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 <u>does not</u> study computers

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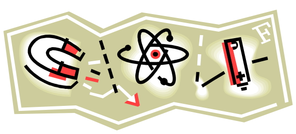
What is Computational Physics?

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

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



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What is Computational Physics?

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


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Example: university physics courses

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= few analytically solvable problems

 +  = solutions to very many problems

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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

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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, …

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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
- ✓ …

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The Best Approach for Avoiding Zombies

Physics could help if you're trapped by the staggering undead.

Sep 28, 2009

By Mike Lucibella
Inside Science News Service

PHYSICAL REVIEW E **80**, 030107(R) (2009)

Target annihilation by diffusing particles in inhomogeneous geometries

Davide Cassi
Dipartimento di Fisica, Università di Parma, Viale Usberti 7/a, 43100 Parma, Italy
(Received 30 June 2009; published 16 September 2009)

The survival probability of immobile targets annihilated by a population of random walkers on inhomogeneous discrete structures, such as disordered solids, glasses, fractals, polymer networks, and gels, is analytically investigated. It is shown that, while it cannot in general be related to the number of distinct visited points as in the case of homogeneous lattices, in the case of bounded coordination numbers its asymptotic behavior at large times can still be expressed in terms of the spectral dimension $\tilde{d}$ and its exact analytical expression is given. The results show that the asymptotic survival probability is site-independent of recurrent structures ($\tilde{d} \leq 2$), while on transient structures ($\tilde{d} > 2$) it can strongly depend on the target position, and such dependence is explicitly calculated.

more …

- 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/

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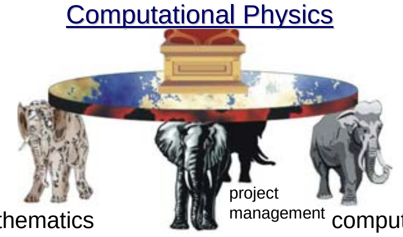
Computational Physics
is a multidisciplinary field

Computational Physics



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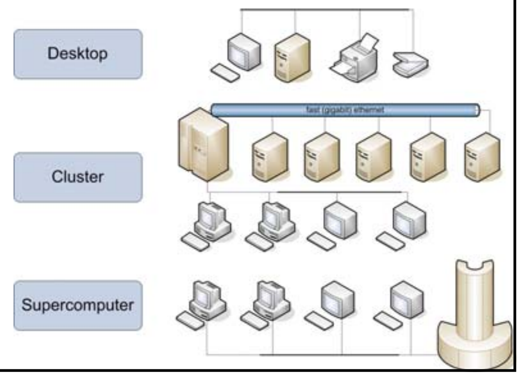
Computers

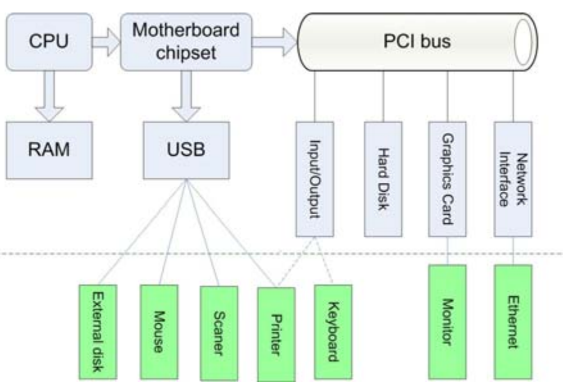
- Hardware
  - Amazing progress: two times more powerful processors in 18 months (Moore's law: the number of transistors per square inch on integrated circuits doubles every 18 months)
  - Do we have twice more results in physics each 18 months?

- Software

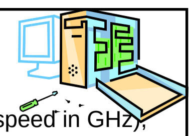
Computers in computational physics



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) (modems 56 Kb/sec)

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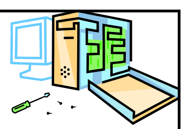
Hardware (peripheral)



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

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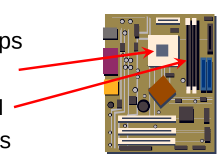
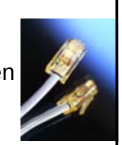
Critical hardware for calculations

- Desktops
  - CPU
  - RAM



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



TOP500 SUPERCOMPUTER SITES http://www.top500.org/

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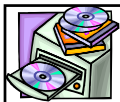
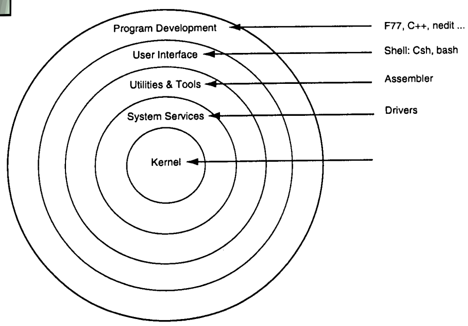


Software



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

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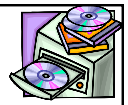
Types of Operating Systems



- 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).

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Some of Operating Systems

Alive	Dead by now
Windows	DOS
Linux	IBM OS/2
Mac OS	VMS
Unix	IBM OS/400

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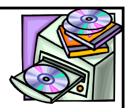
What OS is better for computational physics?



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

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Software 2: Programming Languages

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

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The basic ideas behind computational physics are language independent

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Most common in physics

Fortran

C/C++

Java

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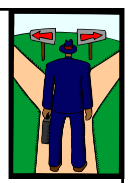
What language to use?



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

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

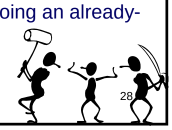
"A First Course in Computational Physics and Object Oriented Programming with C++", by D. Yevick

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



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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

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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

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Languages and Compilers

For effective and efficient work you need to

a) Select a language that is right for you now and in nearest future.
You may need to know/learn more than one language.

b) Have a good book (with examples) to learn the language that you selected

c) Have a compiler that fits you demands (and budget)

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Compilers: C and C++

- Dev-C++ Compiler (open source) a full-featured IDE for the C/C++ The last version was released in 2005 (no activity with the project since that)
- Code::Blocks IDE (open source) for Windows and Mac
- Open Watcom C/C++ compiler, (open source)
- Microsoft Visual C++ 2008 Express Edition (free)
- Borland C++ Compiler. free and proprietary versions
- Intel® C++ Compilers for Windows, Linux and Mac OS (License type - proprietary) Non-commercial customers can download free Intel® C++ Compiler for Linux (registration required)
- Microsoft Visual C++ 2010 (License type - proprietary)
- C++ Builder 2010 C++ (License type - proprietary)
- The Portland Group C and C++ compilers for 32-bit x86 and 64-bit x64 processor-based Linux and Windows workstations, servers and clusters.

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Compilers: Fortran

- Intel® Visual Fortran Compilers for Windows, Linux and Mac OS (License type - proprietary)
- The Portland Group Fortran compilers for Linux and Windows workstations, servers and clusters. (License type - proprietary)
- NAGWare f95 Compiler Available on a wide range of Unix and Windows platforms. (License type - proprietary)
- Absoft Fortran Compiler and associated tools are available for HPC, Linux, Windows and MacOS environments. (License type - proprietary)
- Lahey/Fujitsu Fortran includes full Fortran 95/90/77 and Fortran for .NET compilers. (License type - proprietary)
- Silverfrost FTN95 - Fortran for Windows (free for personal and evaluation use)
- Open 64 – open source for Linux
- Open Watcom Fortran compiler (free): Latest Release (February 2009)
- G95 (free): latest release (March 2009) (Open source)

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Software 3: Problem-solving environment

- Maple
- Mathematica
- MathCad
- Derive

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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

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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.

F.S. Acton "Real Computing made real"

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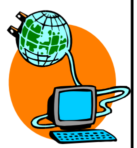
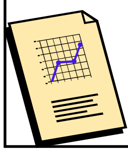
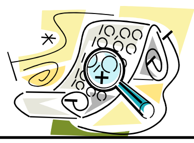
Software 4: Applications



- Graphics
- Spreadsheets
- Word processors
- Internet
- …

Project Management in computational physics

The art or skill of directing and organizing the work