
- Developed mathematical model of a computer called a Turing Machine (before computers)
  - solves same problems as a Pentium III (more slowly)
- Church-Turing thesis
  - All "computers" can solve the same problems
- Showed there are problems that cannot be solved by a computer
- Both a hero and a scientist/ mathematician, but lived in an era hard for gay people



### **Complexity: What's hard, what's easy?**

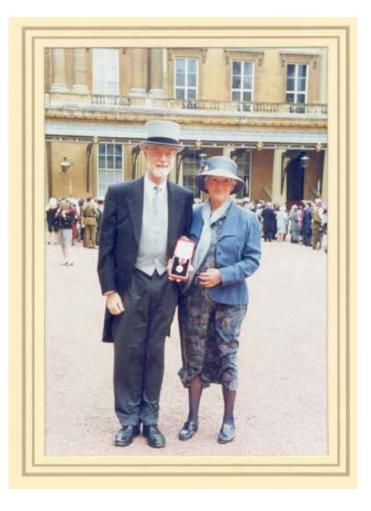
- What is a prime number?
  - > 2, 3, 5, 7, 11, 13, ...
  - > Largest prime?
- 48112959837082048697
- 671998030559713968361666935769
- How do we determine if these numbers are prime?
  - ▶ Test 3, 5, 7, ...
  - If we can test one million numbers a second, how long to check a 100 digit #?
- Why do we care?

- 671998030559713968361666935767
  is not prime, I can prove it but I can't give you the factors.
- Finding factors is "hard", determining primality is "easy"
  - What does this mean?
  - Why do we care?
- Encryption depends on this relationship, without encryption and secure web transactions where would we be?

# C.A.R. (Tony) Hoare (b. 1934)

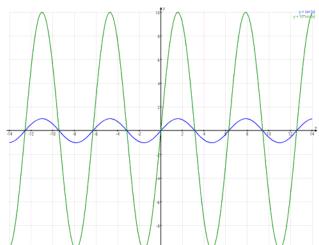
- Won Turing award in 1980
- Invented quicksort, but didn't see how simple it was to program recursively
- Developed mechanism and theory for concurrent processing
- In Turing Award speech used "Emporer's New Clothes" as metaphor for current fads in programming

"Beginning students don't know how to do top-down design because they don't know which end is up"



### What is digital?

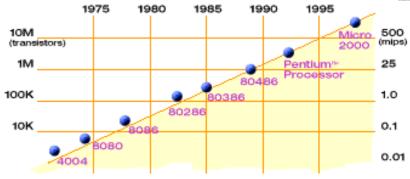
- What's the difference between
  - Vinyl LP and CD/DVD?
  - > Rolex and Timex?



- Sampling analog music for CD's
  - > 44,100 samples/channel/second \* 2 channels \* 2 bytes/sample \* 74 minutes \* 60 seconds/minute = 783 million bytes
- How does MP3 help?

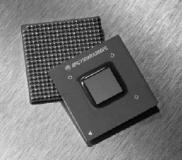
### Chips, Central Processing Unit (CPU)

- CPU chips
  - Pentium (top)
  - G4 (bottom)
  - Sound, video, …
- Moore's Law
  - chip "size" (# transistors) doubles every 12--18 months (formulated in 1965)
  - 2,300 transistors Intel 4004,
    42 million Pentium 4











Genome Revolution: COMPSCI 006G

## Why is programming fun?

What delights may its practitioner expect as a reward?

First is the sheer joy of making things

Second is the pleasure of making things that are useful

Third is the fascination of fashioning complex puzzle-like objects of interlocking moving parts

Fourth is the joy of always learning

Finally, there is the delight of working in such a tractable medium. The programmer, like the poet, works only slightly removed from pure thought-stuff.

Genome Revolution: COMPSCI 006G

**Fred Brooks**