GRID AND HPC WORKSHOP V
IPM TEHRAN, IRAN

Computational Infrastructures Overview

Mohammad Reza Gerami
Institute for Research in Fundamental Sciences
gerami@ipm.ir

Agenda

- Computing resources concepts
  - ✓ Server
  - ✓ Cluster
  - ✓ High Performance Computing (HPC)
  - ✓ Grid
  - ✓ Cloud

New challenges in science

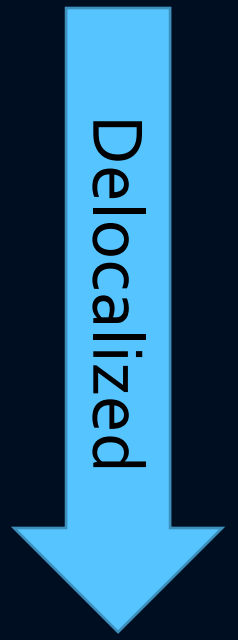
- Going further in scientific knowledge
  - New high sensitivity sensors and instruments
  - Globally distributed collaborations
  - Computing Infrastructures Cluster
- Delocalized knowledge
  - Scientific and technical knowledge is "distributed"
  - Laboratories are distributed
  - Scientific data are distributed

Computing infrastructure (1)

- Anything it allows to solve a computational scientific problem:
  - From laptops to supercomputers
  - From "local" to distributed environments
- Different infrastructures require different approach
- Possibility to use more than one computing infrastructure (CI) to solve the problem

Computing infrastructure (2)

- From localized to distributed:
  - Server
  - Cluster
  - Grid
  - Clouds



Server

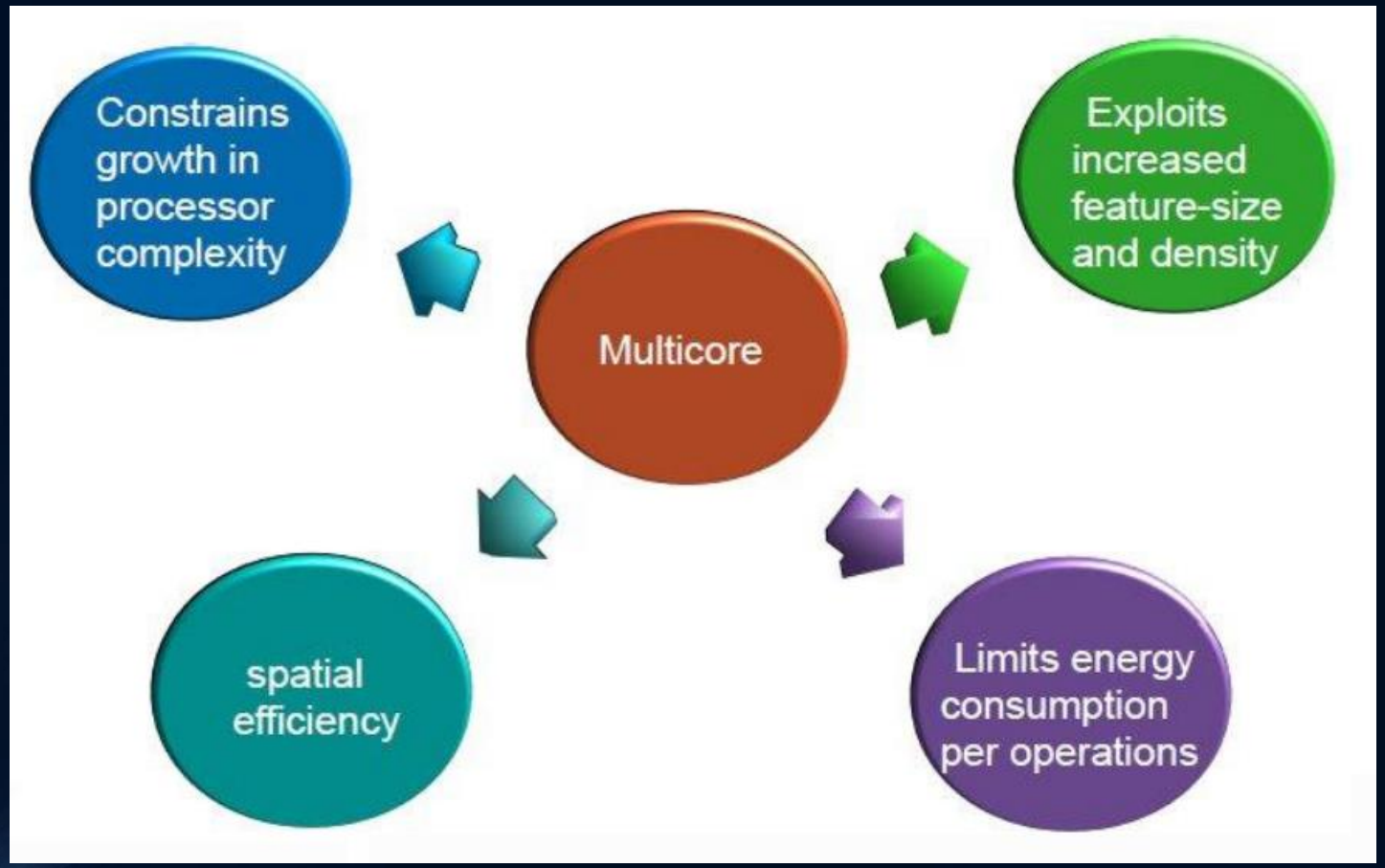
Main server components

- ✓ CPU
  - Multicore architecture
- ✓ RAM
  - Performance impact
- ✓ GPU

Multicore CPUs

- ✓ CPUIntegrated circuit chips (CPU) containing more than one identical physical processor (core) and each core as a unique processor by the OS
- ✓ Each core has its own complete set of resources, and may share the on-die caches
- ✓ What is a multi processor?
  - A collection of multicore CPUs

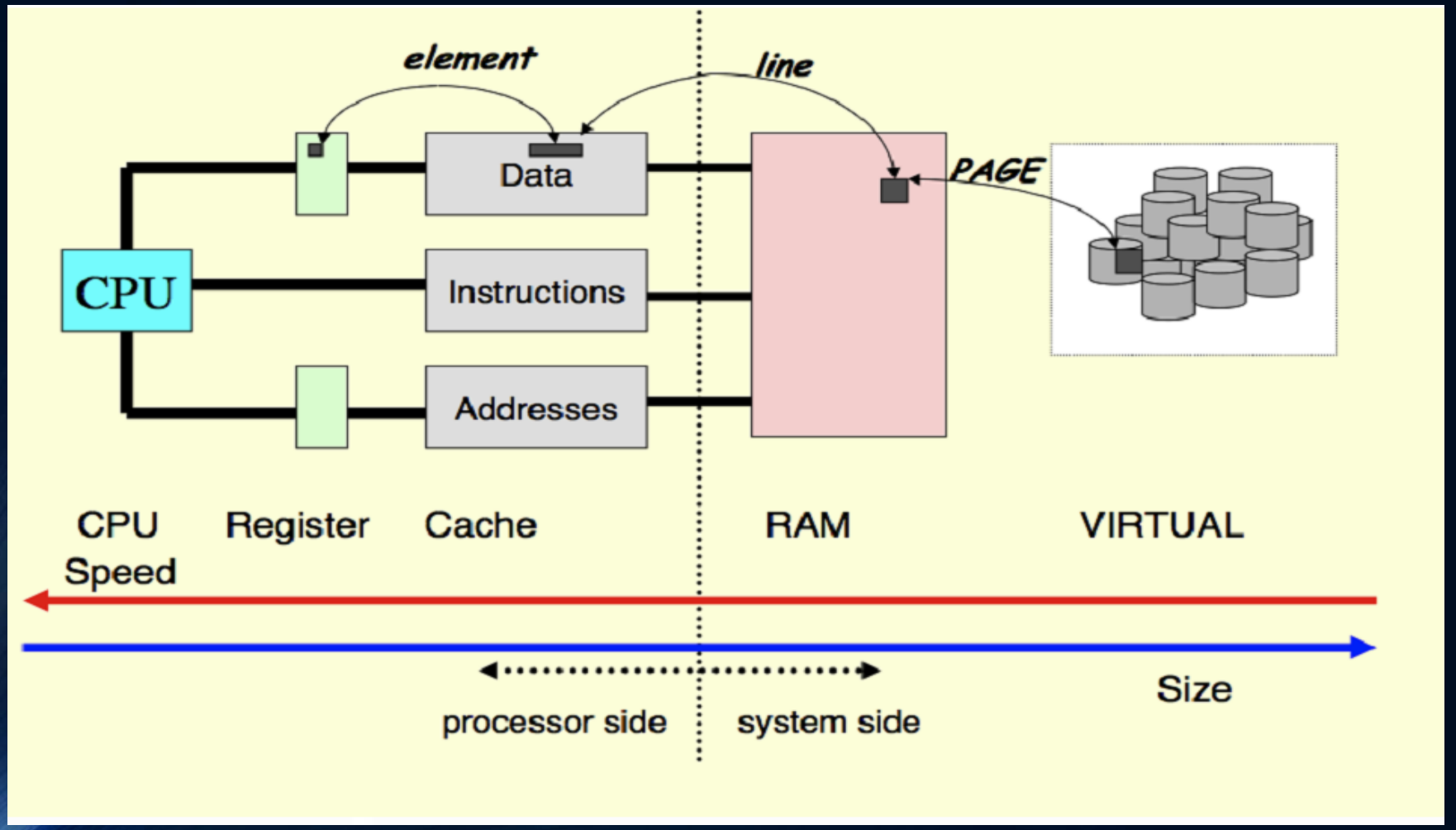
Why using multicore?



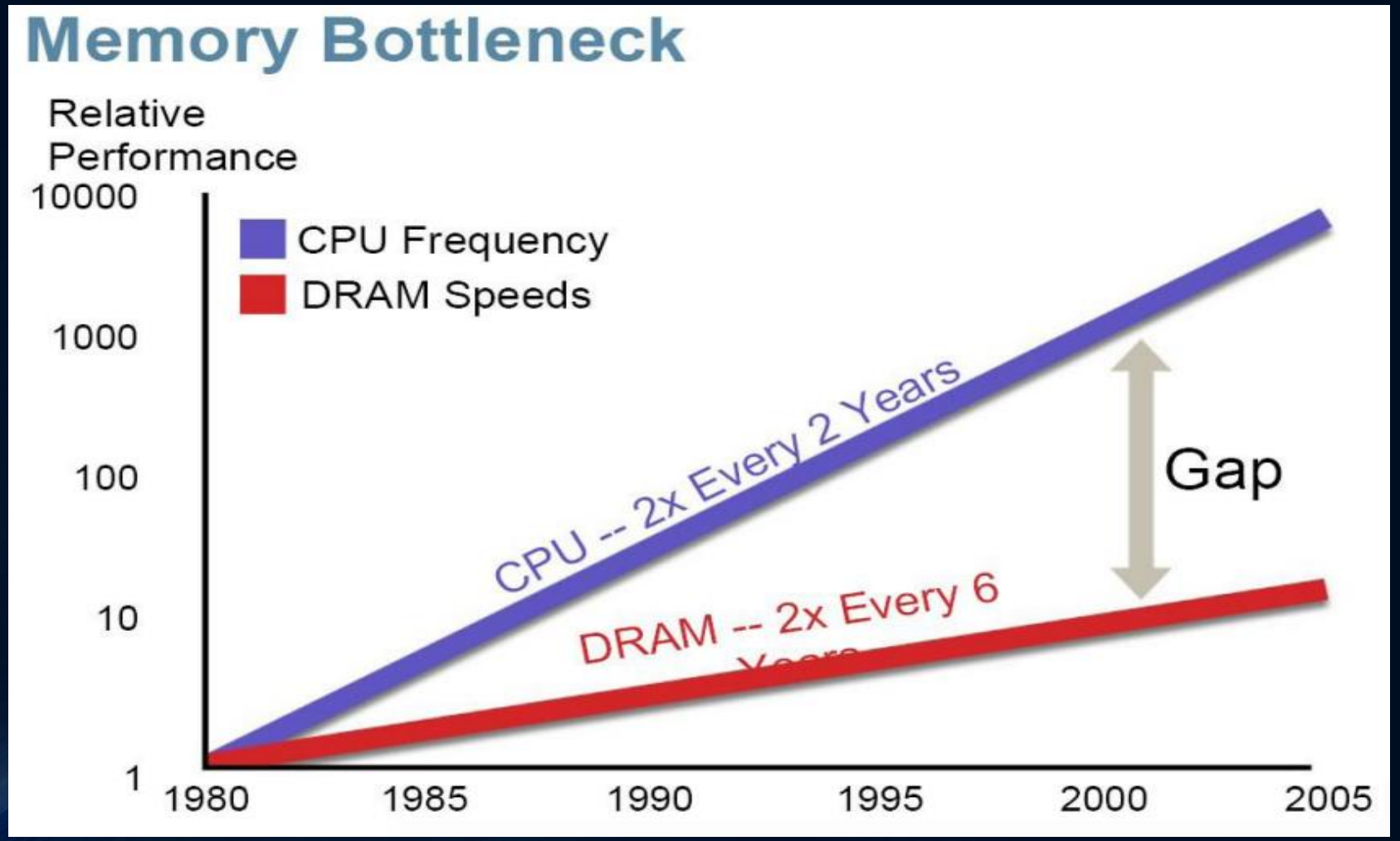
Main CPU producers

- ✓ Intel
  - ✓ Xeon
    - ✓ Nehalem
    - ✓ Sandy Bridge
- ✓ AMD
  - ✓ Opteron
    - ➢ K10 based
      - ✓ Magny-cours (up to 12 cores)
    - ➢ Bouldozzer based
      - ✓ Interlagos (up to 16 cores)

Cache and memory



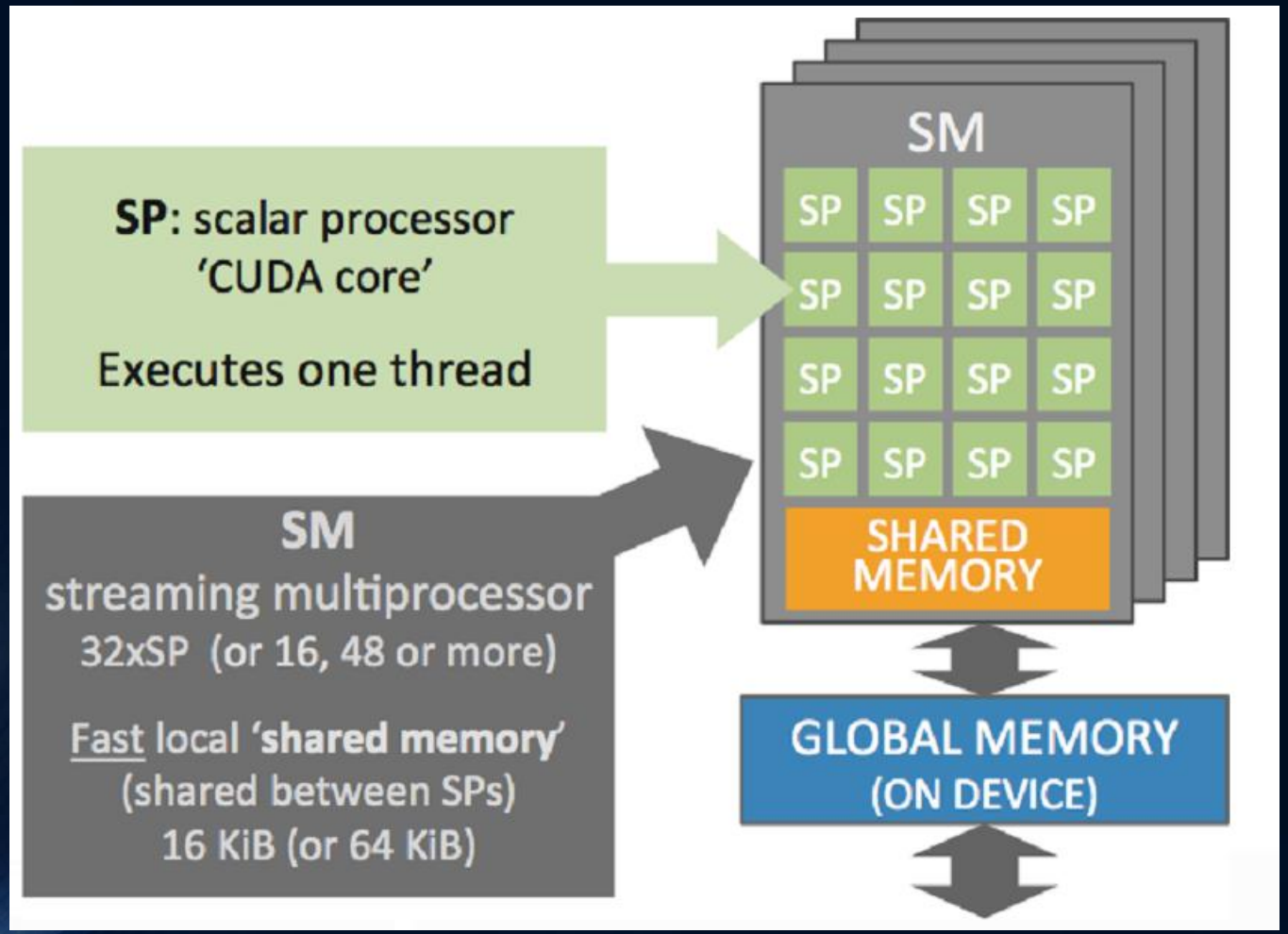
Memory wall problem (2)



GPU (1)

- ✓ Become very popular in past few years
- ✓ General Purpose Computing on GPUs -GPGPU
- ✓ Usage of a GPU (graphics processing unit) to do general purpose scientific and engineering computing
- ✓ Massively parallel architecture
- ✓ CPU and GPU run together in a heterogeneous co-processing computing model

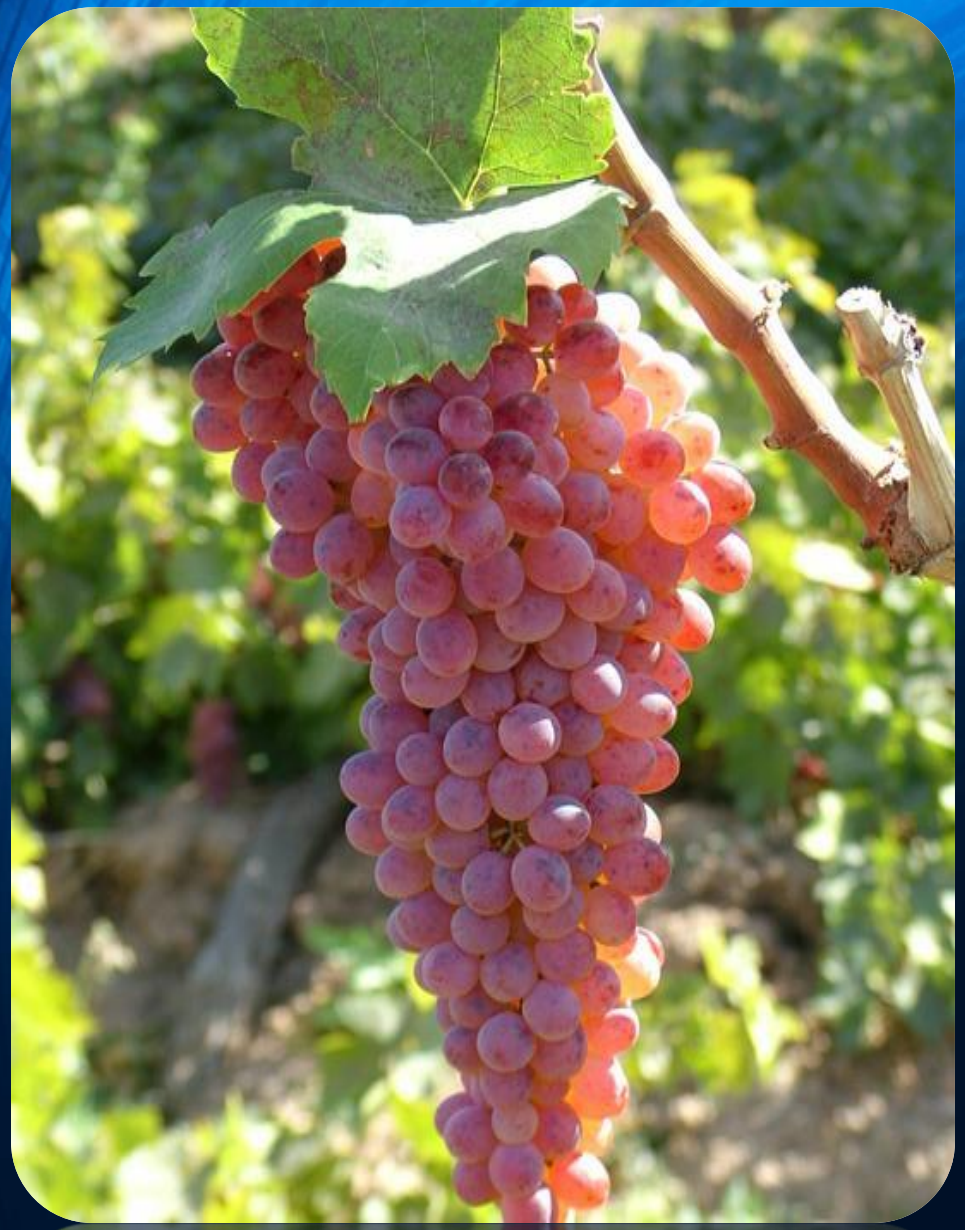
GPU (2)


SP: scalar processor
'CUDA core'
Executes one thread
SM
streaming multiprocessor
32xSP (or 16, 48 or more)
Fast local 'shared memory'
(shared between SPs)
16 KiB (or 64 KiB)
SM
SP SP SP SP
SP SP SP SP
SP SP SP SP
SP SP SP SP
SHARED MEMORY
GLOBAL MEMORY
(ON DEVICE)

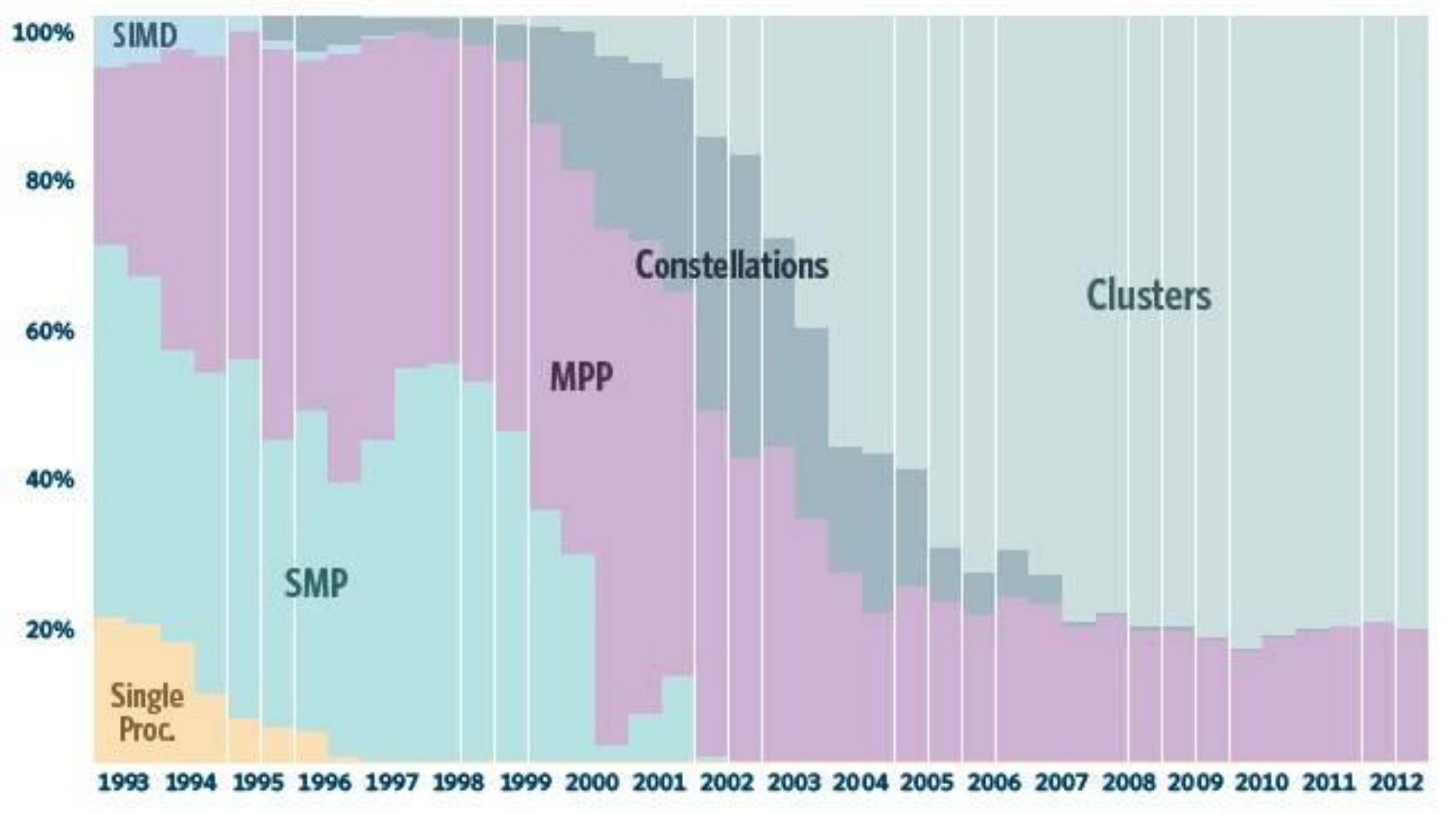
GPU (3)

- ✓ Two main GPUs designers:
  - ❖ Nvidia
    - ✓ CUDA "Compute Unified Device Architecture"
    - ✓ Hardware and software architecture for issuing and managing computations on GPU
    - ✓ C for CUDA (C++ for CUDA) C/C++ language with some additions and restrictions
  - ❖ ATI
    - ✓ Stream Technology
- ✓ OpenCL

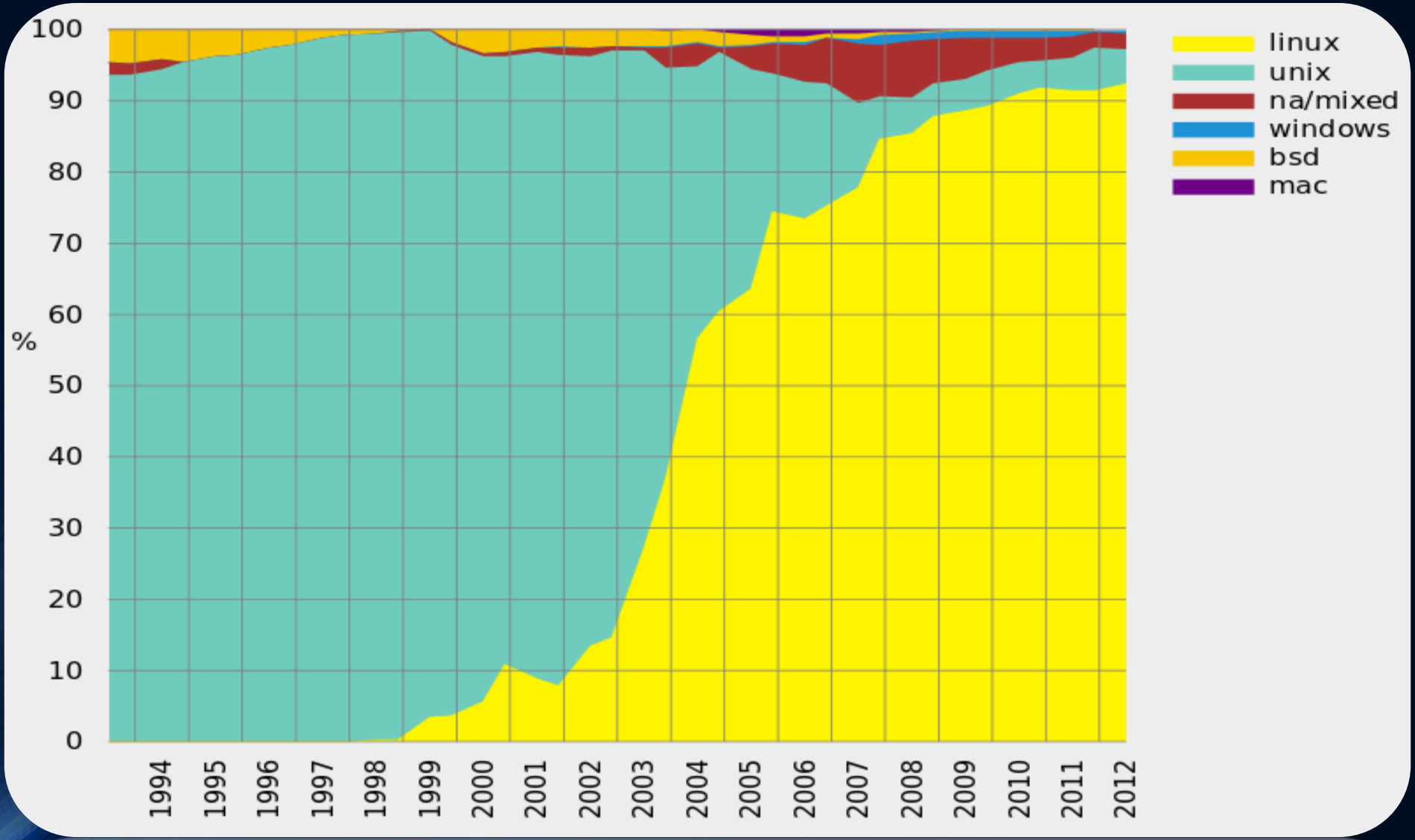
The cluster



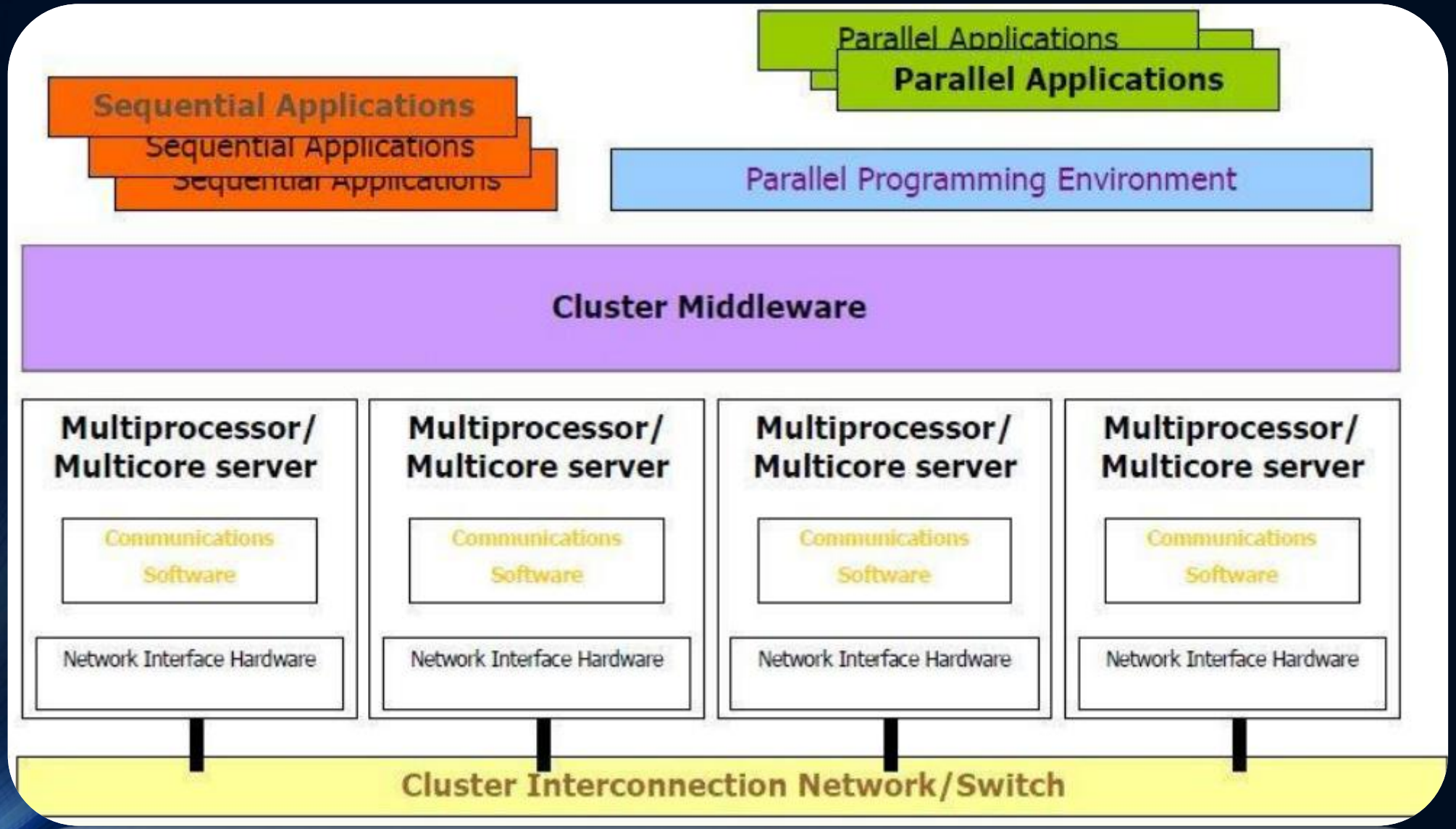
Evolution of cluster architectures in top500



Evolution of operating systems in top500



Cluster architecture (1)



Cluster architecture (2)

- Servers are the nodes (cluster components of different nature: login nodes, computing nodes, service nodes…)
- Nodes are connected using a network
  - ✓ Topology
- Interconnection characteristics
  - ✓ Latency: Initialization time before data can be sent
    - How much does it take to open the channel ?
  - ✓ Per-link Peak Bandwidth: Maximum data transmission rate (varies with packet size)
    - How wide is my channel ?
  - ✓ Bisection Bandwidth:
    - Bandwidth available if one half of nodes try communicating with the other half simultaneously.

Cluster networks

- HIGH SPEED NETWORK
  - parallel computation
    - Low latency /high bandwidth
    - Usual choices: Myrinet / Infiniband…
- I/O NETWORK
  - I/O requests (NFS and/or parallel FS)
    - latency not fundamental/ good bandwidth
- Management network
  - Management traffic
    - Any standard network (fast ethernet OK)

Servers and clusters

- Local resources
  - ✓ Price/performance when compared with a dedicated parallel supercomputer
  - ✓ Great opportunity for low budget institution
  - ✓ Flexibility: many ad hoc solution for different problems…
  - ✓ Open Technology
- Complex to build and maintain

HPC concepts

Resources needed for different problems

- pure CPU
- CPU and memory
- 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!

What is HPC?

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

Why is HPC important?

- We continually demand more and more computing power
- We want to reduce the execution time of our important applications
- We want to overcome the limitations of desktop computing architectures
- HPC-capable architectures are becoming more ubiquitous, user friendly and affordable

HPC architectures

- HPC architectures try to maximize performance simultaneously on all the three important aspects
  - ✓ number crunching (number of floating point operations per second (flops, Mflops, Gflops…)
  - ✓ data access (bit/s transmitted among computers or within the computer)
  - ✓ data storage (size of storage devices: caches, RAM, disks, tapes)

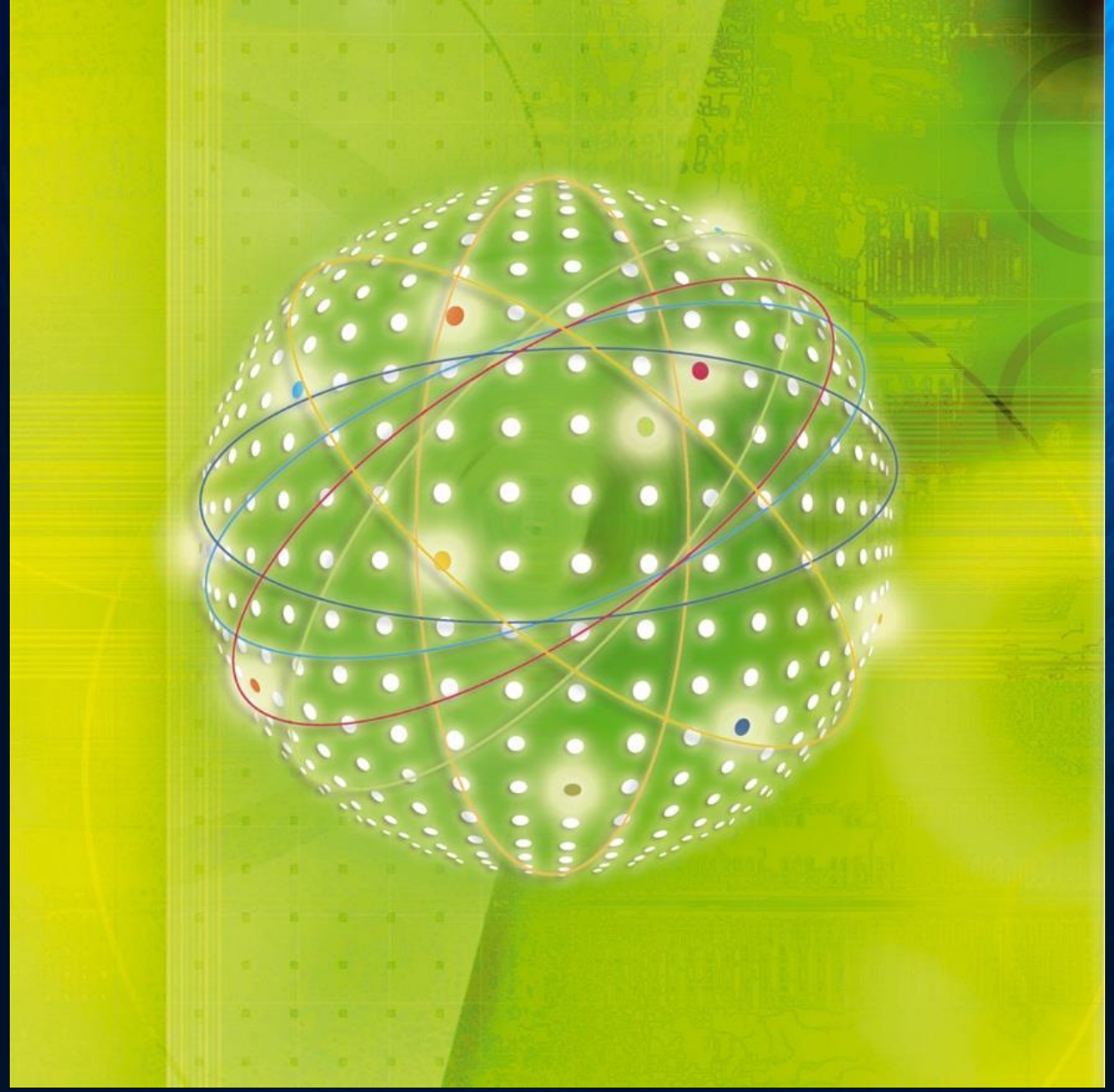
  by using many Processing Elements (CPUs) together to solve a given task

PARALLEL COMPUTING

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]
- The simplest and most useful way to classify modern parallel computers is by their memory model:
  - ✓ SHARED MEMORY
  - ✓ DISTRIBUTED MEMORY

Grid



From clusters to Grids

- Problem 1: clusters cannot be used by end users transparently
- Problem 2: even when access is granted to users to several clusters, they tend to neglect smaller clusters
- Problem 3: distribution of input/output data, sharing of data between clusters

Grid: Cluster of clusters

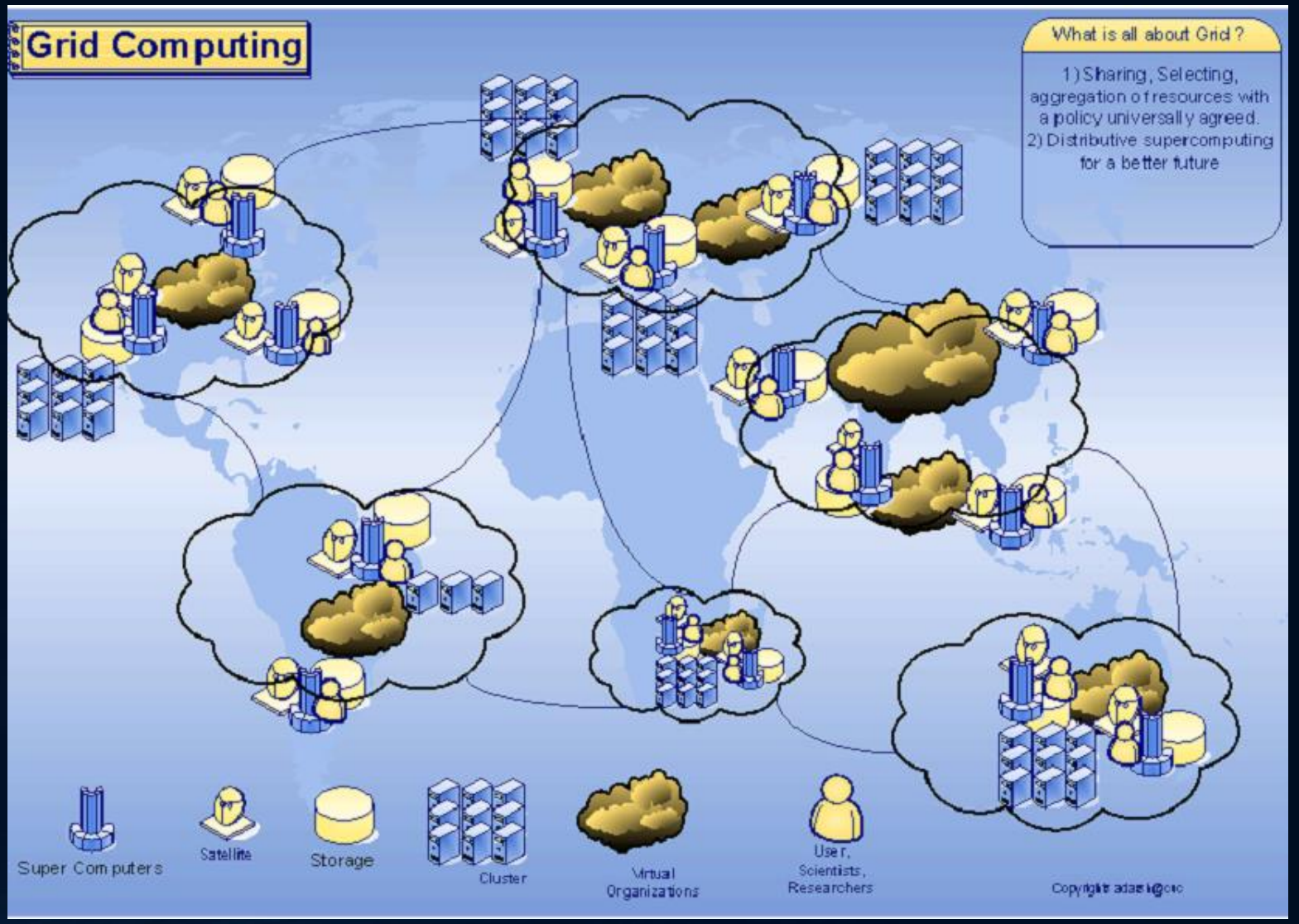
- Motivation:
  - When communication is close to free we should not be restricted to local resources when solving problems
  - Large amount of data produced
  - Large worldwide organized collaborations
    - e.g. Large Hadron Collider (LHC) at CERN
- A Grid Infrastructure built on top of the Internet 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.

Grid definitions

- "a single seamless computational environment in which cycles, communication, and data are shared, and in which the workstation across the continent is no less than one down the hall"
- "wide-area environment that transparently consists of workstations, personal computers, graphic rendering engines, supercomputers and non-traditional devices: e.g., TVs, toasters, etc."
- "[framework for] flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources"
- "collection of geographically separated resources (people, computers, instruments, databases) connected by a high speed network [...distinguished by...] a software layer, often called middleware, which transforms a collection of independent resources into a single, coherent, virtual machine"

Unifying concept: Grid

Resource sharing and coordinated problem solving in dynamic , multi-institutional virtual organizations



Grid analogy

- Electrical power grid
  - You never worry about where the electricity you are using comes from, if it is from coal in Australia, from wind power in the U.S. or from a nuclear plant in France. You simply know that when you plug your toaster in to the wall socket, it will get the electrical power you need to do the job

- Computing Grid
  - You would never worry about where the computer power you are using comes from, if it is from a supercomputer in Germany, a computer farm in India or a laptop in New Zealand. You simply know that when you plug your computer in to the Internet, it will get the computer power you need to do the job -from GridCafe (http://www.gridcafe.org/)

Grid Resources

- Storage systems
- Computer clusters
- HPC clusters
- Supercomputers
- Databases
- Keyword: heterogeneous as regards hardware and software

What problems Grid addresses?

- Too hard to keep track of authentication data (ID/password) across institutions
- Too hard to monitor system and application status across institutions
- Too many ways to submit jobs
- Too many ways to store & access files/data
- Too many ways to keep track of data
- Too easy to leave "dangling" resources lying around (robustness)

Local vs Remote

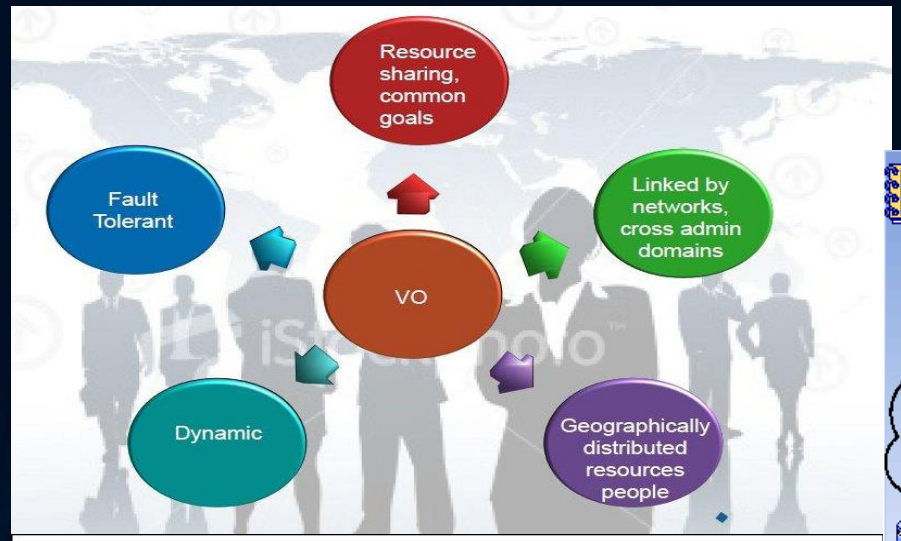
- Resources are locally managed
  - Policies
  - Accountability
  - OS
  - Storage systems
  - Batch systems
- Global policies
- Global accessibility
- Dynamic resource identification
- Remote resource utilization

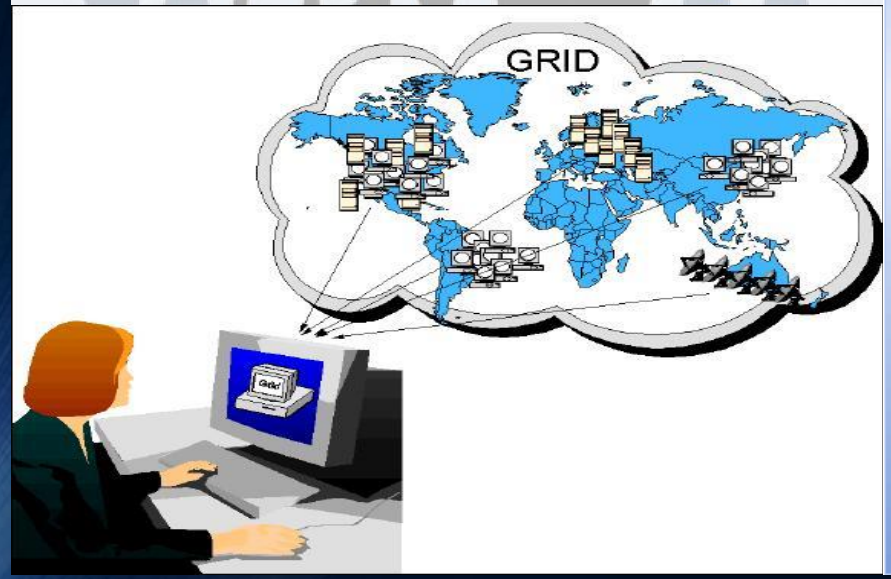
VO Concepts (1)

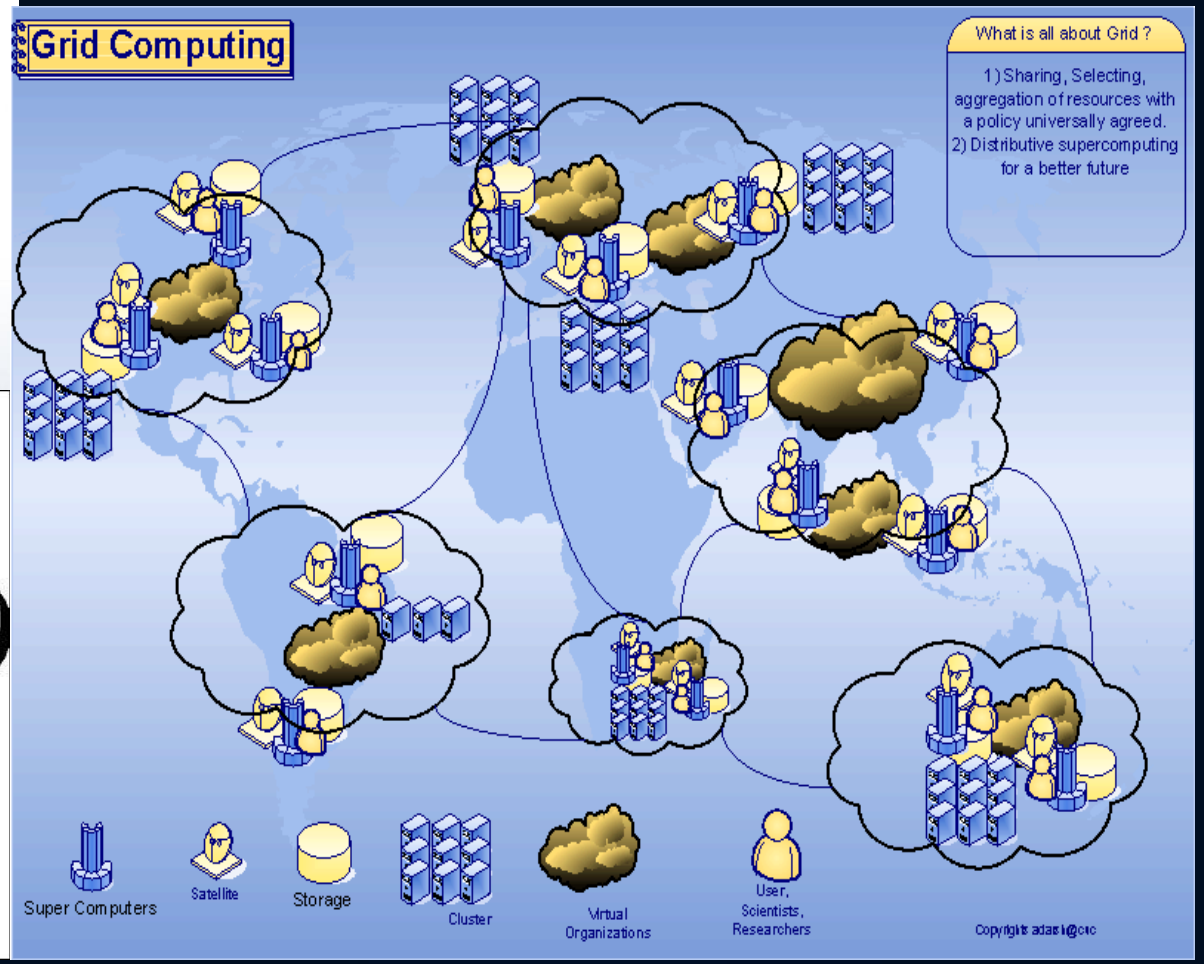
- The size and/or complexity of the problem requires that people in several organizations collaborate and share computing resources, data, instruments

VIRTUAL ORGANIZATIONS

VO Concepts (2)



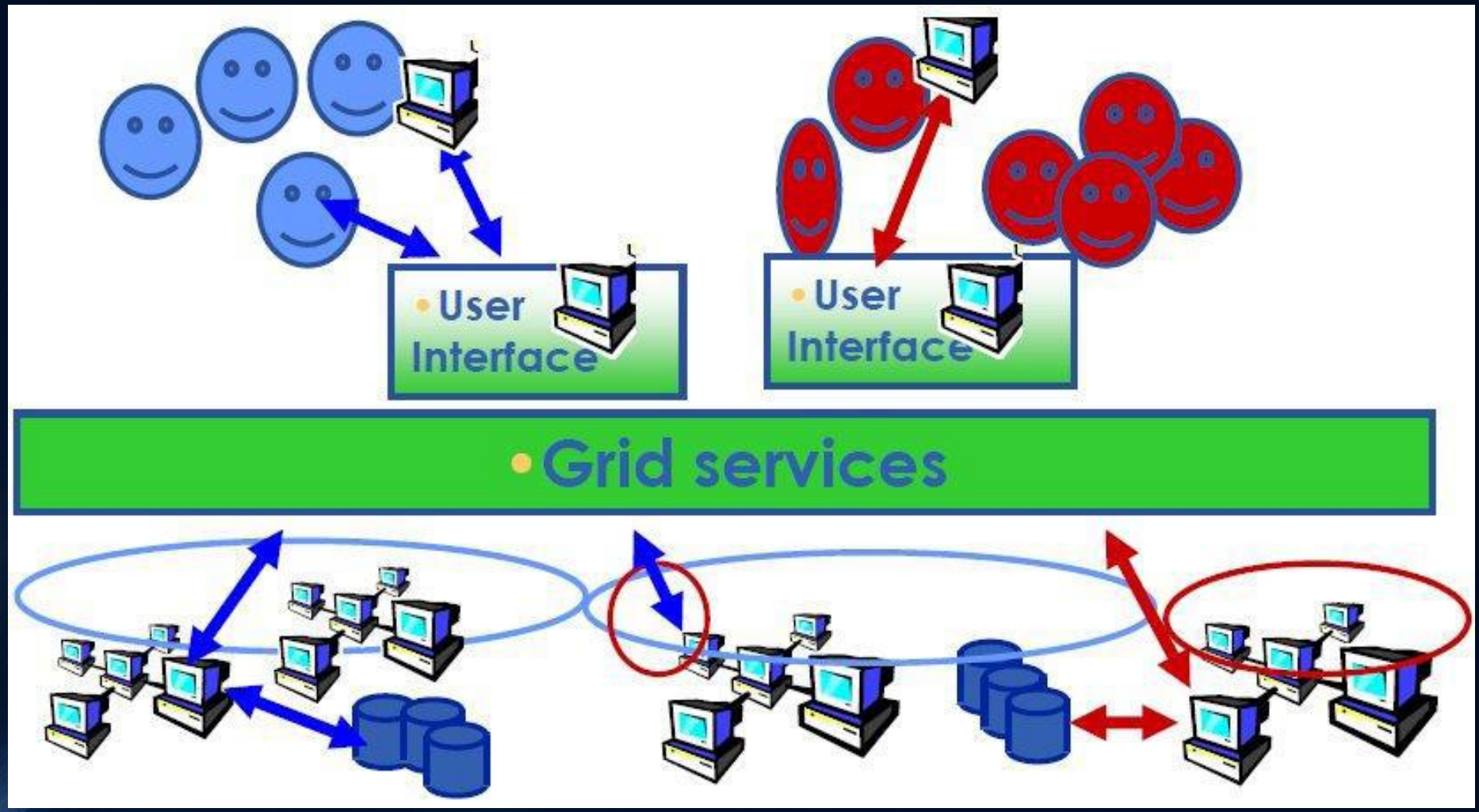




The Grid Middleware

- Its the software layer that glue all the resources
- Everything that lies between the OS and the application
- Grid is as Operating System:
  - different middleware = different Grid
- Globus alliance (Globus Toolkit)
- gLite (EGI middleware)
- Unicore (DE)
- ARC

User view of the Grid



Cloud

Cloud computing (1)

- Even the definition is "cloudy"
- "A computing capability that provides an abstraction between the computing resource and its underlying technical architecture (e.g., servers, storage, networks), enabling convenient , on-demand network access to a shared pool of configurable computing resources that can be rapidly provisioned and released with minimal management effort of service provider interaction." -National Institute of Standards and Technology

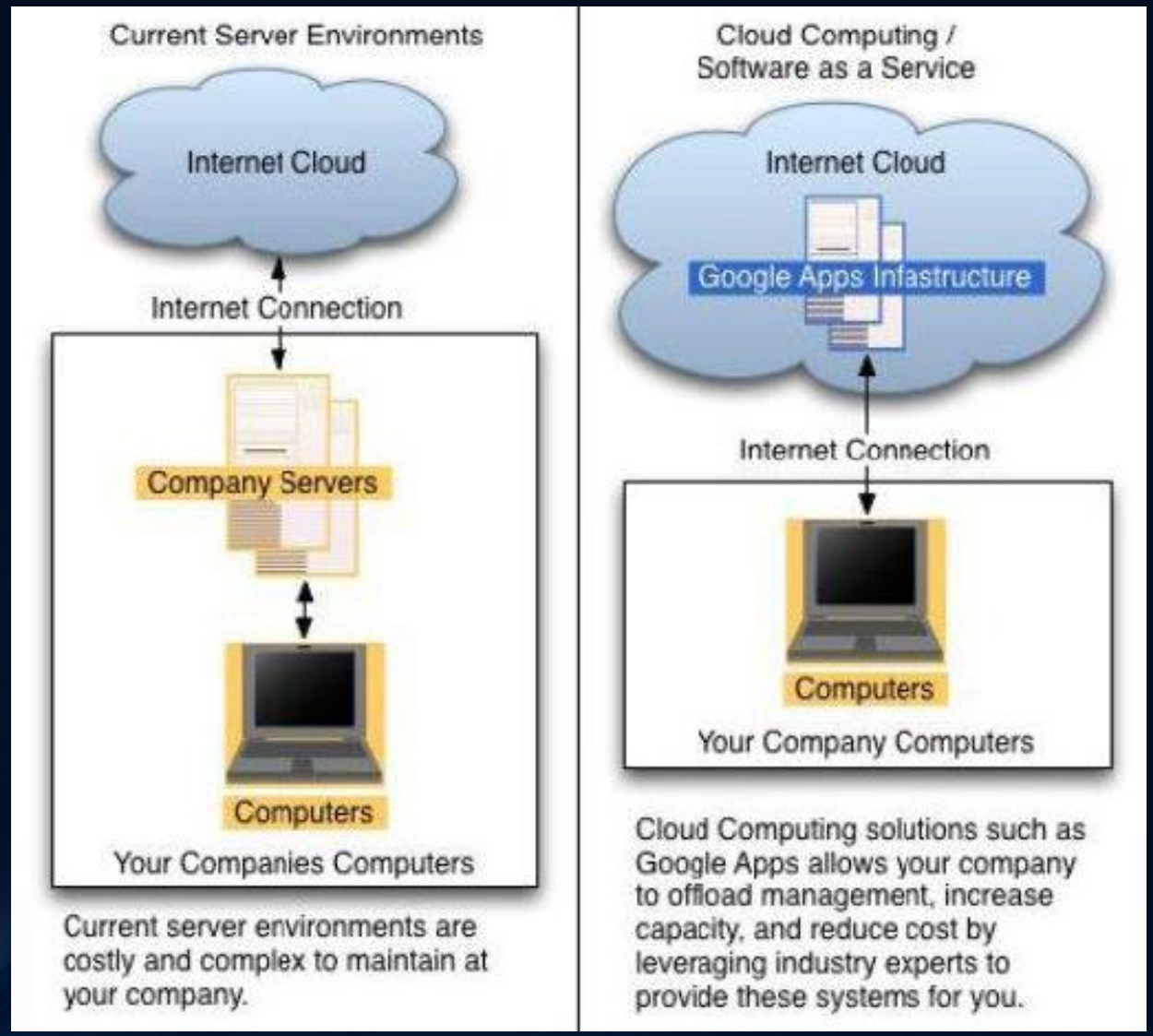
Cloud computing (2)

- A user interacts with the cloud without worrying about how it is implemented
- Commercially based -sold on demand (by the hour)
- Elastic -a user can have as much or as little of a service as they want at any given time
- Service is fully managed by the provider -the consumer needs nothing but a personal computer and Internet access

Cloud computing (3)

- Infrastructure-as-a-Service (IaaS)
  - Virtual server instances with unique IP addresses and blocks of storage on demand (Amazon EC2)
- Platform-as-a-Service (PaaS)
  - Set of software and product development tools hosted on the provider's infrastructure (Google App Engine, Microsoft Windows Azure Platform, Amazon Web Services)
- Software-as-a-Service (SaaS)
  - Vendor supplies the hardware infrastructure, the software product and interacts with the user through a front-end portal (anything from Web-based email to inventory control and database processing-GoogleApps)

Cloud computing (4)



Thanks for your attention

Question
?