Software development for computational science

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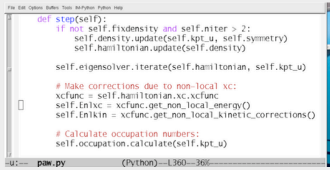
Software Engineering

CSC – The finnish IT center for science



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Outline

- **CSC – The finnish IT center for science**
- **Computational science**
- **Software development in high performance computing**
  - General needs
  - Programming languages
  - Optimization
  - Parallel processing
- **Summary**

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CSC – The finnish IT centre for science

- **Limited non-profit company, owned by the Finnish Ministry of Education**
- **~ 150 emplyees**
- **Computational services for Finnish universities and research institutes**
  - Supercomputing
  - Scientific applications and databases
  - Network service
  - Information management services

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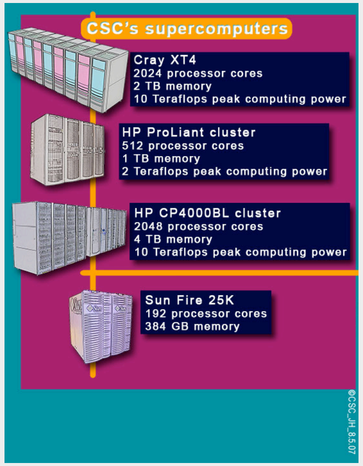
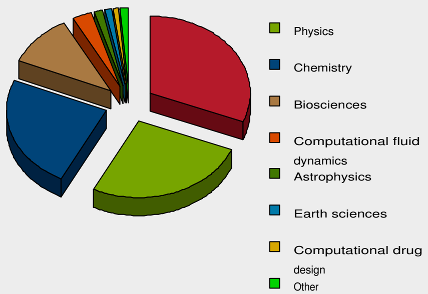
Computing environment of CSC



Usage of processor time by discipline 2006



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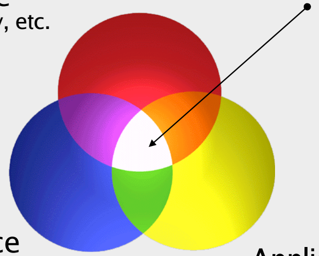
What is computational science?

Computational Science
Teamwork and Collaboration

Science Discipline
Physics, Chemistry, Biology, etc.



Computer Science
Hardware/Software

Applied Mathematics
Numerical Analysis, Modeling, Simulation

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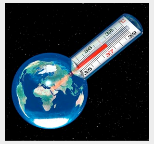
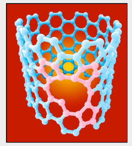
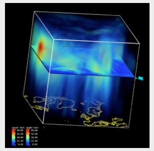
Applications of computational science



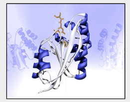
Climate change



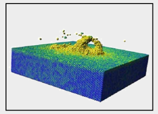
Nanoscience



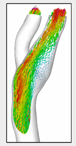
Weather forecasts



Drug design



Material physics



Fluid dynamics

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Ingredients of computational science

- **Modeling**
  - set up the mathematical equations describing the problem
  - the governing equations are often known e.g. Navier-Stokes equation, Schrödinger equation etc.
- **Simulation**
  - write or use existing computer program which solves the equations numerically
  - high performance computing
- **Analysis and visualization**
  - analysis of results may also require programming

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Software development in high performance computing

- **General development needs**
  - version control
  - choice of programming language(s)
  - debugging tools
  - testing schemes
- **Specific needs in high performance computing**
  - achieving high performance with single processor in different platforms
  - efficient parallel processing
  - profiling tools

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Development tools

- **Version control**
  - cvs, svn, etc.
  - easy access to version history
  - code syncronization with multiple developers
- **Regression testing**
  - test sets
  - automatic testing
- **Programming tools**
  - syntax highlighting in editors
  - automated building
  - debugging utilities
  - integrated development environments (IDE)
- **Profiling tools**
  - help to pinpoint the bottlenecks of the program efficiency

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Programming languages

- **Efficiency of development vs. execution efficiency**
  - human work is expensive
  - ease of development and maintanance
- **Portability**
  - (super)computers have life cycle of few years
  - programs may be run in different architectures
- **Access to external libraries**
  - most time consuming parts e.g. linear algebra operations can be performed by optimized external libraries
- **Traditional languages**
  - Fortran, C
- **"Modern" languages**
  - C++, Java, Python, Perl

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Programming languages

- **Compiled, "low" level languages**
  - Fortran, C, C++
  - produce typically fast code
  - development may be more cumbersome, e.g. each code change requires recompiling
  - interfaces to external libraries
- **Interpreted scripting languages**
  - Python, Perl
  - fast development and prototyping
  - native code relatively slow
  - possible to combine with compiled languages
  - special (e.g. parallel) profiling tools do not necessarily support these languages

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Optimization

- **Find the bottlenecks of the program**
  - timing calls in program
  - profiling tools
  - typically, a program spends 90 % of time in 10 % of code
- **Efficiency of algorithm**
  - optimization of the algorithm is typically the most efficient way to improve the performance of the program
- **Try to use optimized external libraries**
  - many vendors provide highly tuned libraries for linear algebra (BLAS, LAPACK), FFTs etc.
- **Optimize the actual code**
  - in current systems, memory access is often the crucial factor

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Basic linear algebra subprograms (BLAS)

- **Many algorithms can be written in terms of matrix-vector operations**
- **BLAS provides standard building blocks for many vector and matrix operations**
- **In addition to standard BLAS (www.netlib.org/blas) there are implementations optimized for specific architectures**
- **Interfaces to Fortran, C and Java**
- **Example: matrix-matrix multiplication in Opteron 2.6 GHz**
  - 600x600 double precision matrix
  - simple implementation with compiler optimizations takes 0.58 s
  - BLAS call 0.094 s

Parallel processing

- **Parallel processing is used to**
  - speed-up program execution
  - recuce the needed memory per processor
- **Todays desktop processors start to contain multiple cores (dual core, quad core, ...)**
- **Current supercomputers can use thousands of commodity processor**
  - Top 10 supercomputers have all over 10000 processing cores, the top one having over 200 000 processors!
- **Utilization of large number of processors is major challenge in software development**

Classes of parallel computers

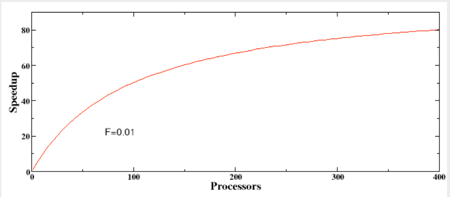
- **Shared memory systems**
  - all the processors can access all of the memory
  - OpenMP compiler directives
  - simple to use
  - limited scalability
- **Distributed memory systems**
  - message passing is used to communicate between processors
  - MPI interface
  - requires more work from the programmer
  - in trivial problems can scale to arbitrarily large number of processors

Speedup of parallel program

- **Upper limit by Amdahl's law:**

$$Speedup = \frac{1}{F + (1-F)/N},$$

where F is sequential fraction and N number of processors



- **Maximum speedup is 1/F**
  - if 1 % of program is sequential, maximum speedup is only 100!
  - When number of processors is doubled from 200 to 400, program will execute only 20 % faster
- **In practice, scaling is much worse**

Software development projects in CSC

- **Elmer**
  - multiphysical modeling with finite element method
  - Fortran90, MPI-parallelization
- **GPAW**
  - atomistic modeling within density functional theory
  - Python + C, MPI-parallelization
- **FinHPC**
  - optimization of selected programs
  - only implementations are optimized
- **Chipster**
  - user-friendly interface for DNA microarray data analysis
  - Java
- **SOMA**
  - molecular modelling environment
  - Perl programs and XML-schemas, operated through www-browser

Open vs. closed source software

- **Proprietary software**
  - there are high quality commercial programs for some problems
  - user friendly graphical interfaces
  - “black boxes”
  - no access to source code, no own extensions
- **Open source software**
  - correct functioning of program (i.e. correct results) can be checked
  - code can be extended depending on users needs