PARADOXical Training
Institute of Physics Belgrade, 14 October 2011

Introduction to High Performance Computing

Antun Balaz
Institute of Physics Belgrade
http://www.scl.rs/

Academic and Educational Grid Initiative of Serbia
AEGIS

PRACE

HP-SEE

egi

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Agenda

- Introduction:
  - or why scientists need HPC & GRID
- Section 1: HPC concepts
- Section 2:
  - Parallel computing
  - Parallel machines
- Section 3: GRID concepts
- Conclusions
  - Computer infrastructure for everybody

Why computer simulations in science ?

- **numerically solve theories** which could not be solved otherwise (i.e. get numbers out of theories, much in the same way as experiments get numbers out of nature)
- **perform virtual experiments** when real experiments are not possible, or under conditions controlled in ways not possible in the lab
- **benchmark** the soundness of ideas and theories

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Examples of numerical simulations at SCL

- Ultra-cold quantum gases
  - Global and local properties of BEC
  - Parametric resonance
- Strongly correlated systems
  - Fractional quantum Hall effect
  - Bose-Hubbard
- Granular materials
  - Classical MD simulations of collective behavior

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What resources are needed to perform them?

- Example 1: pure CPU
  - Monte Carlo for global properties of BEC
- Example 2: CPU and memory
  - Exact diagonalization for study of BEC and FQHE
  - Large number of particles in studies of granular material
- Example 3: CPU and storage
  - Single runs sometimes produce large (TBs) outputs, or may need to process large inputs
- Ad hoc, fast, powerful, reliable computational platform - in short HPC!

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What HPC stands for?

- High Performance Computing
- The term is most commonly associated with computing used for scientific research. [from Wikipedia]
- It involves not only hardware, but software and people as well!
- HPC encompasses a collection of powerful:
    - hardware systems
    - software tools
    - programming languages
    - parallel programming paradigms

which make previously unfeasible calculations possible

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Only performance?

- High Throughput Computing
- High Availability Computing
- Capacity Computing
- Capability computing
- To reflect a greater focus on the productivity, rather than just the performance, of large-scale computing systems, many believe that HPC should now stand for High Productivity Computing

How to run applications faster ?

- There are 3 ways to improve performance:
  - Work Harder
  - Work Smarter
  - Get Help
- Analogy in computer science
  - Use faster hardware
  - Optimize algorithms and techniques used to solve computational tasks
  - Use multiple computers to solve a particular task
- All 3 strategies can be used simultaneously!

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Measures of performance

- How fast can I crunch numbers on my CPU?
- How fast can I move the data around?
  - from CPUs to memory
  - from CPUs to disk
  - from CPUs to/on different machines
- How much data can I store?

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CPU crunching

- Number of floating point operations per second (flops, Mflops, Gflops…)
- Comparison of theoretical and sustained peak performance
- Theoretical peak performance:
  - determined by counting the number of floating-point additions and multiplications that can be completed during a period of time, usually the cycle time of the machine
  - IPC=Instruction per Cycle

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Peak performance of modern systems

- My laptop: 9.6 Gflops
  - 4 IPC x 2 cores x 2.4 GHz
- Cluster at SCL: 6.6 Tflops
  - 4 IPC x 712 cores x 2.33 GHz
- sp6.cineca.it: 100 Tflops
  - 5300 Power6 processors @ 4.7Ghz
- Cray Jaguar, ORNL: 2331 Tflops
  - Opteron Six Core 2.6 GHz
  - 224162 cores

Sustained performance

- What your application is actually able to get from the computer hardware

- Example from previous century:

Table 1: Benchmark Results for NERSC's 644-PE Cray T3E

Benchmark	System Performance	Single Processor Performance	% of Peak
Theoretical peak	580.0 Gflop/s	900 Mflop/s	100.0%
Linpack	444.2 Gflop/s	690 Mflop/s	76.6%
LSMS code (Locally Self-consistent Multiple Scattering), 1998 Gordon Bell Prize-winning application	256.0 Gflop/s	398 Mflop/s	44.1%
Average of seven major NERSC applications	67.0 Gflop/s	~104 Mflop/s	11.6%
NAS Parallel Benchmarks	29.6 Gflop/s	~46 Mflop/s	5.1%

Data movement

- bit/s transmitted
- among computers: networks
  - default (commodity): 1 Gb/s
    - 1000 Mb/s = 1 Gb/s
  - custom (high speed)
    - 10Gb/s, 20 Gb/s and now 40Gb/s
- within the computer:
  - CPU – Memory: thousands of Mb/s
    - 10 - 100 Gb/s
  - CPU - Disks: MByte/s
    - 50 ~ 100 MB/s up to 1000 MB/s

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Storage sizes

- Size of storage devices:
  - kbyte/Mbyte ----> caches / RAM
  - Gigabyte ----> RAM / hard disks
  - Terabyte ----> Disks / SAN
  - Petabyte ----> SAN / Tapes

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HPC architecture

HPC architectures try to maximize performance simultaneously on all the three aspects (number crunching/ data access /data storage) by using many Processing Elements (CPUs) together to solve a given task

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What is parallel computing?

- Parallel computing is the simultaneous execution of the same task (split up and specially adapted) on multiple processors in order to obtain results faster
- The process of solving a problem usually can be divided into smaller tasks, which may be carried out simultaneously with some coordination

[from Wikipedia]

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High performance problem example:

picture from http://www.f1nutter.co.uk/tech/pitstop.php

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Analysis of the parallel solution

- Functional decomposition
  - different people are executing different tasks

- Domain decomposition
  - different people are solving the same global task but on smaller subset

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HPC parallel computers

- The simplest and most useful way to classify modern parallel computers is by their memory model.

- How CPUs view and can access the available memory?
  - SHARED MEMORY
  - DISTRIBUTED MEMORY

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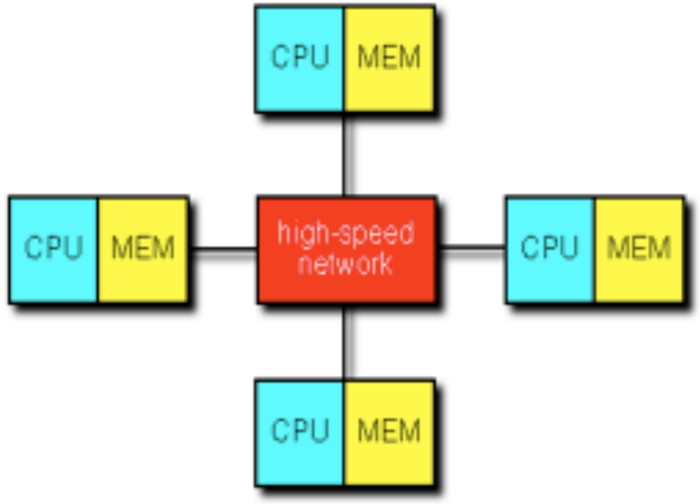
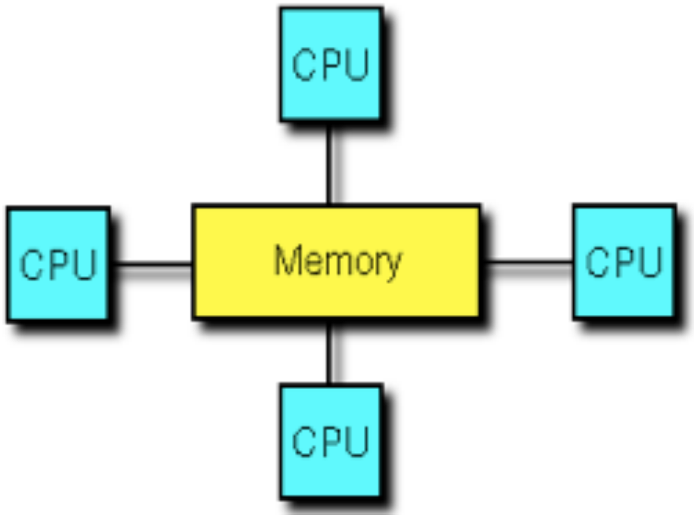
Shared vs. Distributed

- Distributed Memory:
  - Each processor has its own local memory. Must do message passing to exchange data between processors.
  - Multi-computers



- Shared Memory
  - Single address space. All processors have access to a pool of shared memory.
  - Multi-processors



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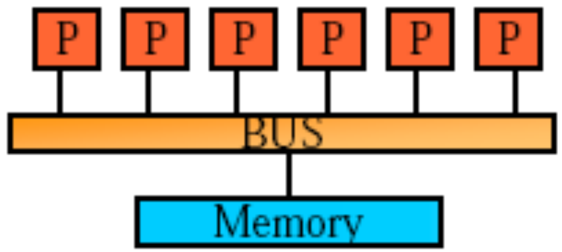
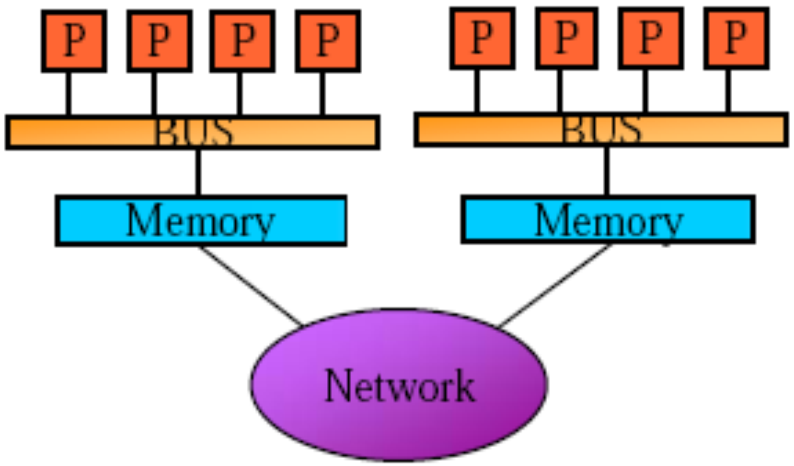
Shared Memory: UMA vs. NUMA

- Uniform memory access (UMA): Each processor has uniform access to memory. Also known as symmetric multiprocessors (SMP).



- Non-uniform memory access (NUMA): Time for memory access depends on location of data. Local access is faster than non-local access.



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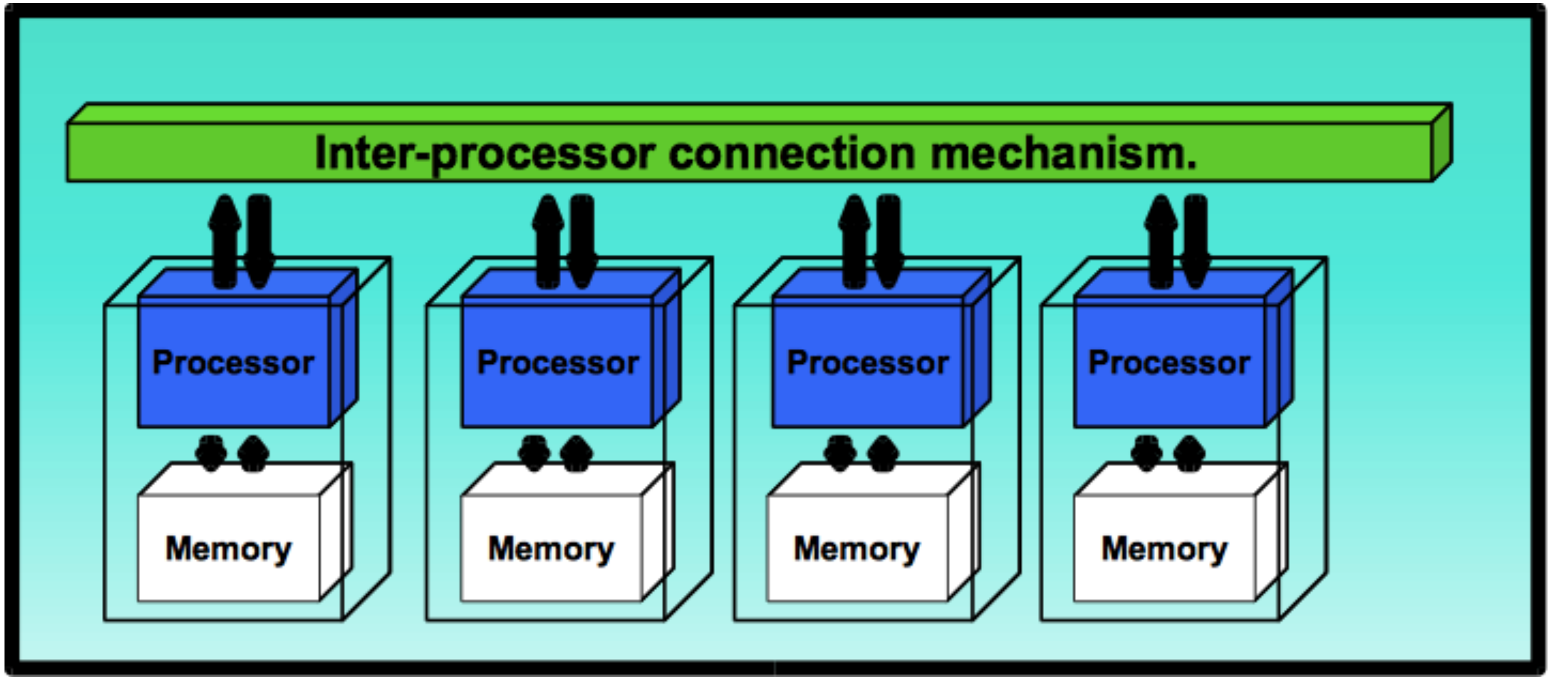
Clusters: distributed memory

- Independent machines combined into a unified system through software and networking



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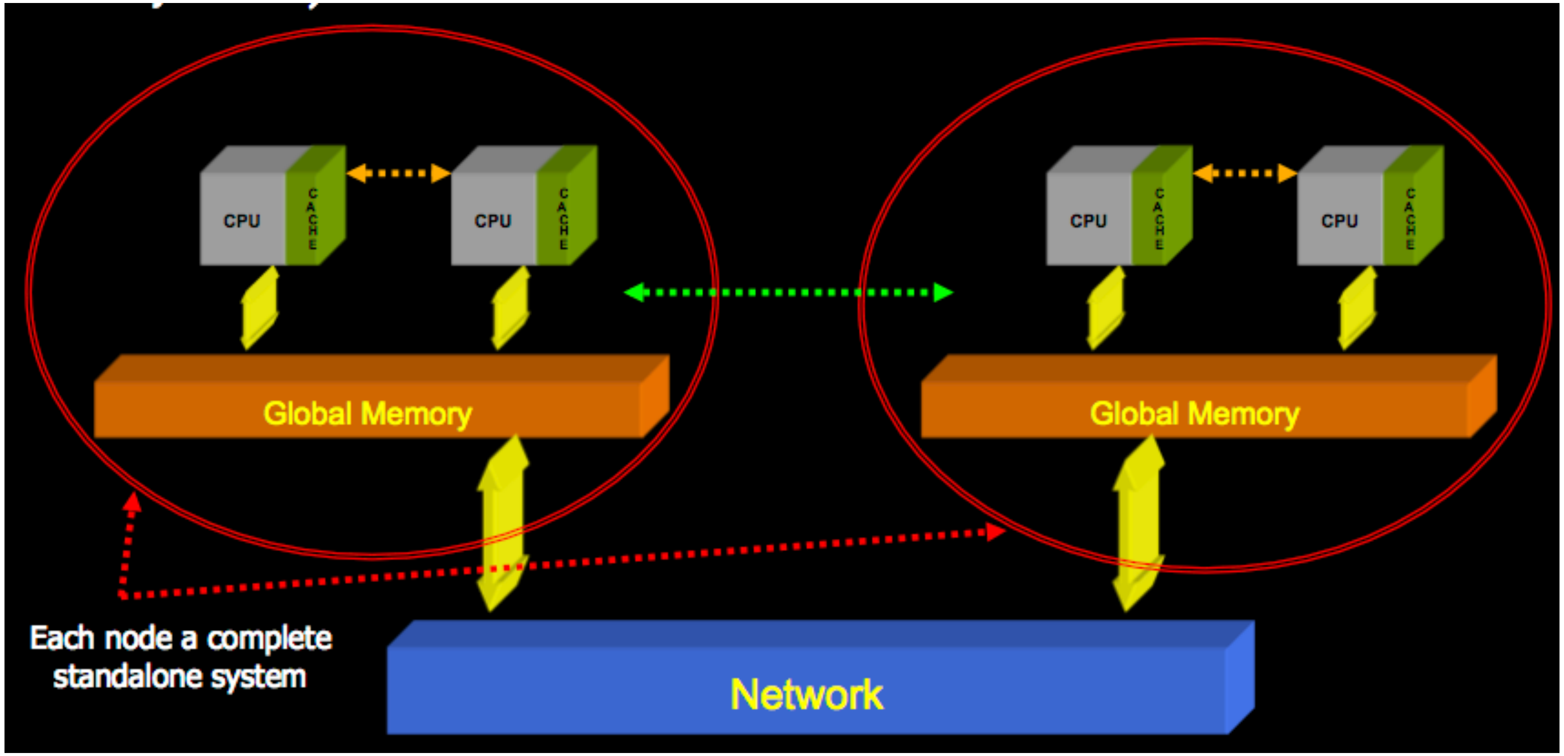
Hybrids

- Modern clusters have hybrid architecture
- Many-core CPUs make each node a small SMP system



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Parallel Programming Paradigms

- Memory models determine programming paradigms

Parallel machines	
Distributed memory	Shared memory
Parallel paradigms	
Message passing	Data parallel
All processes could **directly access only their local memory.** Explicit messages are requested to access remote memory of different processors.	Single memory view. all processes (usually threads) could **directly access the whole memory.**

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Parallel performance

- The speedup of a parallel application is

  Speedup(p) = Time(1) / Time(p)

  where

  Time(1) = execution time for a single processor

  Time(p) = execution time using p parallel processors
- If **Speedup(p) = p**, we have a perfect speedup (also called linear scaling)

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Absolute performance

- Speedup compares performance of an application with itself on one and on p processors
- More useful to compare:
  - The execution time of the best serial application on 1 processor

  vs.

  - The execution time of best parallel algorithm on p processors

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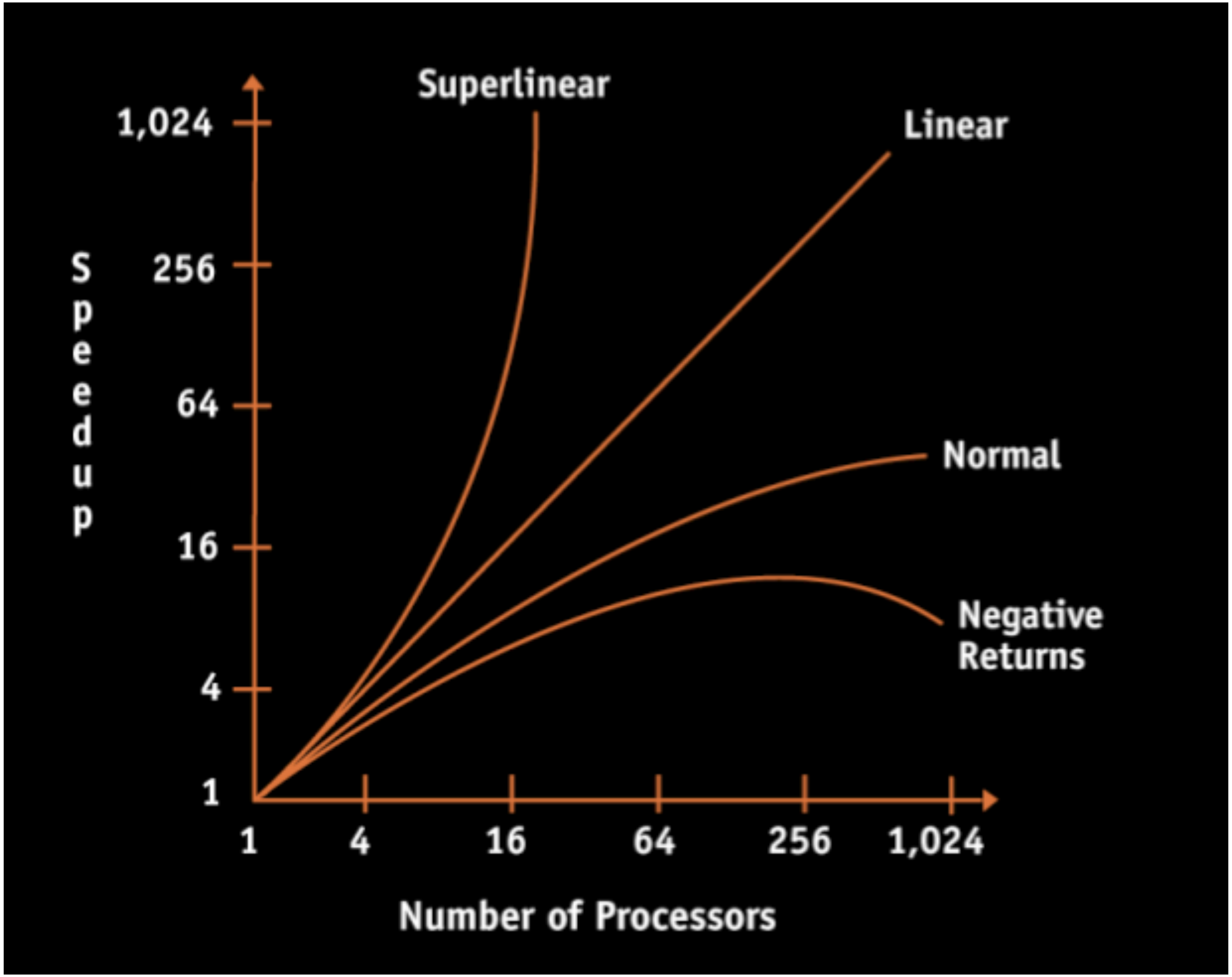
Speedup



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Superlinear speedup?

- Can we find **superlinear** speedup, i.e.

  Speedup(p) > p
- Yes, we can:
  - Choosing a bad “baseline” for T(1)
    - Old serial code has not been updated with optimizations
  - Shrinking the problem size per processor
    - May allow it to fit in small fast memory (cache)
    - Total time decreased because memory optimization tricks can be played.

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Question

- Algorithm A and algorithm B solve in parallel the same problem
- We know that on 64 core:
  - Program A gets a speedup of 50
  - Program B gets a speedup of 4
- Which one do you choose ?
  - 1) program A
  - 2) program B
  - 3) None of the above

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Answer

- None of the above, since we do not know the **overall execution time** of each of them!
- What if A is sequentially 1000 time slower than B?
- Always use the best sequential algorithm for computing speedup (absolute speedup)
- And the best compiler to produce the executable, for both serial and parallel version of the application!

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Limits to speedup

- All parallel programs contain:
  - Parallel sections
  - Serial sections
- Serial sections limit the speed-up:
  - Lack of perfect parallelism in the application or algorithm
  - Imperfect load balancing (some processors have more work)
  - Cost of communication
  - Cost of contention for resources, e.g., memory bus, I/O
  - Synchronization time
- Understanding why an application is not scaling linearly will help finding ways improving the applications performance on parallel computers.

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Amdahl's law (1)

- Let *s* be the fraction in an application representing the work done serially
- Then, 1-*s* = *P* is fraction done in parallel
- What is the maximum speedup for N processors?

$$speedup = \frac{1}{(1-P)+\frac{P}{N}} \Rightarrow \lim_{N\to\infty} \frac{1}{1-P}$$

- Even if the parallel part scales perfectly, we may be limited by the sequential portion of the code!

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Amdahl's law (2)

- The presence of a serial part of the code is quite limiting in practice:

>	2	4	8	32	64	256	512	1024
5%	1.91	3.48	5.93	12.55	15.42	18.62	19.28	19.63
2%	1.94	3.67	6.61	16.58	22.15	29.60	31.35	32.31
1%	1.99	3.88	7.48	24.43	39.29	72.11	83.80	91.18

- Amdahl's Law is relevant only if serial fraction is independent of the problem size
- Fortunately, the proportion of the computations that are sequential (non parallel) usually decreases as the problem size increase (a.k.a. Gustafson's law)

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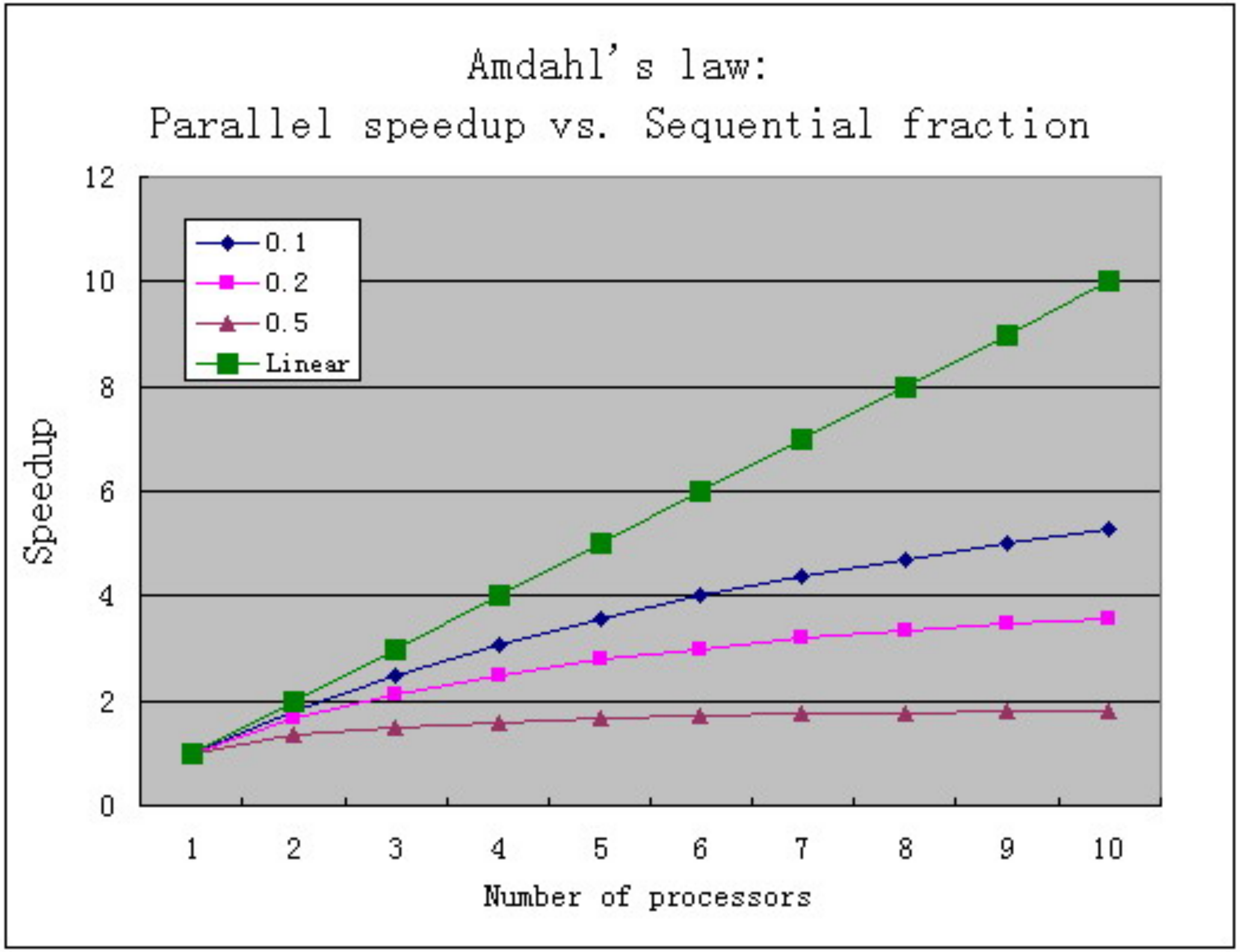
Effective parallel performance



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Linux cluster revolution

- The adoption of clusters virtually exploded since the introduction of the first Beowulf cluster in 1994
- The ingredients / attraction lies in:
  - low costs of both hardware and software
  - affordable interconnect technologies
  - the control that builders / users have over their own systems
- The problems:
  - you should be an expert to build and run efficiently your clusters
  - not always the problem you have fits into a cluster solution (even if this is cheap!)

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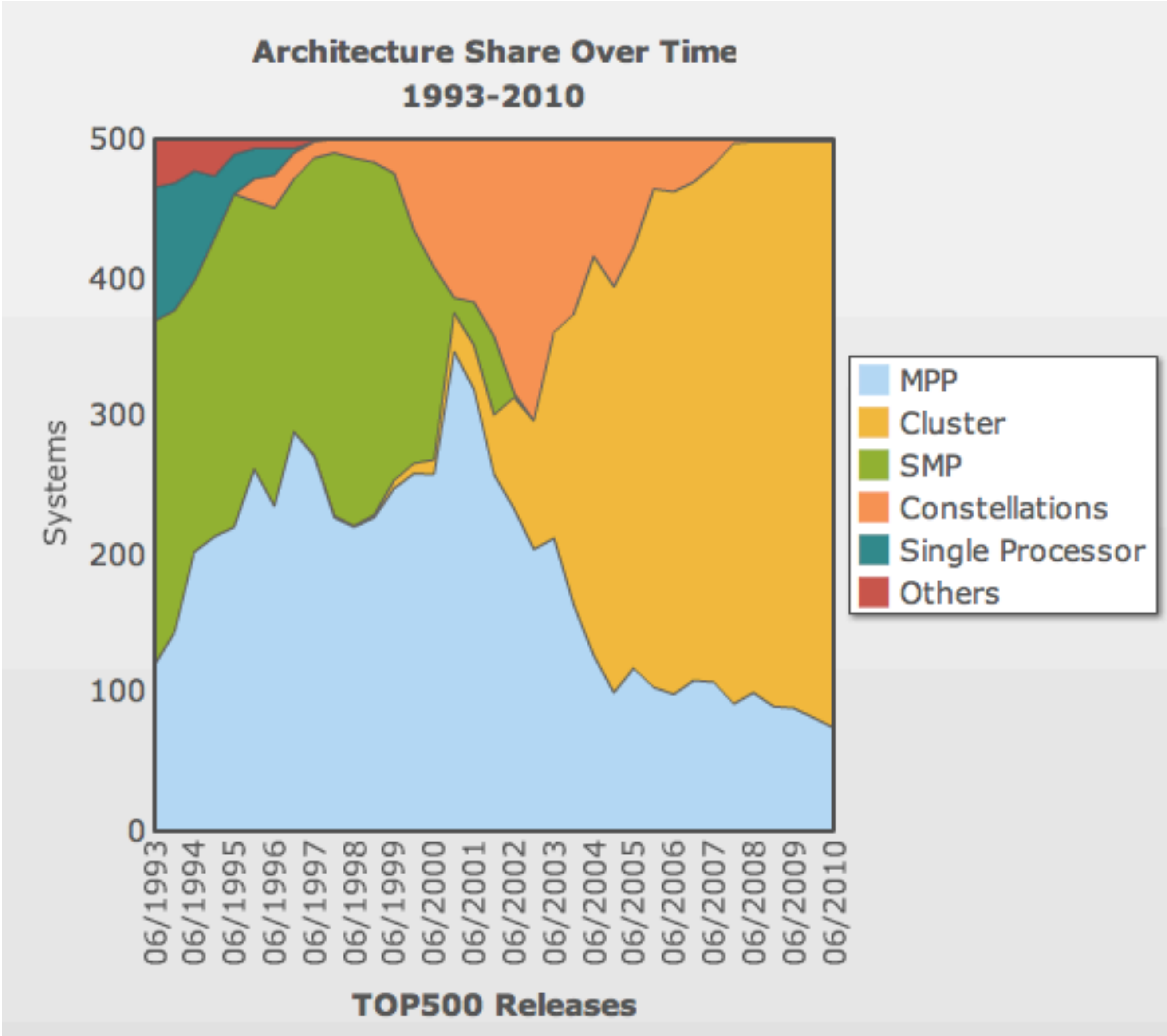
Clusters on Top500



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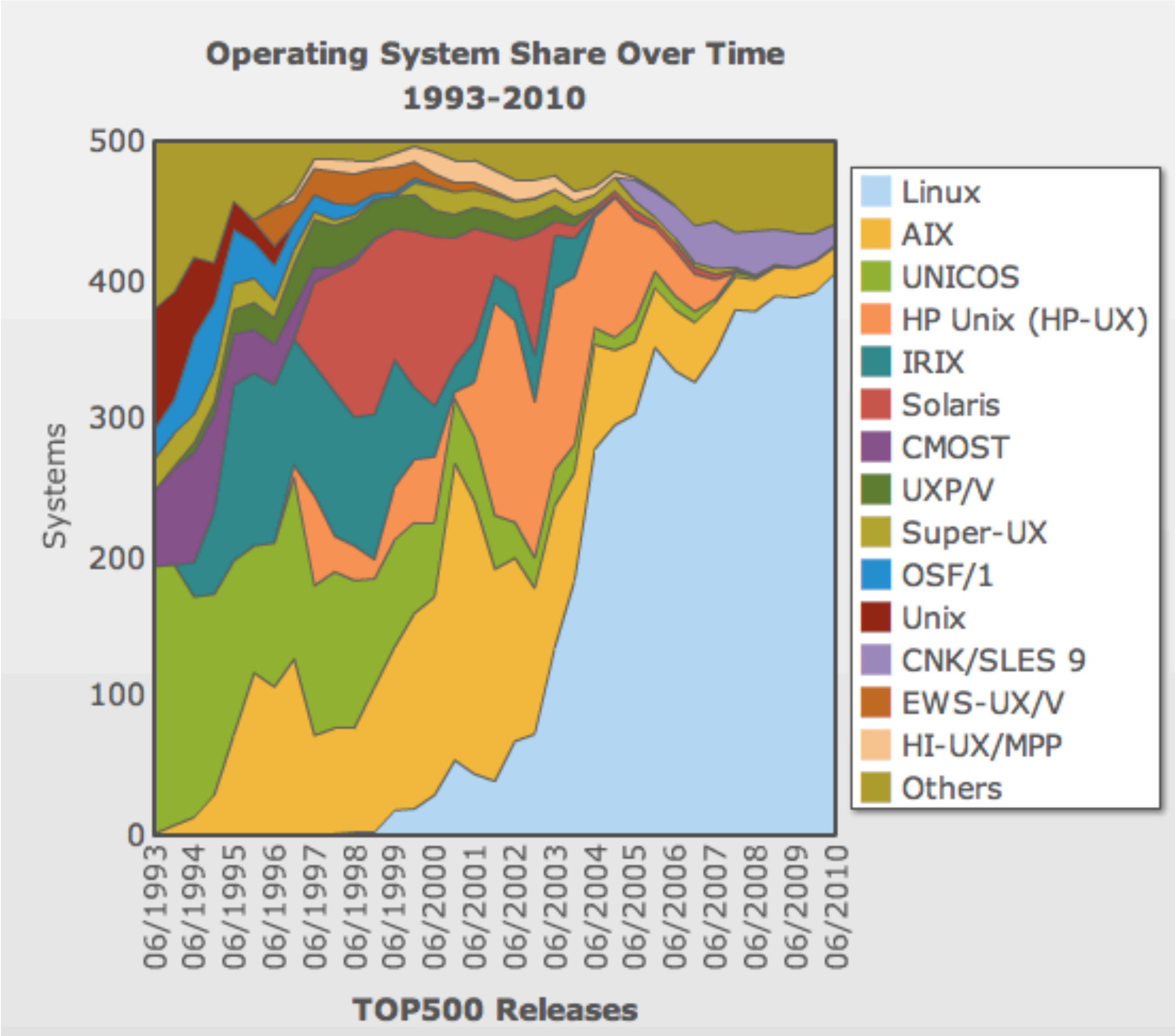
Linux clusters on Top500



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GRID: cluster of clusters

- Motivation: When communication is close to free we should not be restricted to local resources when solving problems.
- A Grid Infrastructure built on top of the Internet and the Web to enable and exploit large scale sharing of resources
- It should provides **Scalable, Secure, Reliable** mechanisms for discovery and for remote access of resources.

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Resource sharing

- **Applications**: web services technology
- **CPU and Storage**: Grid computing, Cloud Computing, etc.
- **Data**: Data Grid, Virtual Observatory, Google Filesystem, etc.
- **Instruments**: Virtual Labs, collaboration tools, etc.

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Building a computational infrastructure

- Open source software + commodity (off the shelf) hardware provide now tools to build low cost HPC infrastructure based on clusters
- GRID infrastructures are just two clicks away and can provide large amounts of resources
- Planning of a computational infrastructure depends on your needs

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Elements of a computational infrastructure

- Hardware
  - The basic bricks
- Software
  - To make hardware usable
- People
  - Installers / sys admins / planners / users etc..
- Problems to be solved
  - Any action in building such an infrastructure should be motivated by real needs

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What infrastructure do you need?

- Applications
  - Parallel
    - Tightly coupled
    - Loosely coupled
    - Embarrassingly parallel
  - Serial
    - Memory / I/O requirements
- User community
  - Large /Small
  - Distributed or not?
  - Homogeneous /heterogeneous
- Budget considerations

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HPC projects

- HP-SEE regional HPC project
- PRACE-1IP: European Tier-0 systems
- PRACE-2IP: European Tier-1 systems

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Conclusions (1)

- Modern scientific research need lots of computational resources provide by HPC/GRID infrastructures
- HPC means parallel computing
- GRID means pooling of geographically distributed resources
- HPC and GRID computing are not mutually exclusive but can be both used to address computational resources in a transparent way.
- The challenge is now to build your own computational infrastructure **driven by real needs**

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Conclusions (2)

- With access to commodity HPC hardware and a free OS such as Linux, entry-level HPC is within reach of even the most modest budget.
- It is relatively easy to join large Grid infrastructures that make available large amount of computational resources.

However:

- To fully exploit HPC/GRID one needs to obtain detailed knowledge of HPC/GRID architectures as well as master HPC/GRID development tools and advanced programming techniques.
- We hope to give some insight about these in this two week school!

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