Computer Organization and Programming for Scientific Computing

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Particulars

- Course on aspects of Computer Science necessary to achieve good performance in Scientific Computing
- Directed mostly at non CS majors who use computers extensively, but do not necessarily know how they are organized
- CS majors cannot use this as a “core” course
- Part of the Scientific Computing Certificate

Instructor

- Faculty member in computer science
- Research interests in scientific computing, machine learning, computational acoustics, fast algorithms, computer vision, etc.
  - Fluid mechanics research in a previous career
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- Office hours: by appointment via email

Prerequisites

- Undergraduate numerical methods or numerical analysis course (460 or 466)
- Background Needed
  - Linear Algebra
  - Numerical Analysis
  - Programming
    - Matlab, C/C++ and/or FORTRAN 9x
  - Experience and/or interest in scientific computing
- Participation essential!

Homework

- Will try to have it at least every other week
- Will not be excessive
- Essential for learning --- must do as opposed to just read.
- Homework handed out last class of a week.
- Due last class of next week
- Thanksgiving week no homework

Projects & Exams

- There will be a final project that will require you to implement an algorithm in a field of your choice,
  - account for 20% of the grade.
  - Demonstrate how you use knowledge of the computer to improve performance
- Project to be chosen latest by October 13.
  - If you already have a project in mind you can discuss it with us
- Exams
  - intermediate exam worth 20%, week of October 1
  - final exam worth 20%. Finals Week

Scientific Computing

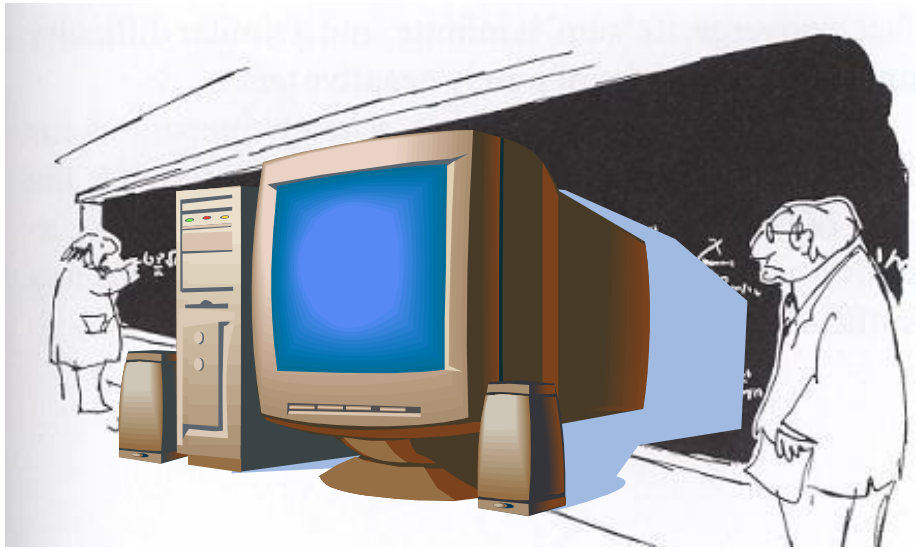
Big Picture

- Object of all science
- Efficiency and better understanding
- Scientific Method: Experiment/Hypothesis
- Now Simulation/Hypothesis

algorithms

experimentation

Algorithm: graham scan
Find rightmost lowest point; label it p_0.
Sort all other points angularly about p_0 .
    In case of tie, delete the point closer to p_0
    (or all but one copy for multiple points).
Stack S = (p_1, p_0)=(p_t, p_{t-1}) ; indexes top.
i = 2
while $i < n$ do
    if p_i is strictly left of $p_{t-1}p_t$
    then Push(p_i , S) and set $i \leftarrow i + 1$
        else Pop(S).



computation

Slide from
Chazelle, 2006

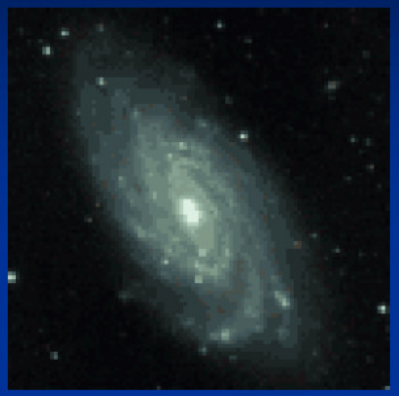
Problem Sizes Continue to Grow in all Fields

- Sensors are getting varied and cheaper; and storage is getting cheaper
- Cameras, microphones
- Text (all the newspapers, books, technical papers)
- Genome data
- Medical/biological data (X-Ray, PET, MRI, Ultrasound, Electron microscopy …)
- Climate (Temperature, Salinity, Pressure, Wind, Oxygen content, …)
- Finer detail in meshes

Google

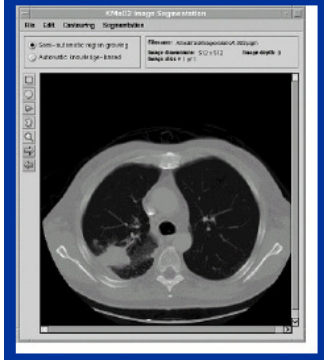
10 petabytes
(~1MG)

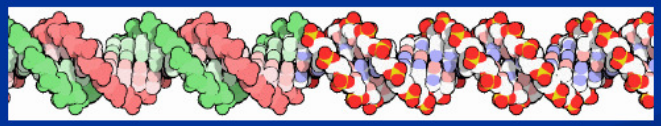
Sloan Digital
Sky Survey



10 petabytes/yr

Biomedical imaging





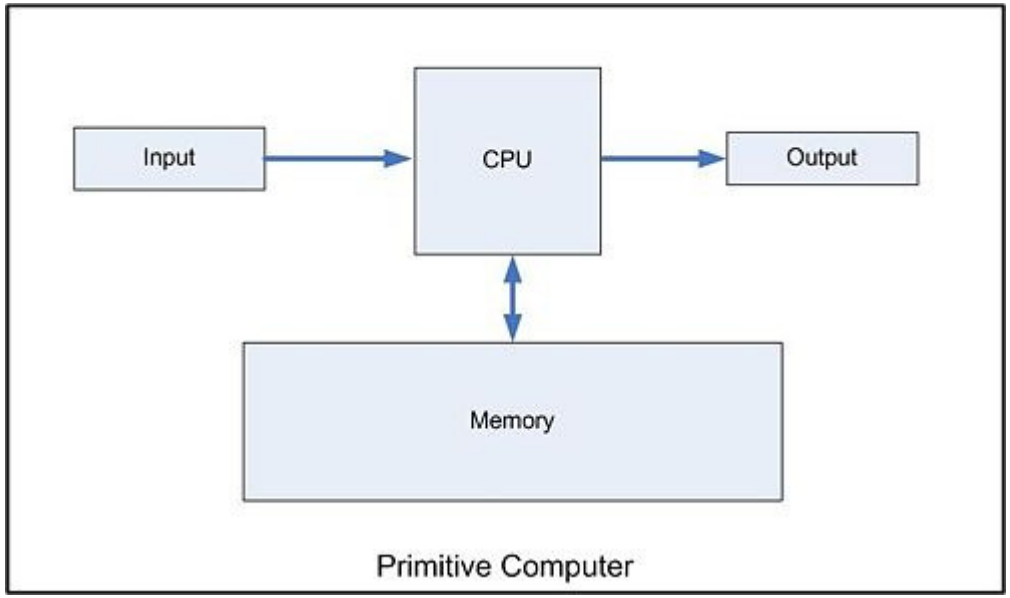
150 petabytes/yr

10,000 times the
Library of Congress

- From a 2006 talk by B. Chazelle

Good workmen know their tools

- Primitive model



Other models