INTRODUCTION TO HPC

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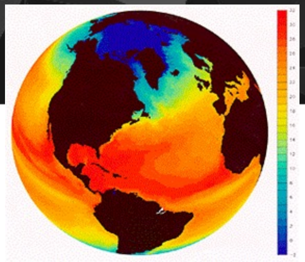
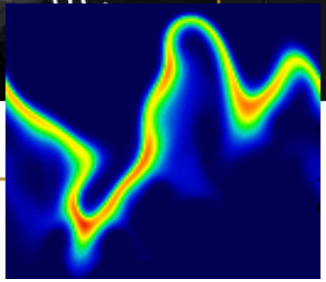
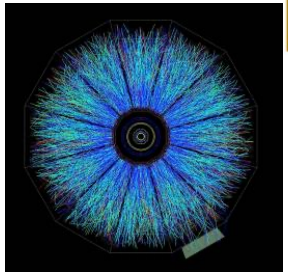
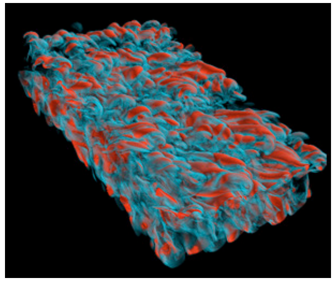
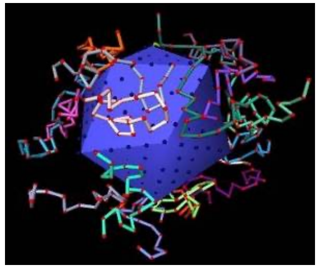
Why supercomputing?

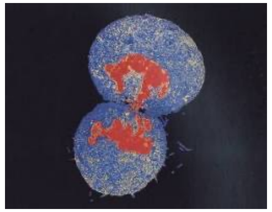




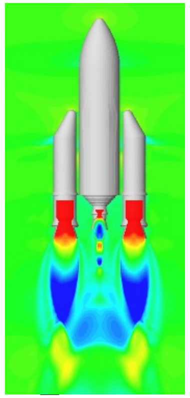


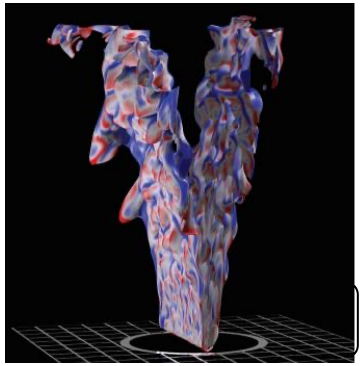






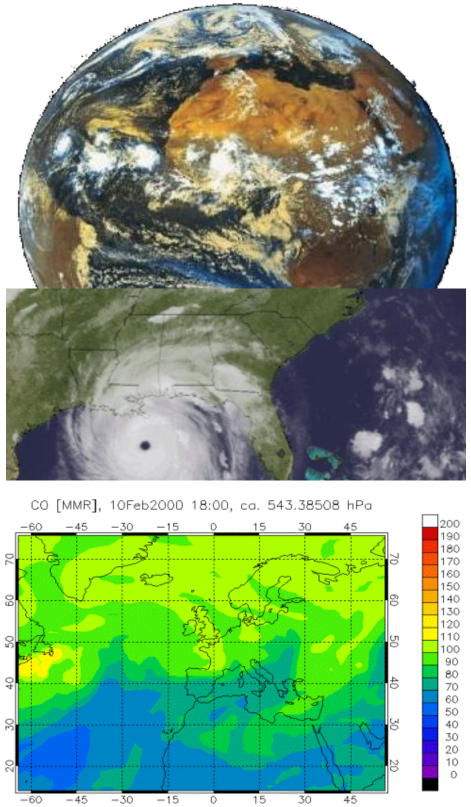
- **Weather, Climatology, Earth Science**
  - degree of warming, scenarios for our future climate.
  - understand and predict ocean properties and variations
  - weather and flood events
- ***Astrophysics, Elementary particle physics, Plasma physics***
  - *systems, structures which span a large range of different length and time scales*
  - *quantum field theories like QCD, ITER*
- ***Material Science, Chemistry, Nanoscience***
  - *understanding complex materials, complex chemistry, nanoscience*
  - *the determination of electronic and transport properties*
- ***Life Science***
  - *system biology, chromatin dynamics, large scale protein dynamics, protein association and aggregation, supramolecular systems, medicine*
- ***Engineering***
  - *complex helicopter simulation, biomedical flows, gas turbines and internal combustion engines, forest fires, green aircraft,*
  - *virtual power plant*



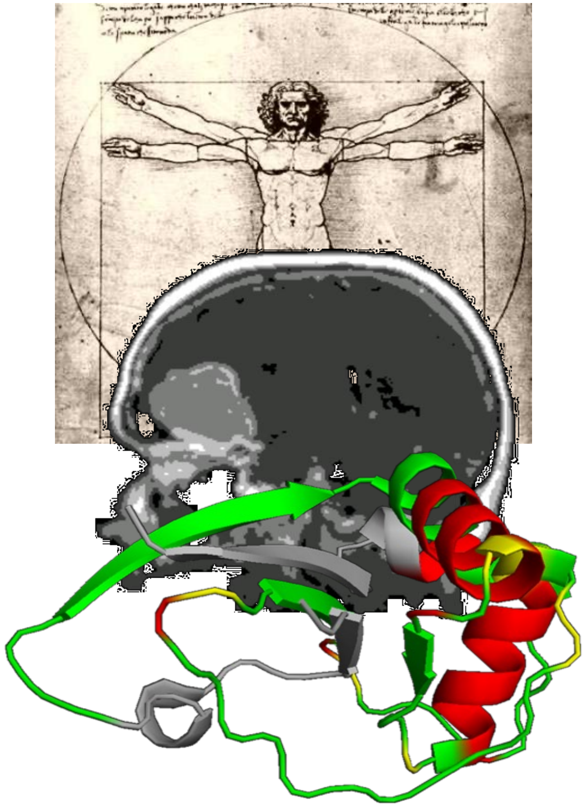


Why supercomputing?

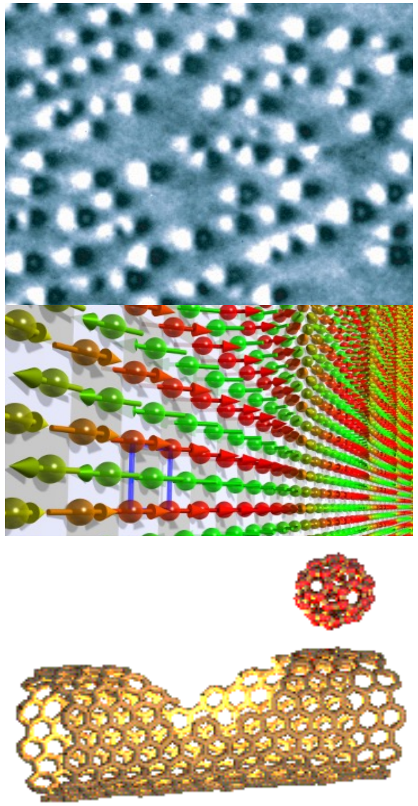
Supercomputing drives science with simulations



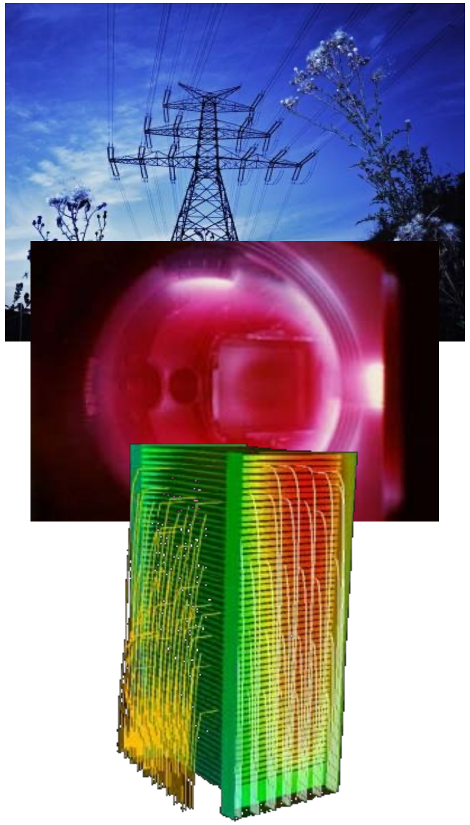
Environment
Weather/ Climatology
Pollution / Ozone Hole



Ageing Society
Medicine
Biology



Materials/ Inf. Tech
Spintronics
Nano-science



Energy
Plasma Physics
Fuel Cells

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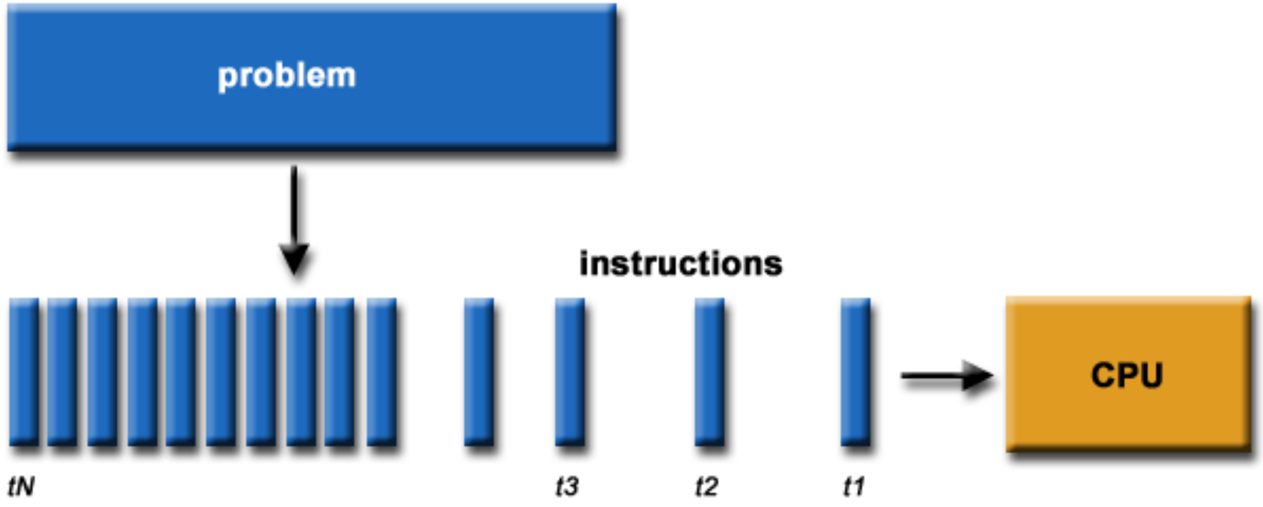
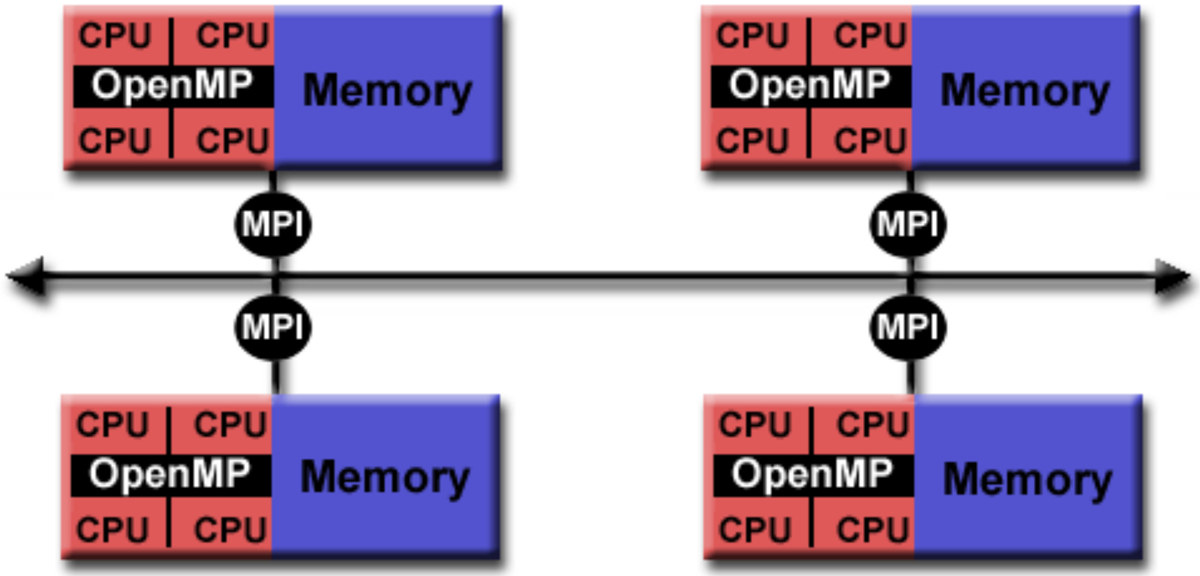
Introduction to parallel computing

- Usually the program is written for serial execution on one processor
- We divide the problem into series of commands that can be executed in parallel
- Only one command at a time can be executed on one CPU



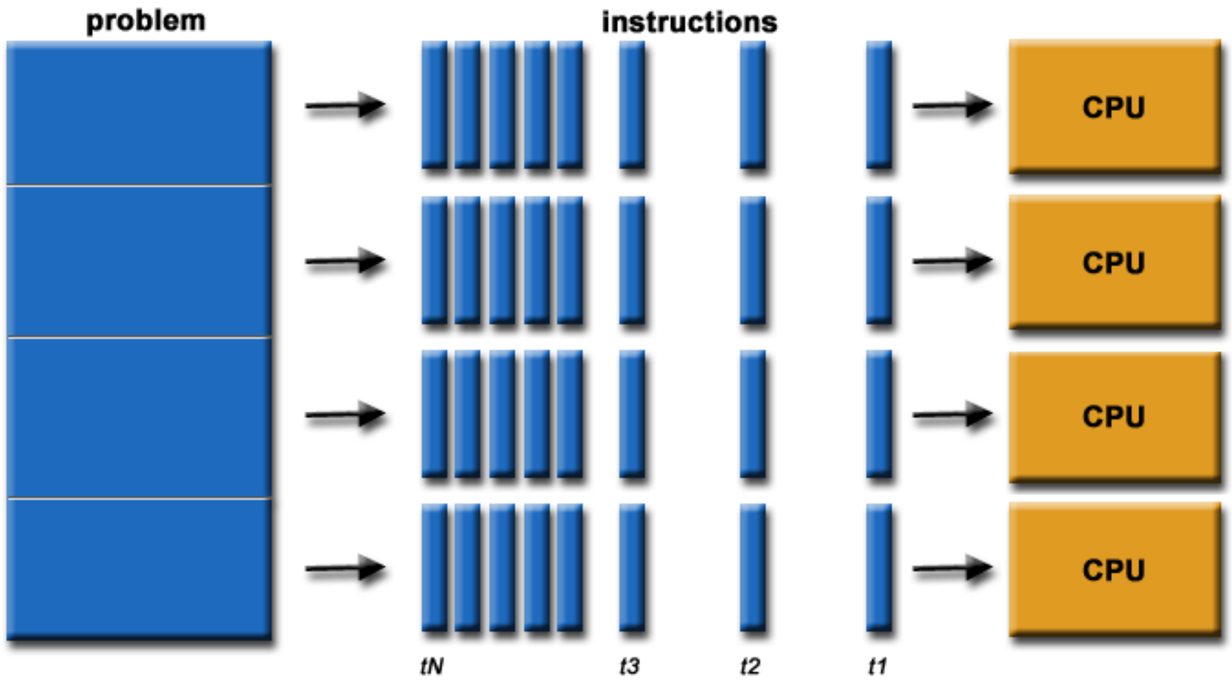
Parallel programming models

- Threading
- ***OpenMP** – **automatic parallelization***
- Distributed memory model = ***Message Passing Interface (MPI)** – **manual parallelization needed***
- ***Hybrid model OpenMP/MPI***



Embarrasingly simple parallel processing

- Parallel processing of the same subproblems on multiple prooocessors
- No communication is needed between processes



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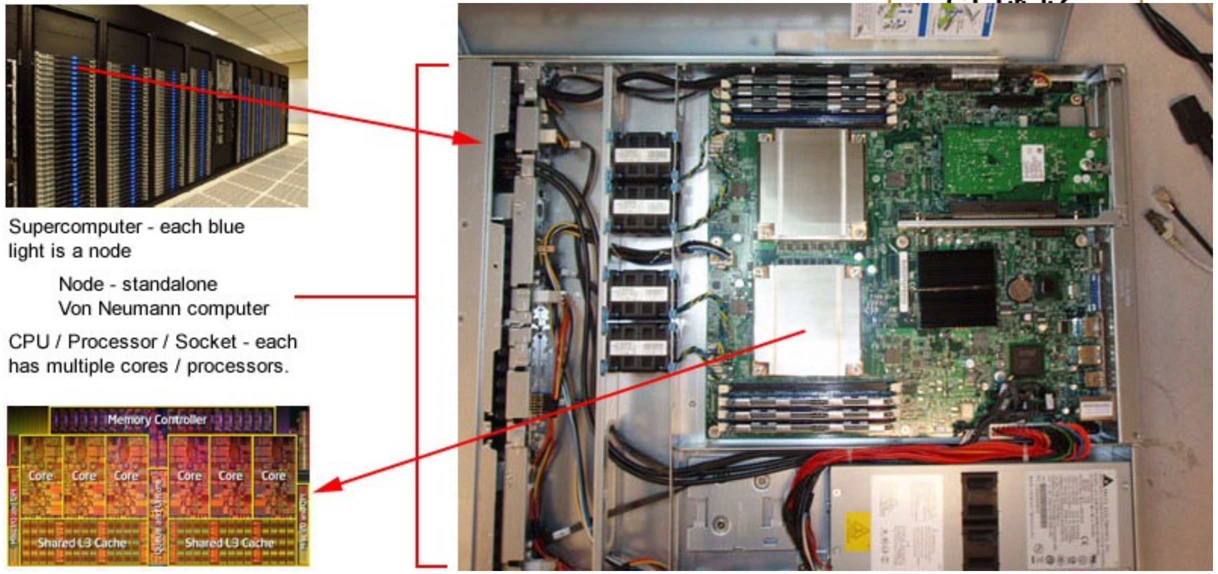
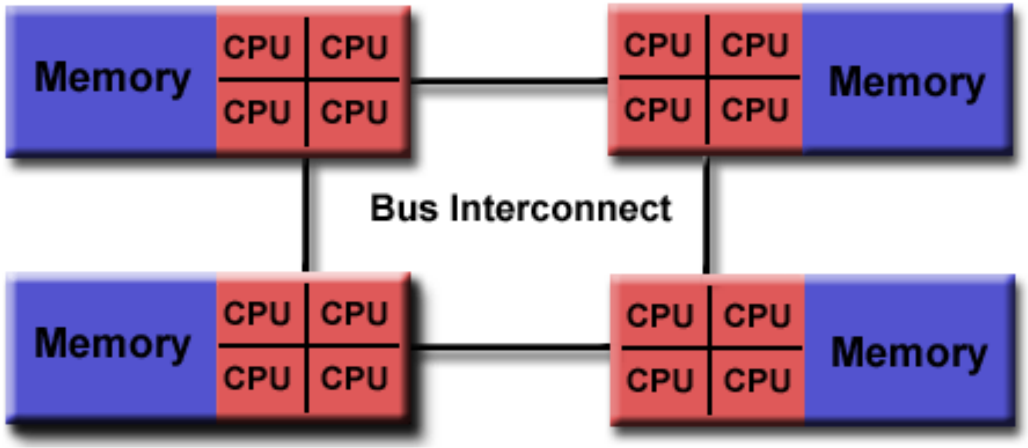
Logical view of a computing node

- Need to know computer architecture
- ***Interconnect bus for sharing memory between processors (NUMA interconnect)***





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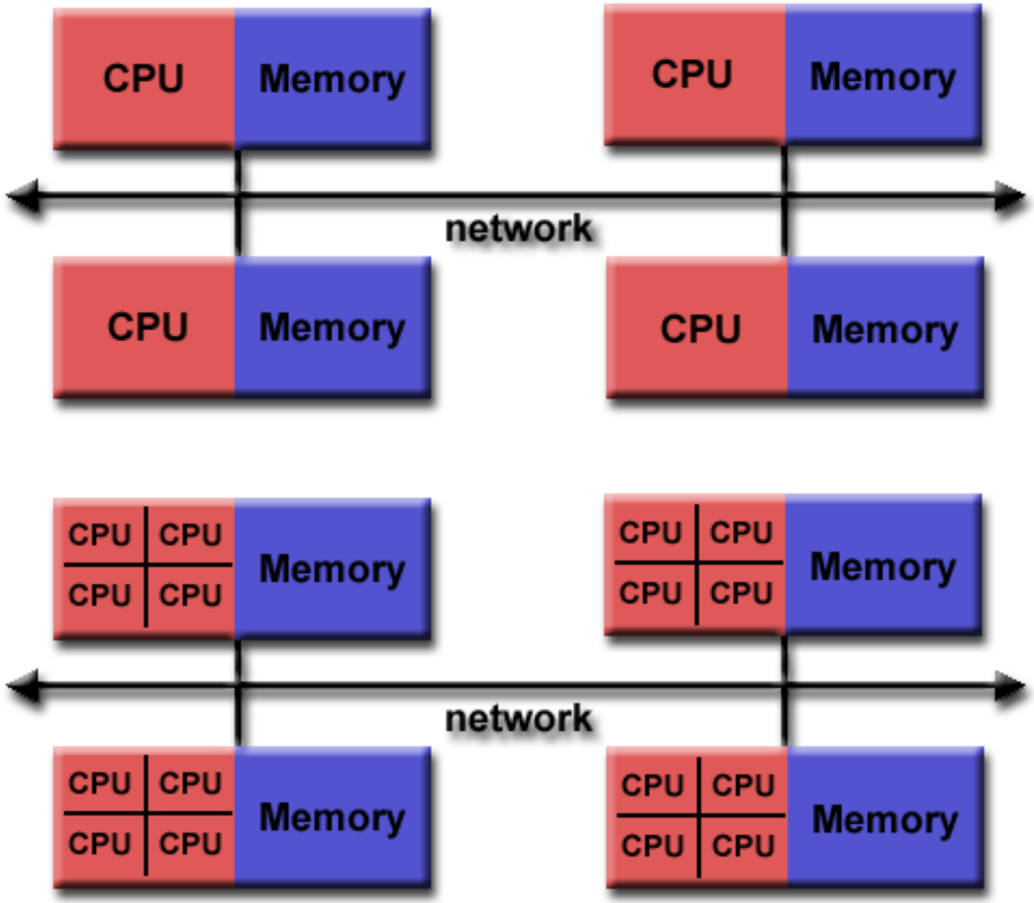
Nodes interconnect

- Distributed computing
- Many nodes exchange messages on:
  - ➢high speed,
  - ➢low latency interconnect such as **Infiniband**



Development of parallel codes

- Good understanding of the problem being solved in parallel
- How much of the problem can be run in parallel
- Bottleneck analysys and profiling gives good picture on scalability of the problem
- We optimize and parallelize parts that consume most of the computing time
- Problem needs to be disected into parts functionally and logically

Interprocess communications

- Having little and infrequent communication between processes is the best
- Determining the largest block of code that can run in parallel and still provides scalability
- Basic properties:
  - ***response time***
  - ***transfer speed - bandwidth***
  - ***interconnect capabilities***

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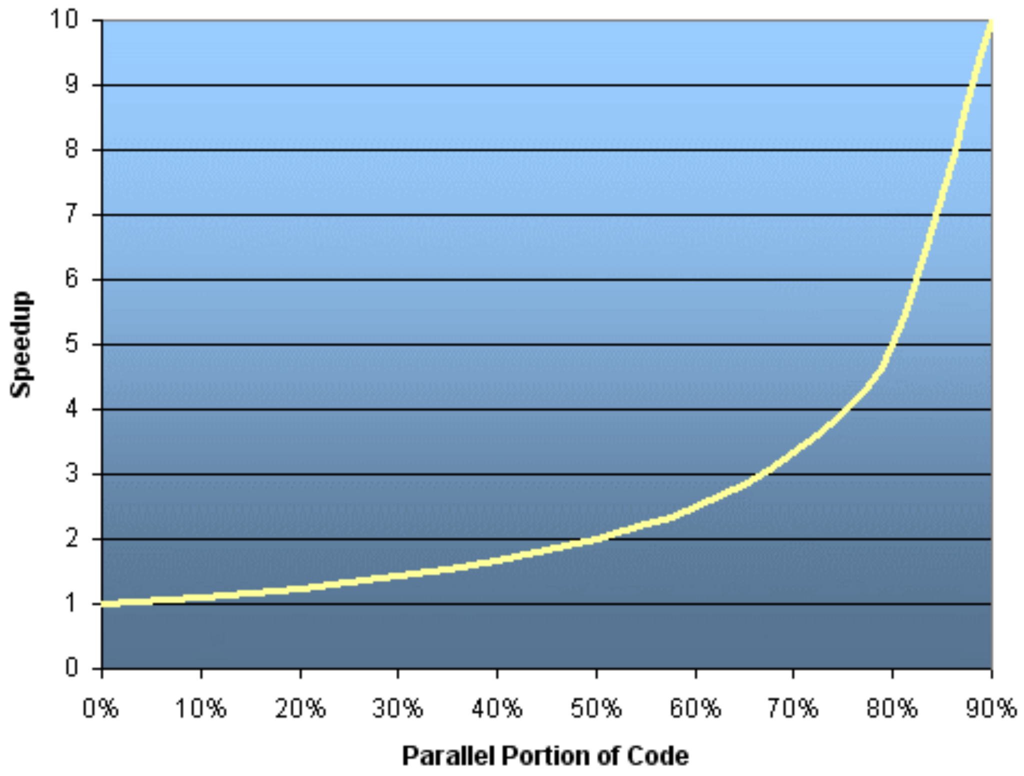
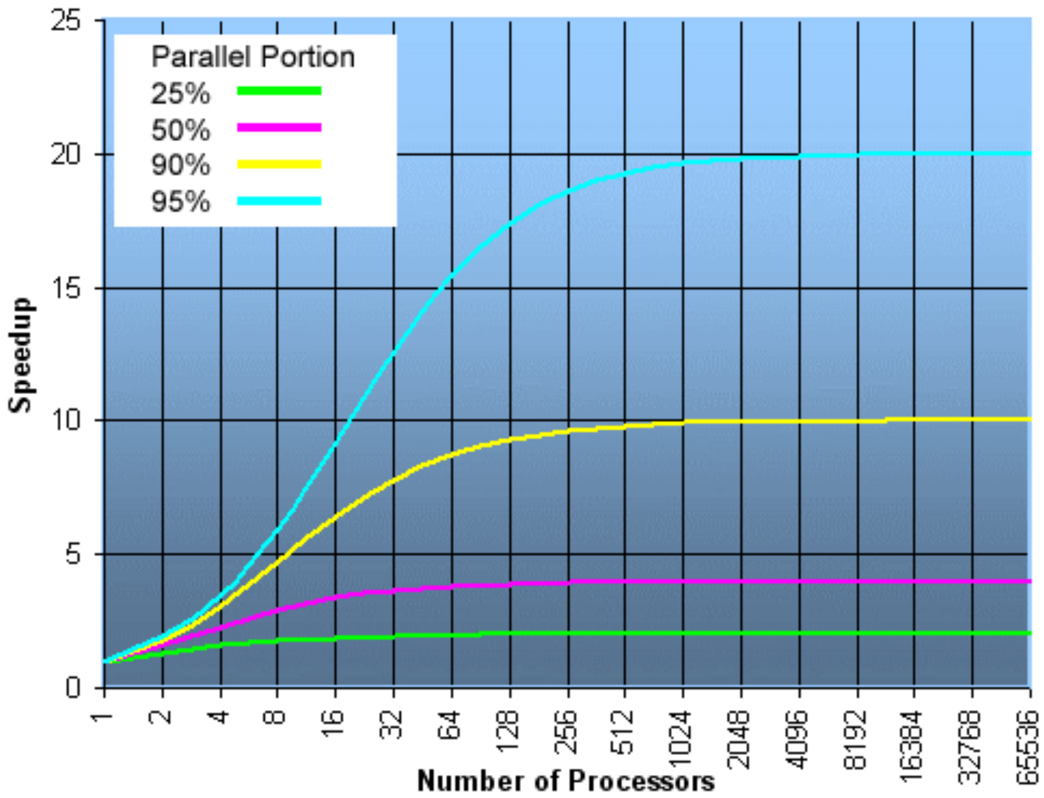
Parallel portion of the code determines code scalability

- Amdahlov law: ***Speedup = 1/(1-p)***





Questions and practicals on the HPCFS cluster

- Demonstration of the work on the cluster by repeating
- Access with NX client
- Learning basic Linux commands
- SLURM scheduler commands
- Modules
- Development with OpenMP and OpenMPI parallel paradigms
- Excercises and extensions of basic ideas
- Instructions available at http://hpc.fs.uni-lj.si/

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