Basics of Computational Physics

- What is Computational Physics?
- Basic computer hardware
- Software 1: operating systems
- Software 2: Programming languages
- Software 3: Problem-solving environment

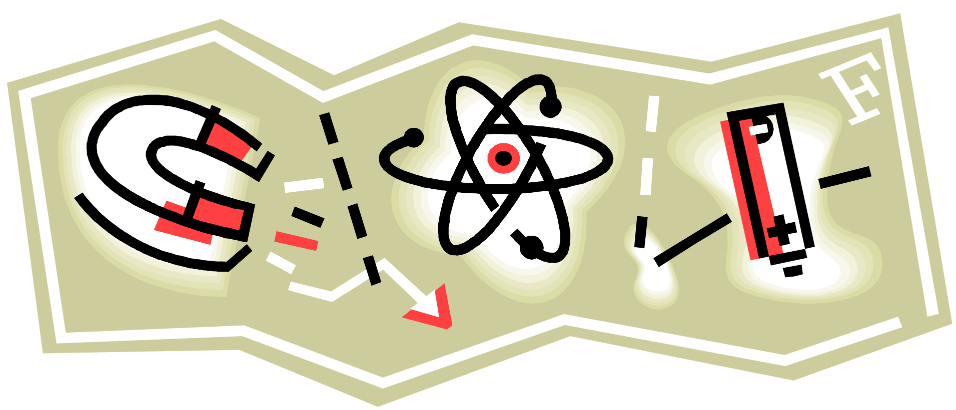
What does Computational Physics do?

- Atomic Physics studies atoms
- Nuclear Physics studies nuclei
- Plasma Physics studies plasmas
- Solid State Physics studies solids
- Computational physics does not study computers

What is Computational Physics?

"Computational physics is a synthesis of theoretical analysis, numerical algorithms, and computer programming."

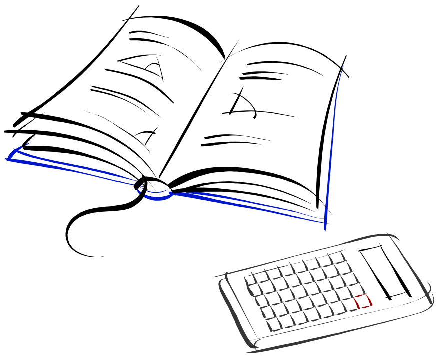
P. L. DeVries Am. J. Phys., vol. 64, 364 (1996)



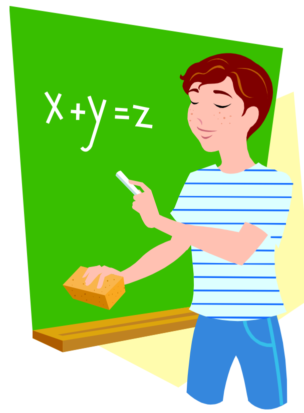
What is Computational Physics?

Computational physics is a tool for solving complex numerical problems in physics

Example: university physics courses



+



=

few analytically solvable problems

+

=

solutions to very many problems

Why do we need computational physics?

- In physics we answer how nature works.
- Quite often we need equations
  (*unless you are a poet or a philosopher*)
- Using equations we create models to describe nature
- Exact (analytic) solutions are very rare unless a model is a very simple one
- We need computational physics when
  – we cannot solve problems analytically
  – we have too much data to process

Many, if not the most, problems in contemporary physics could never be solved without computers

Computational physics in contemporary physics

- Numerical calculations: solutions of well defined mathematical problems to produce numerical solutions
  Examples: systems of differential equations, integration, systems of linear equations, …
- Visualization and animation: the human eye + the visual processing power of the brain = very sophisticated tool
  traditional presentation: 2D and 3D plots
  new presentations: animation, using colors and textures
- Computer simulation: testing models of nature
  Examples: weather forecast, …
- Data collection and analysis in experimental research
  Example: LabView
- Symbolic manipulation:
  Examples: Maple, Mathematica, …

Classification of computational models

Deterministic or Stochastic models

⇨ Deterministic models: Results of deterministic models depend on initial conditions.

⇨ Stochastic models: an element of chance exists.

Dynamic or Static models

⇨ A dynamic models changes in time.

⇨ A static model does not consider time

Computer Simulation (few examples)

- ✓ Molecular Dynamic Simulation
- ✓ Weather forecast
- ✓ Design of complex systems (aircrafts, …)
- ✓ Financial markets
- ✓ Traffic
- ✓ War games
- ✓ …

Computer simulations for non-linear problems

- Many natural phenomena are *nonlinear*, and a small change in a variable might produce a large effect.
  But just few nonlinear problems can be solved analytically.
- Interest in systems with many variables or many degrees of freedom

Millennium Simulation - the largest N-body simulation carried out thus far (more than 10^{10} particles).
A 3-dimensional visualization of the Millennium Simulation shows a journey through the simulated universe
http://www.mpa-garching.mpg.de/galform/millennium/

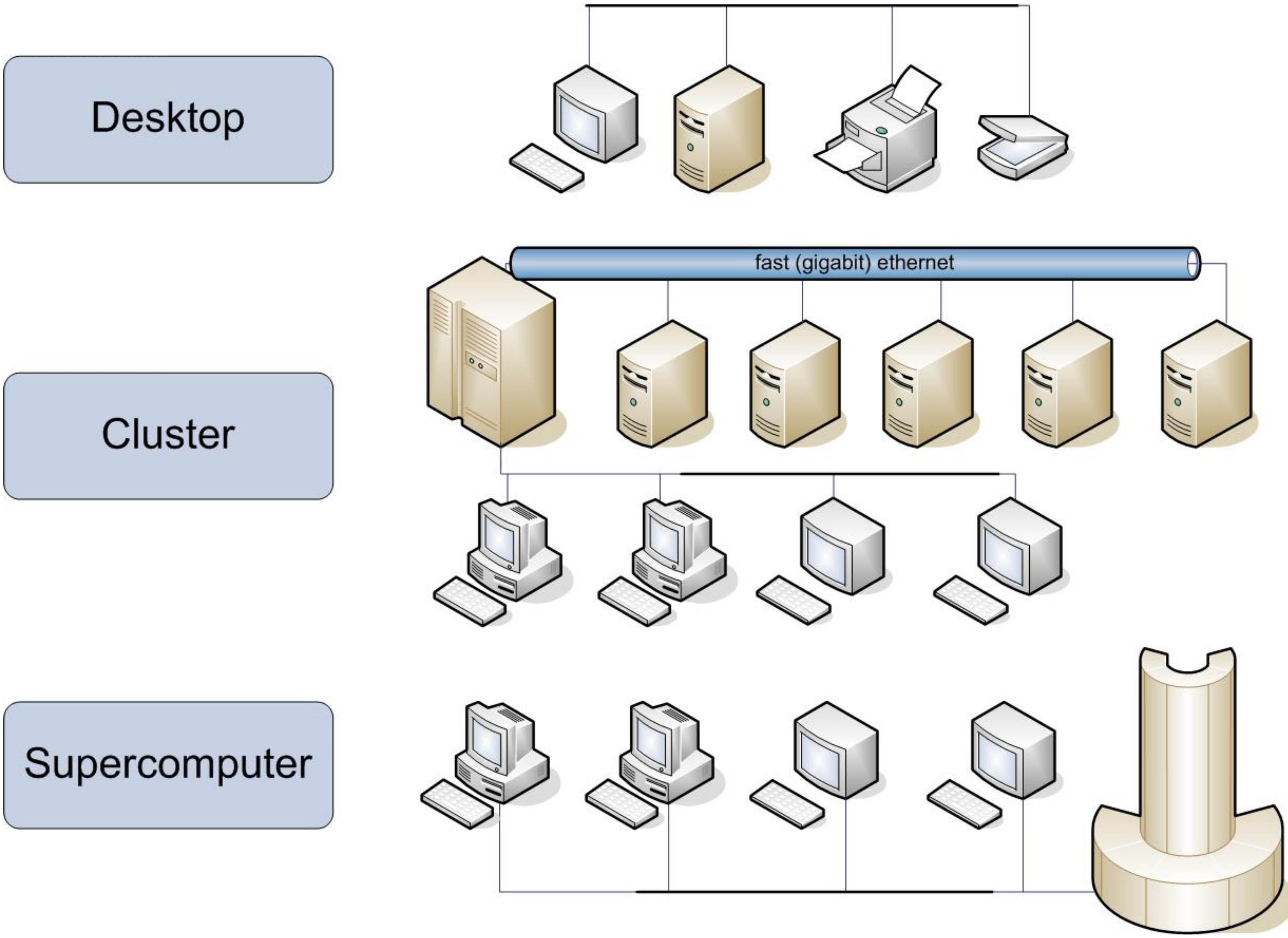
Computational Physics is a multidisciplinary field

Computers

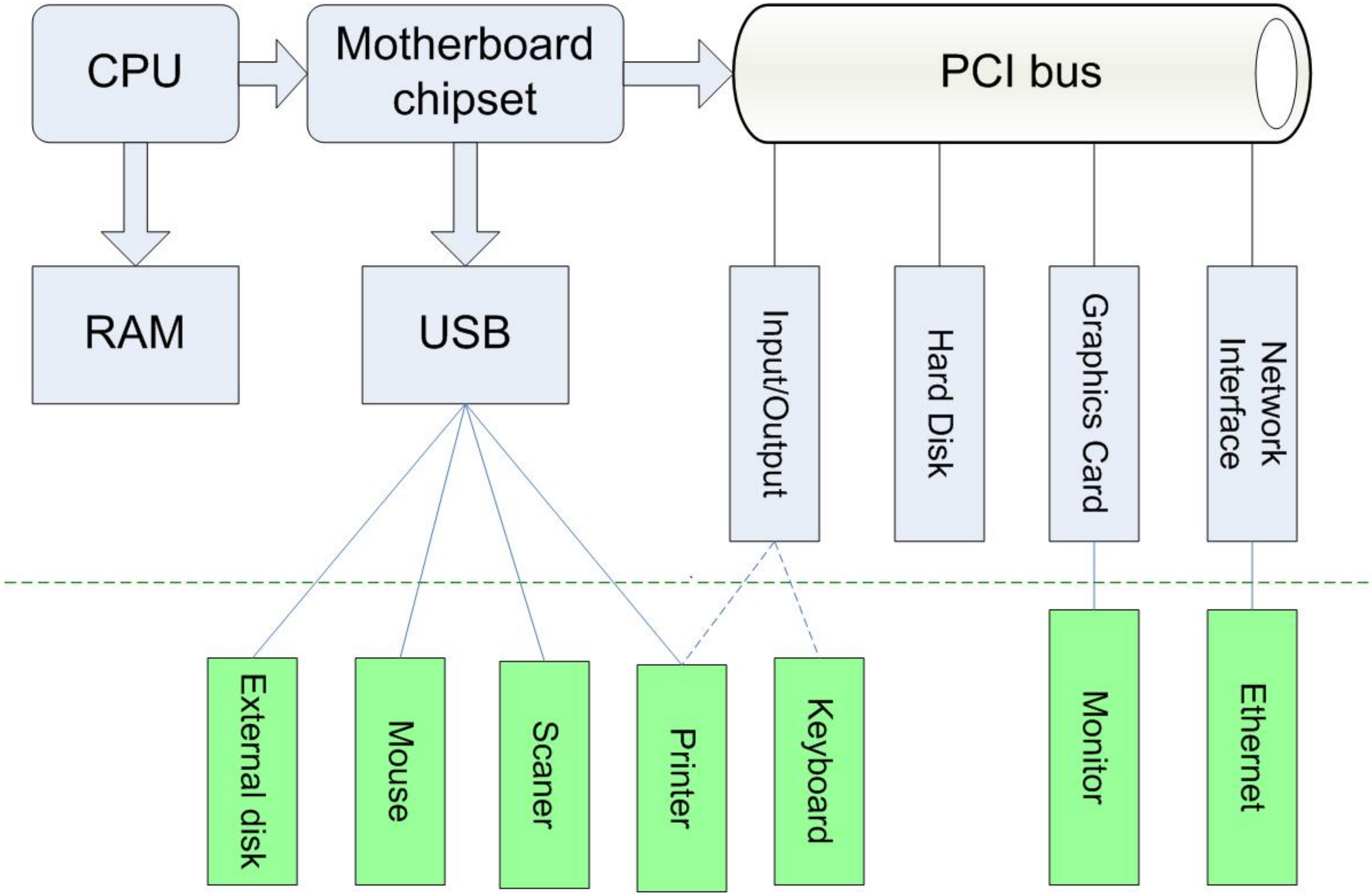
- Hardware
  - Amazing progress: two times more powerful processors in 18 months (Moore's law: the number of transistors per square inch on integrated circuits doubles every 18 months)
  - Do we have twice more results in physics each 18 months?

- Software

Computers in computational physics



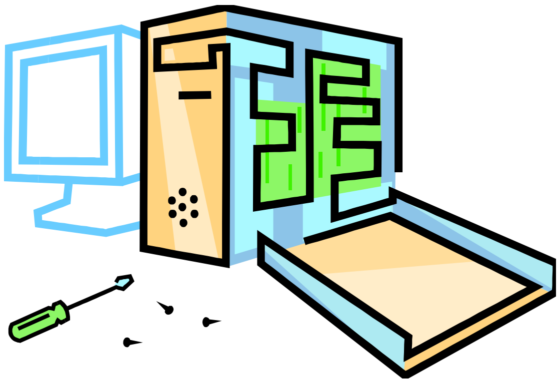
Basic computer hardware



Hardware (internal)

- CPU - central processing unit (speed in GHz), cache memory: cache 1, cache 2
- RAM -random-access memory (MB or GB) communication with CPU by bus (MHz)
- PCI – Peripheral Component Interconnect
- USB – Universal Serial Bus
- HDD – Hard Disk Drive (GB)
- Graphic card
- Network Interface (Mb/sec)

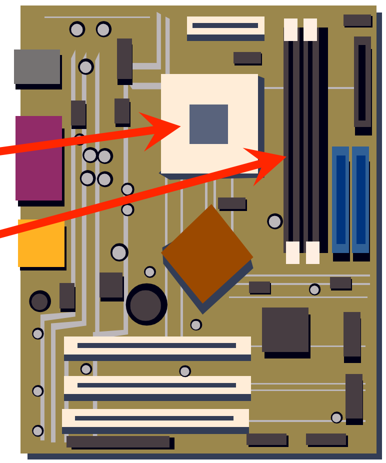
Hardware (peripheral)



- Keyboard (I/O)
- Mouse (I/O)
- Printer (I/O)
- Monitor (Graphic card)
- Ethernet (network)
- Scanner, external storage, …

Critical hardware for calculations

- Desktops
  - CPU
  - RAM

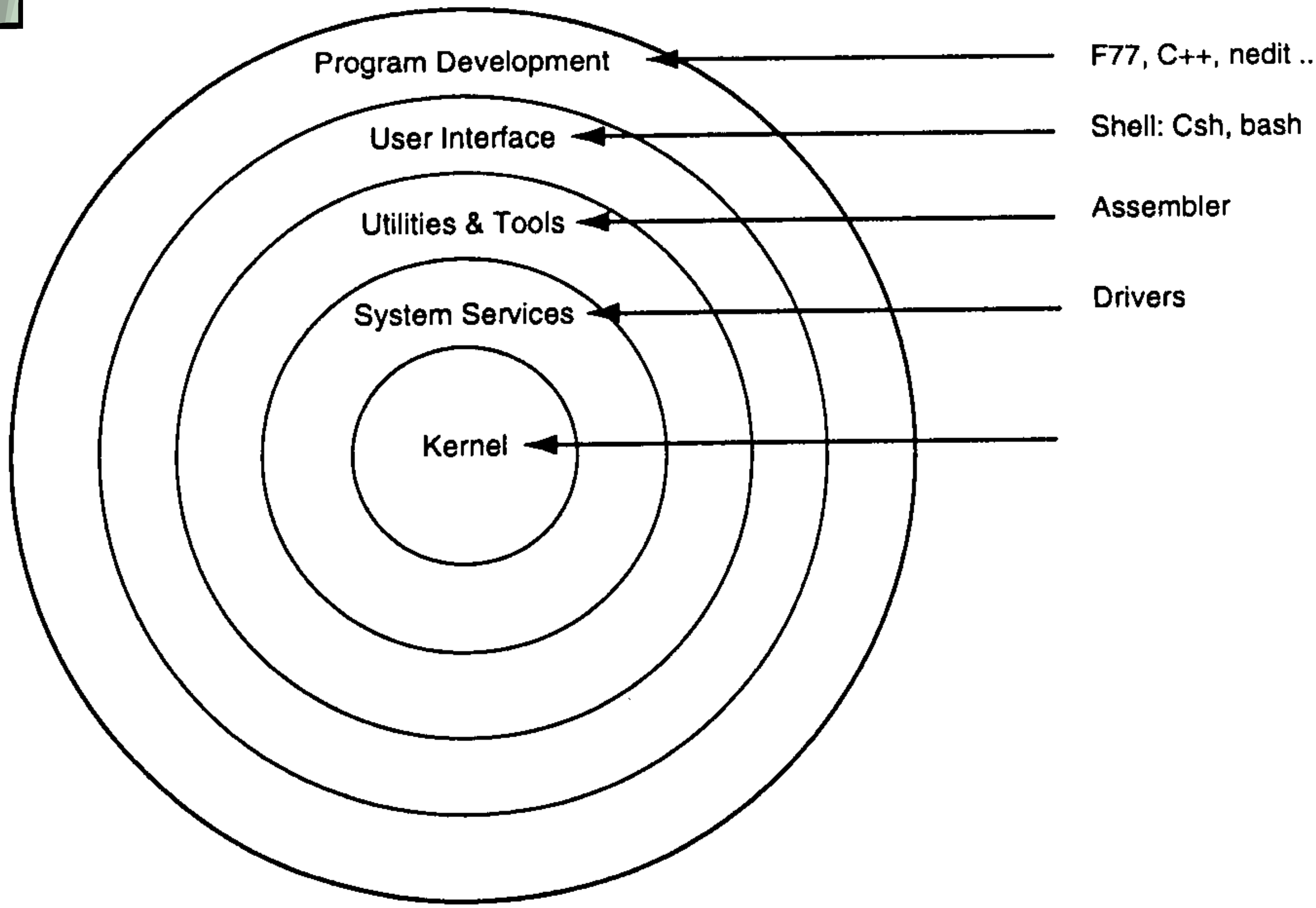


- Clusters
  - CPU and RAM
  - number of CPUs
  - fast network communication between nodes

TOP500 SUPERCOMPUTER SITES

http://www.top500.org/

Software


Program Development
User Interface
Utilities & Tools
System Services
Kernel
F77, C++, nedit ...
Shell: Csh, bash
Assembler
Drivers

Software 1: Operating Systems

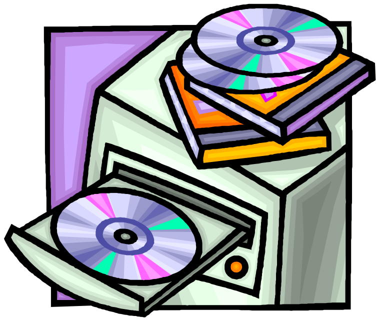
Operating system – a set of programs to manage

- communication between hardware (device drivers)
- communication between a user and a computer
- running applications (software)
- file system
- security

Types of Operating Systems

- multi-user: Allows two or more users to run programs at the same time. Some operating systems permit hundreds or even thousands of concurrent users.
- multiprocessing: Supports running a program on more than one CPU.
- multitasking: Allows more than one program to run concurrently.
- multithreading: Allows different parts of a single program to run concurrently.
- real time: Responds to input instantly. General-purpose operating systems, (Windows, Linux are not real-time).

Some of Operating Systems



Alive

- Windows
- Linux
- Mac OS
- Unix

Dead by now

- DOS
- IBM OS/2
- VMS
- IBM OS/400

What OS is better for computational physics?

The answer depends on a problem

- Desktops – Windows, Linux, Mac OS
- Clusters – Linux
- Supercomputers – Unix, Linux
- Parameters to consider:
  - Available hardware, software and computer codes
  - Stability
  - Analysis of results and presentation

Software 2: Programming Languages

http://www.engin.umd.umich.edu/CIS/course.des/cis400/

The basic ideas behind computational physics are language independent

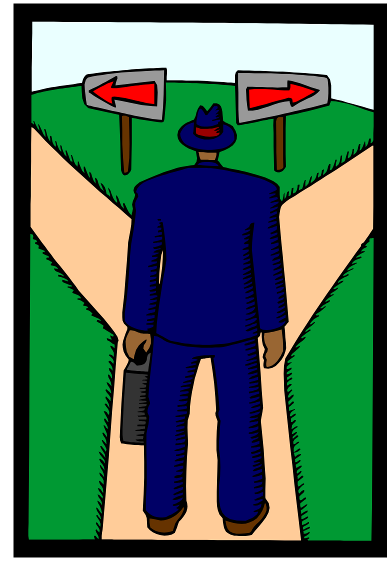
Most common in physics

Fortran

C/C++

Java

What language to use?



- choice depends on a problem
  - numerical simulation
  - system programming
  - web programming
- available libraries and computer codes
- experience

"The relevance of C++ to scientific computing is somewhat controversial"

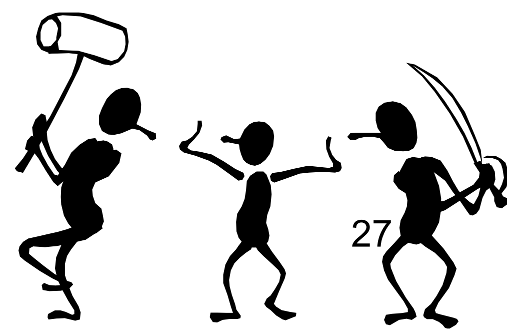
"A First Course in Computational Physics and Object Oriented Programming with C++", by D. Yevick

C++ is also one of the most complex programming languages, with many pitfalls for the unwary.

"C a reference manual" (5th edition) by S.P. Harbison and G. L. Steele Jr.

Spend your intellectual energies on the current problem - not on fancy tools. When the volume and sophistication of your problems demand these weapons you will know it. That is the time to learn a new tool - and learn it by re-doing an already-solved problem, not a new one.

F.S. Acton "Real Computing made real



Fortran, C/C++, and others

- Fortran – legacy! Very many computer codes and libraries
- Fortran – easy-to-learn and easy-to-use
- Normally, scientific C++ programs cannot be effectively optimized as Fortran programs (C++ codes run slower - from 10% to 10 times)
- Java and C# poses formal advantages (however, C++ is rather for industry)
- Scientific software – may solve problems faster

Fortran 77, C, C++, Fortran 90

Table 1: Relative Rank of Languages for Computational Science.

functionality	F77	C	C++	F90
numerical robustness	2	4	3	1
data parallelism	3	3	3	1
data abstraction	4	3	2	1
object oriented programming	4	3	1	2
functional programming	4	3	2	1
average	3.4	3.2	2.2	1.2

1 – excellent
2 – good
3 – fair
4 – poor
http://www.phy.ornl.gov/csep/CSEP/PL/PL.html

Free C++ Compilers

Windows 7/8 :

Microsoft Visual Studio 2010 or 2012:

http://www.microsoft.com/visualstudio/eng/downloads

NB: You must register to obtain a free product key for ongoing use after 30 days.

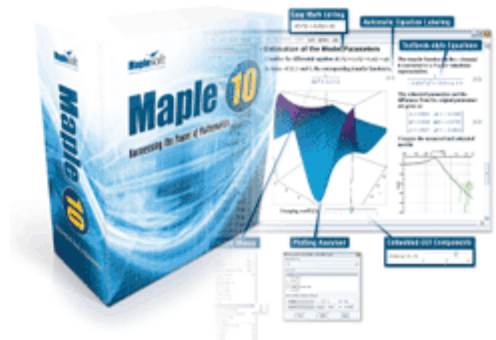
Mac OS up to 10.9: Xcode (versions 3 or 4)

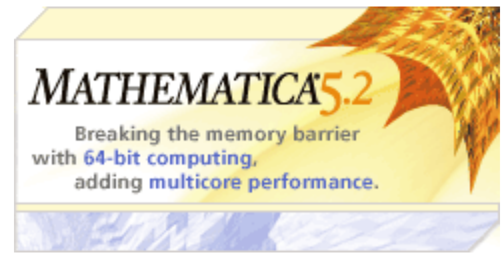
Mac HD -> Developer -> Applications -> Xcode

Mac OS 10.9 or higher: free download

Software 3: Problem-solving environment

- Maple
- Mathematica
- MathCad
- Derive





mathcad →13
driving innovation excellence

Problem-solving environment

- Problem-solving environment is good for small and medium projects
- Programming with compiled languages gives more control, power, flexibility for numerically and logically intensive tasks

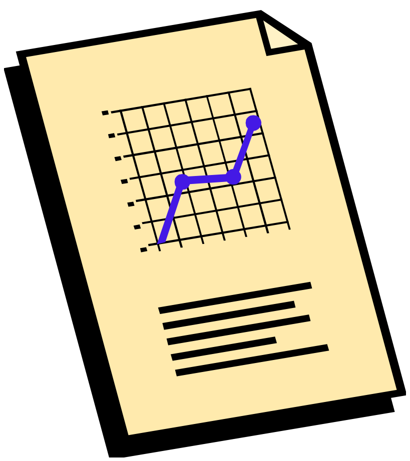
comments:

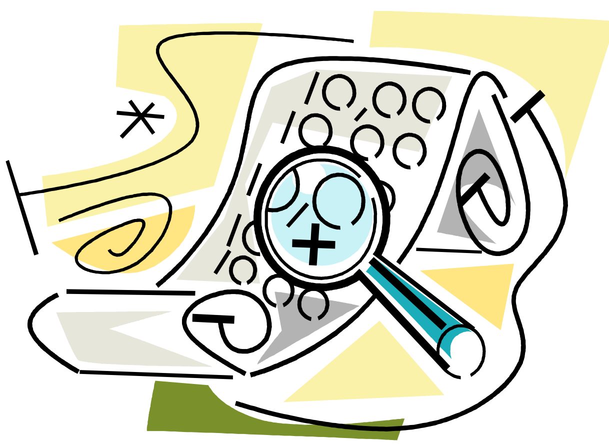
Mathematica is a huge system of remarkable capabilities cloaked in a stupefying variety of commands. But after six months of frequent experimentation, I still find that three-quarters of my time goes into trying to discover why I got an error message instead of the answer I was expecting.

F.S. Acton "Real Computing made real"

Software 4: Applications

- Graphics
- Spreadsheets
- Word processors
- Internet
- …





Project Management in computational physics

The art or skill of directing and organizing the work