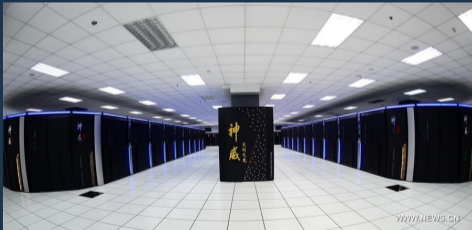


Introduction to High Performance Computing

Pierre Aubert

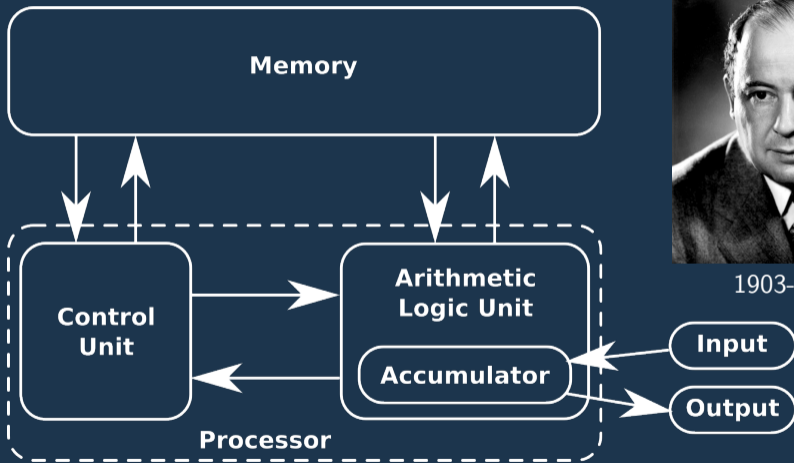


- ▶ Part of the computer science
- ▶ Get the best performances by using the right algorithms on the right architectures



Computing Processing Unit (CPU)

John Von Neumann architecture (1945)



1903-1957

ALU

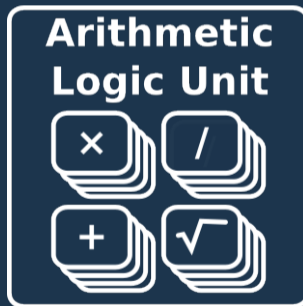


Arithmetic Logic Unit (ALU)

ALU



ALU Vectorized

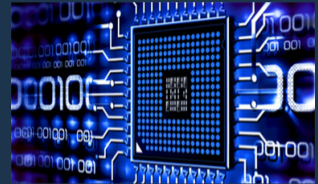


- ▶ C :
 - ▶ MKL, Atlas, BLAS, Lapack
- ▶ C++ :
 - ▶ TBB, Eigen, Armadillo, HPX
- ▶ Python :
 - ▶ Numpy
 - ▶ Numba (JIT, Just In Time)



Aim of this tutorial

- ▶ How HPC libraries work
- ▶ How to measure performances of a function
- ▶ Focus on **float** computation (simple precision)
 - ▶ Sufficient in most cases and get very good speed up
- ▶ Precision of the Computation :
 - ▶ Optimized version is **MORE** precise than scalar version !!!
 - ▶ So, asking to have exactly the same result as scalar version is a non sense !!!
 - ▶ To claim scalar was checked is not a plea because errors can compensate each other
 - ▶ Optimized **float** version can reach same precision as scalar **double** version



Prerequisites for this tutorial

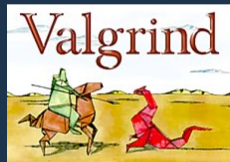
- ▶ Tools for compilation :
 - ▶ **GCC/G++** : version **7.2** (I do not know what is going on with the version 8)
 - ▶ **CMake** : version ≥ 3.0
 - ▶ **Make** : version ≥ 4.0
- ▶ Versioning Tool :
 - ▶ **Git** : version $\geq 2.14.1$
- ▶ Tool for drawing plot :
 - ▶ **Gnuplot** : version ≥ 5.0
- ▶ Optional Tools :
 - ▶ **hwloc-ls**
 - ▶ **jupyter-notebook**
 - ▶ **anaconda**



- ▶ Warm up
- ▶ Creation of a HPC/Timer library
- ▶ Optimisation of Hadamard product (+ python wrapper)
- ▶ Optimisation of saxpy (homework)
- ▶ Optimisation of a vector reduction
- ▶ Application/exercice : Optimisation of barycentre computation (homework)
- ▶ Optimisation of Dense Matrix-Matrix multiplication
- ▶ What about branching ? (bonus)
- ▶ Conclusion

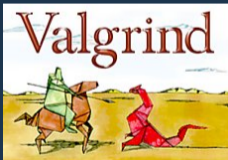
Basically with a timer.

- ▶ Instrumenting the code
 - ▶ GProf
 - ▶ Perf
- ▶ Emulate the binary
 - ▶ Valgrind (<http://www.valgrind.org/>)
 - ▶ Maqao (<http://www.maqao.org/>)
- ▶ Python :
 - ▶ cprofile (+ snakeviz)
 - ▶ time



How to evaluate time spent in a function ?

- ▶ Tools :
 - ▶ GProf
 - ▶ Perf
 - ▶ Valgrind
 - ▶ Maqao
- ▶ Functions :
 - ▶ **clock** : to get a time in seconds (not very precise).
 - ▶ **rdtsc** : to get a time in cycles (very precise).
- ▶ Method :
 - ▶ To evaluate N calls of the function and then to average the results.



The Kernel approach

- ▶ What is a kernel ?
 - ▶ The function which does the computation and which does not call any other function.
So a pure mathematic function.
- ▶ Elapsed time of compilation :
 - ▶ GCC always tries to make a short compilation (typically 1 second per file).
 - ▶ It is the same if the file has 100 000 lines or not.
 - ▶ So, short files implies better optimisations.



Where to get the tutorial ?

Web Tutorial : `https://lappweb.in2p3.fr/~paubert/ASTERICS_HPC/index.html`

Minimal repository : `https://lappweb.in2p3.fr/~paubert/ASTERICS_HPC/ressource/build/Correction/ExampleMinimal.tar.gz`

Correction :

`https://lappweb.in2p3.fr/~paubert/ASTERICS_HPC/ressource/build/Correction/Examples.tar.gz`