

# C2115

# Practical introduction to supercomputing

## Lesson 1

Petr Kulhánek

[kulhanek@chemi.muni.cz](mailto:kulhanek@chemi.muni.cz)

National Centre for Biomolecular Research, Faculty of Science  
Masaryk University, Kamenice 5, CZ-62500 Brno

# Content

- **History, use and future of computer technology**
- **Overview of computer centers in the Czech Republic**  
MetaCentrum, CERIT-SC, IT4 Innovation
- **Foreign data centers**  
centers available for those interested from the Czech Republic, Top500

# History

[http://en.wikipedia.org/wiki/History\\_of\\_computing\\_hardware](http://en.wikipedia.org/wiki/History_of_computing_hardware)

1800 beginnings of punched cards

1946 ENIAC

1947 discovery of the transistor

1971 Intel 4004 (4 bit)

1974 Intel 8080 (8 bit)

1976 Intel 8086 (16 bit)

1985 Intel 80386 (32 bit)

2001 IA-64 (64 bit)

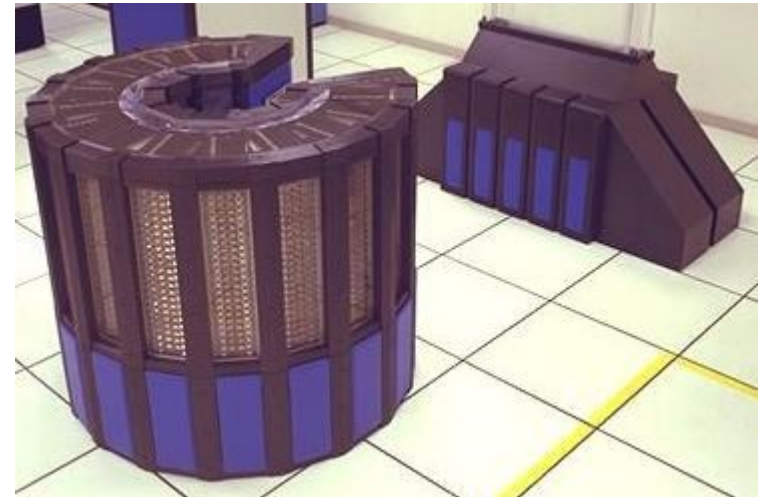
2003 AMD64/EM64T (64 bit)

**2010 Intel Core i7 980X: @3,33 GHz  
(6C/12T, Turbo@3,46 GHz): 109 GFLOPS**



<http://www.root.cz>

**Pavel Tišnovský, Unixové vykopávky**



**1985 Cray 2 1,9 GFLOPS**

proprietary vector CPU

source: wikipedia.org, intel.com

# Use of computer technology

Computer technology (computers) has affected all branches of human activity and has become an integral part of our lives. This was brought especially by **rapid development** in the last 20 years. We use computer technology for entertainment, to process and consume information.

Computer technology (and foremost supercomputers) are used for **numerically demanding solutions** of problems such as:

- simulation of weather, climatological and geological changes (spread of floods, tsunamis, earthquakes)
- design of new materials and drugs
- modeling of economic development
- **scientific and technical calculations** (**chemistry**, physics, mathematics)
- military purposes (nuclear weapons simulation)
- finding context in data (big data)
- artificial intelligence, autonomous management...

# Future

Human brain simulator...

<http://www.humanbrainproject.eu/>

<https://www.humanbrainproject.eu/en/follow-hbp/news/animation-exploring-brain-scales-in-90-seconds/>

Big Data ...

## Artificial Intelligence ...

Autonomous management ...

Quantum computing....

Hardware:

- consumption reduction....
- increasing performance....
- massive use of GPGPU ...
- special hardware: TPU, Intel Phi, ARM
- quantum accelerators



D-wave  
dwavesys.com



Tensor processing unit (TPU)  
google.com

# Computer centers in Czech Republic

# MetaCentrum

<http://www.metacentrum.cz/>

**MetaCentrum** acts in the role of the Czech National Grid Infrastructure (NGI\_CZ), which is part of the European Grid Infrastructure (EGI). Virtual work environment of MetaCentrum significantly contributes to **more efficient use** of installed technology, allows the use of available computing resources to solve very demanding computing tasks, which cannot be managed by a single independent workplace in the Czech Republic.

For those interested from academic and research institutions, MetaCentrum offers an environment for (cooperation) in **areas of calculations and data storage** not only in the Czech Republic, but also on an international scale (support for integration into the International Research Area (ERA) and connection to the European Grid Infrastructure (EGI)).

MetaCentrum coordinates the acquisition of expensive software and application equipment, ensures the central purchase and management of licenses of selected licensed software. At the same time, MetaCentrum actively participates in the research and development necessary to ensure optimal functionality, security and high performance of the entire infrastructure.

MetaCentrum is activity of **CESNET** association.

**CERIT-SC Center (CERIT Scientific Cloud)** is a national center operating computing and data storage infrastructure for research and development. With its capacity of approx. 5500 CPU cores and over 4 PB storage capacity it is the largest node of Czech national e-Infrastructure MetaCentrum.

Center CERIT-SC is a part of the national e-infrastructure recognized in the Roadmap of Large Infrastructures for Research, Experimental Development and Innovation of the Czech Republic, complementary to the **CESNET** association and **IT4Innovations** supercomputing center, with emphasis on experimental ("leading edge" and even disruptive) use of the e-infrastructure to meet the evolving user needs.



# MetaCentrum VO

<http://metavo.metacentrum.cz/>

Combines computing resources provided by MetaCenter, CERIT-SC project and other partners.

- National grid infrastructure
- OS Debian
- **Status 2019**
  - ca **15000 CPU** cores
  - **CEITEC/NCBR own resources approx. 1100 CPU** cores
  - ~3 PB storage disk arrays, ~20 PB hierarchical storage space
- **An account can be obtained by a student of any university in the Czech Republic.**
- Access is not tied to a specific project and is granted for 1 year.
- Extension of access is conditional on the submission of an annual report.

# MetaCentrum VO

<http://metavo.metacentrum.cz/>

Combines computing resources provided MetaCentrem, the CERIT-SC project and other partners.

- National grid infrastructure
- OS Debian
- **Status 2019**
  - ca **15000 CPU** cores
  - **CEITEC / NCBR own resources approx. 1100 CPU** cores
  - ~ 3 PB storage disk arrays, ~ 20 PB hierarchical storage spaces

**Practical: infrastructure,**  
**clusters, data storage,**  
**submitting tasks**

- **An account can be obtained by a student of any university in the Czech Republic.**
- Access is not tied to a specific project and is granted for 1 year.
- Extension of access is conditional on the submission of an annual report.

**IT4Innovations National Supercomputer Center** at VŠB - Technical University of Ostrava is a leading research, development and innovation center in the field of high-performance computing (HPC), data analysis (HPDA) and artificial intelligence (AI), operating the most powerful supercomputer systems in the Czech Republic. IT4Innovations together with institutions **CESNET** and **CERIT-SC** form strategic research infrastructure of the Czech Republic **e-INFRA CZ**.

- **The solvers of successful projects in a public grant competition gain access.**

The project is jointly prepared by five entities: the University of Mining and Technology in Ostrava, the University of Ostrava in Ostrava, the Silesian University in Opava, the Brno University of Technology and the geonics AS CR.

# Computer centers abroad

## Project Types:

- **Multi-year Access** is available to major European projects or infrastructures that can benefit from PRACE resources and for which Project Access is not appropriate.
- **Project Access** is intended for individual researchers and research groups including multi-national research groups and has a one year duration. Calls for Proposals for Project Access are issued twice a year (February and September).
- **Preparatory Access** is intended for resource use required to prepare proposals for Project Access. Applications for Preparatory Access are accepted at any time.

# PRACE - members

Austria: JKU - Johannes Kepler University of Linz

Belgium: DGO6-SPW - Direction general operational of the economy, de the Empire and the Search - Public Service de Wallonia

Bulgaria: NCSA - Executive agency "Electronic communication networks and information systems"

Cyprus: CaSToRC - Computation-based Science and Technology Research Center, The Cyprus Institute

## **Czech Republic: VŠB - Technical University of Ostrava**

Denmark: DeIC - Danish e-Infrastructure Cooperation

Finland: CSC - IT Center for Science Ltd.

France: GENCI - Grand Equipment National of Calcul Intensive

Germany: GCS - GAUSS Center for Supercomputing eV

Greece: GRNET - Greek Research and Technology Network SA

Hungary: NIIFI - National Information Infrastructure Development Institute

Ireland: ICHEC - Irish Center for High-End Computing

Israel: IUCC - Inter-University Computation Center

Italy: CINECA - Consortium Interuniversity

Norway: SIGMA - UNINETT Sigma AS - The Norwegian Metacenter for Computational Science

The Netherlands: SURFSARA: SARA Computing and Networking Services

Poland: PSNC - Institute Chemistry Bioorganic Pan - Institute of Bioorganic Chemistry - Poznan Supercomputing and Networking Center

Portugal: University of Coimbra

Serbia: IPB - Institute of Physics Belgrade

Slovenia: ULFME - University of Ljubljana, Faculty of Mechanical Engineering

Spain: BSC - Barcelona Supercomputing Center - Centro National of Supercomputation

Sweden: Vetenskapsrådet - Swedish Research Council

Switzerland: ETH - Eidgenössische Technical University of Applied Sciences Zurich - Swiss Federal Institute of Technology, Zurich

Turkey: UYBHM - Ulusal Yuksek Basarimli Hesaplama Merkezi, Istanbul Technical University - National Center for High Performance Computing

UK: EPSRC - The Engineering and Physical Sciences Research Council

# TOP500

<http://www.top500.org/>

**TOP500** is a project that holds a list of the 500 fastest computers in the world.

## TOP500 benchmark

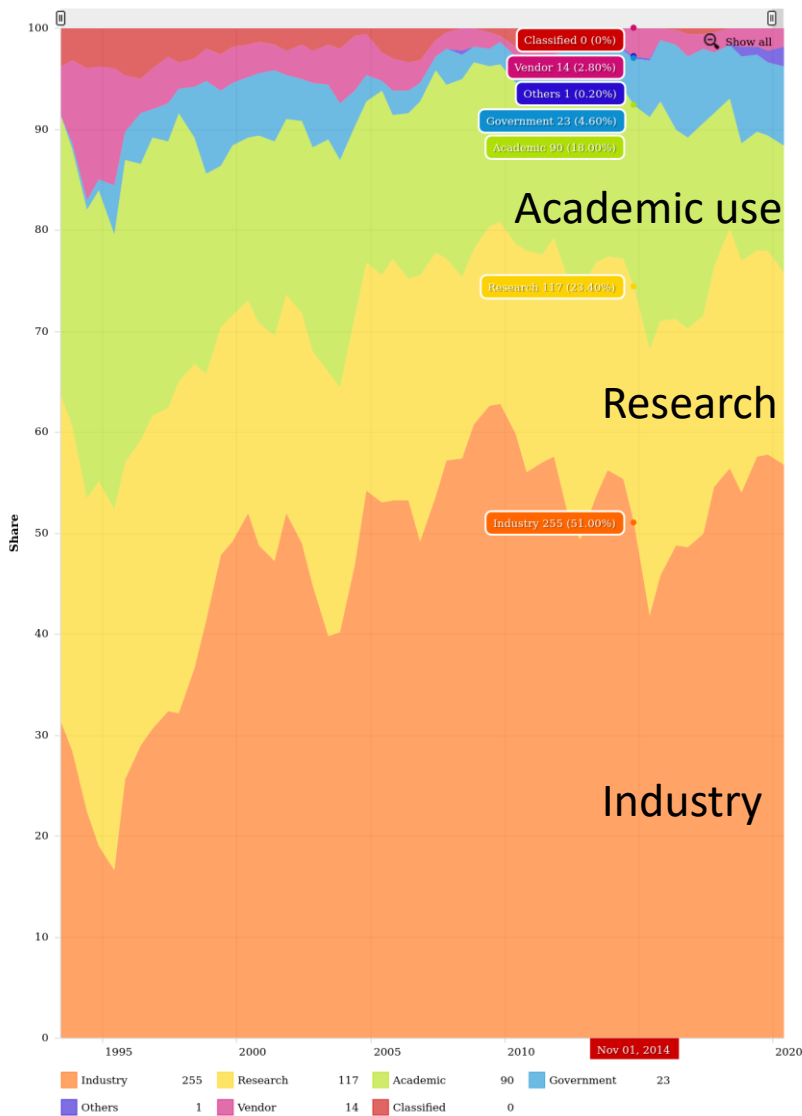
Our simple **TOP500** approach does not define “supercomputer” as such, but we use a benchmark to rank systems and to decide on whether or not they qualify for the TOP500 list. The benchmark we decided on was **Linpack**, which means that systems are ranked only by their ability to solve a set of linear equations,  $Ax = b$ , using a **dense random matrix A**.

November 2020

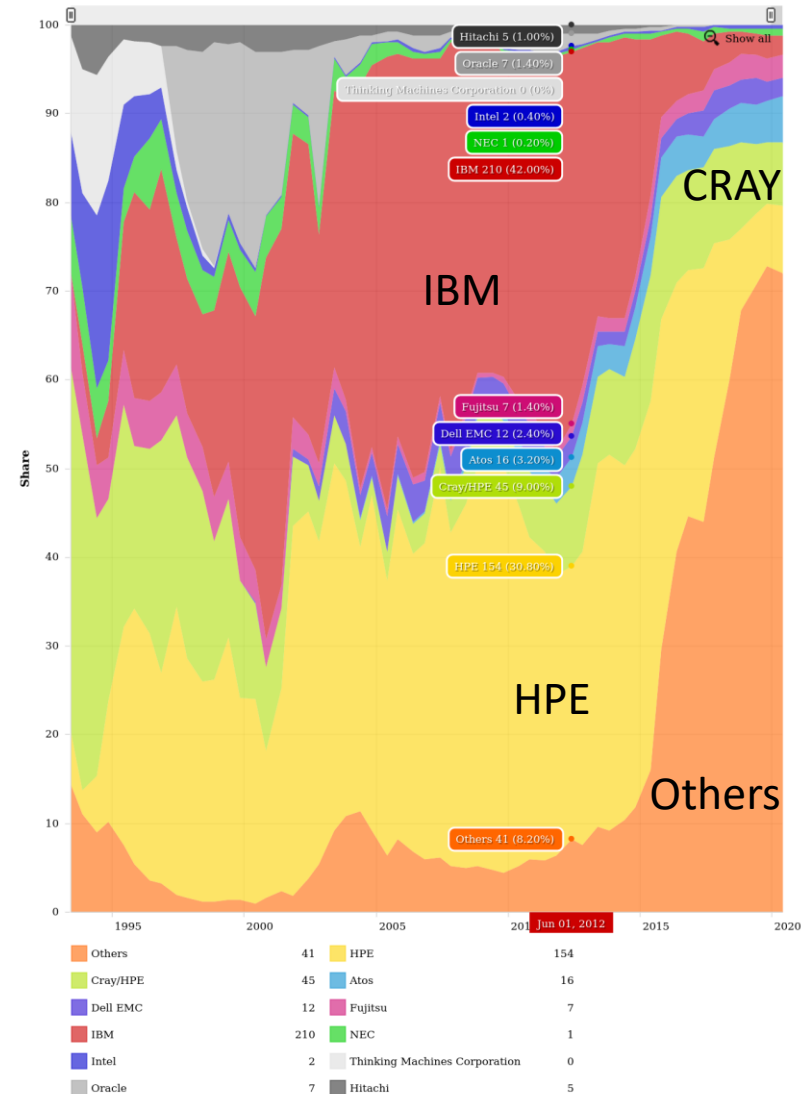
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	<b>Supercomputer Fugaku</b> - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	<b>Summit</b> - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	<b>Sierra</b> - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438

# TOP500 – Usage / Manufacturer

Segments - Systems Share



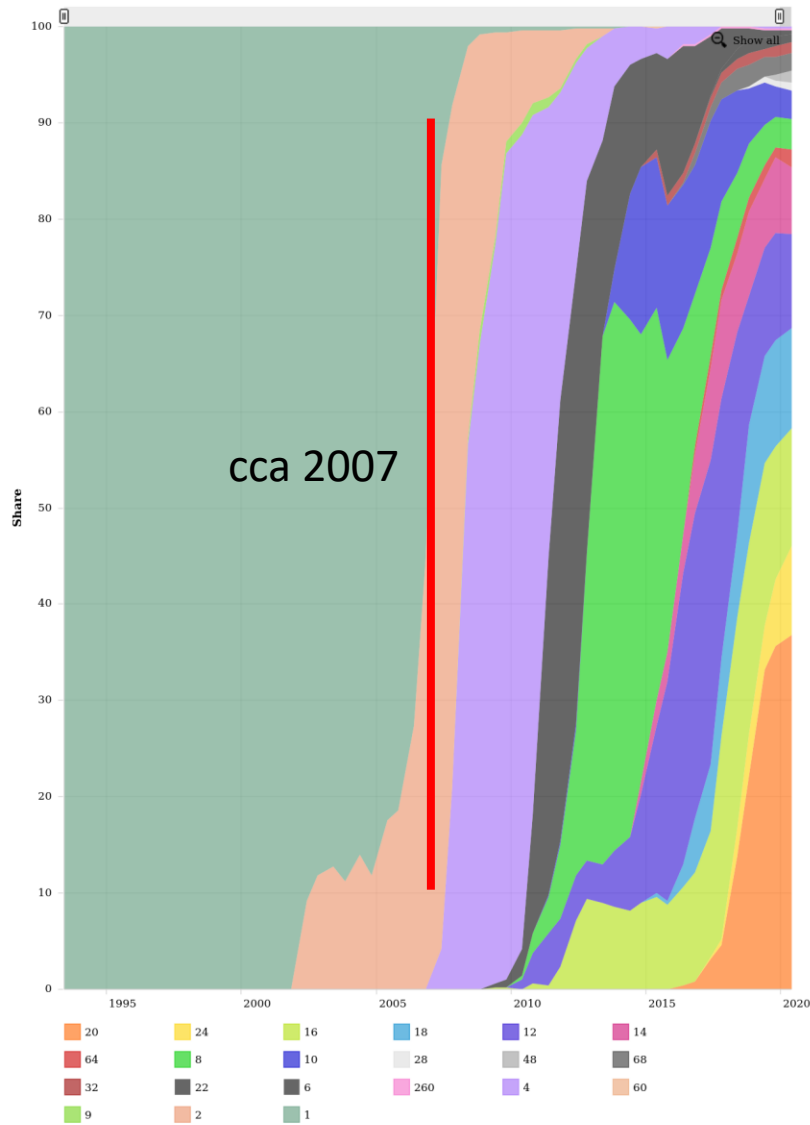
Vendors - Systems Share



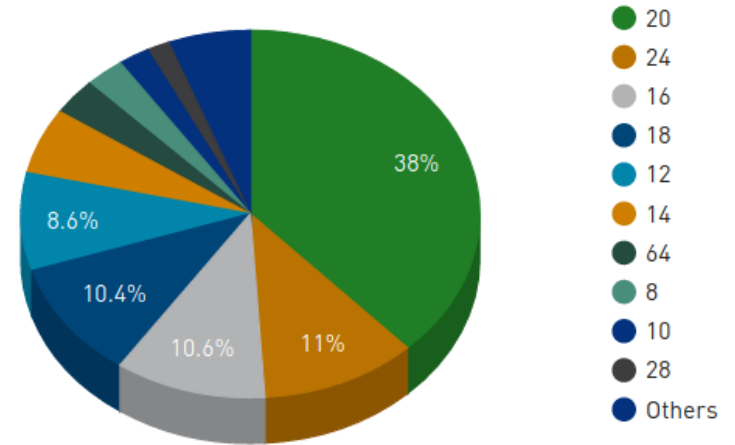


# TOP500 - CPU cores

Cores per Socket - Systems Share

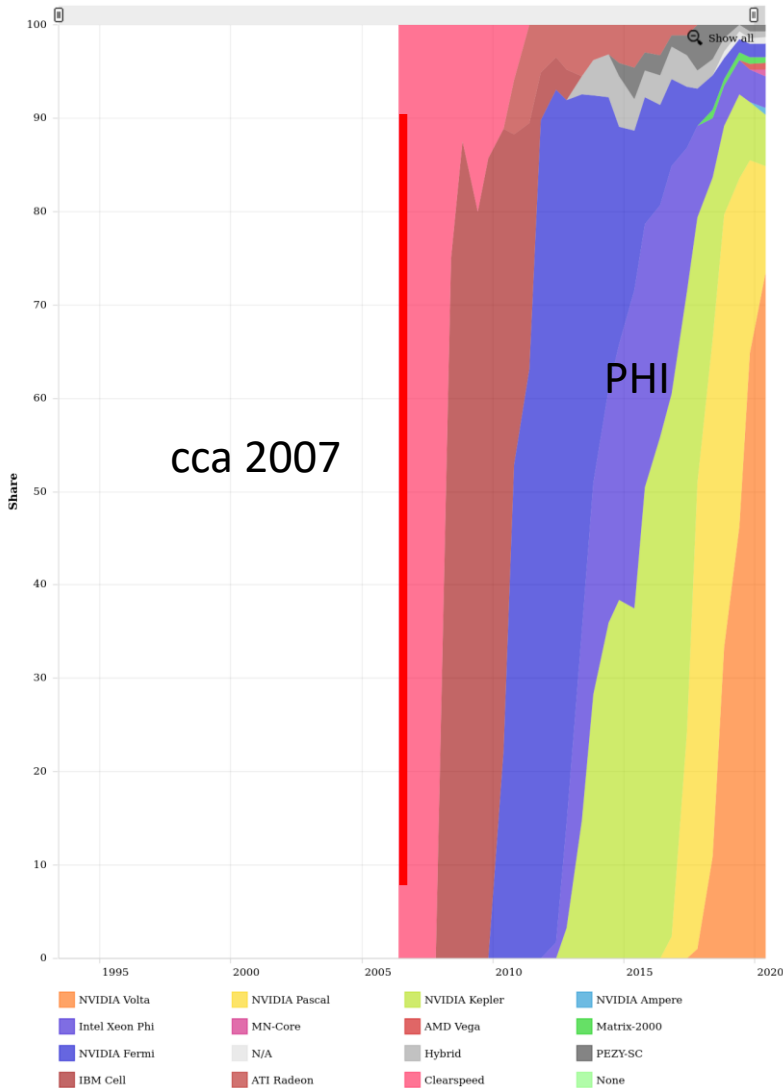


Cores per Socket System Share 2020

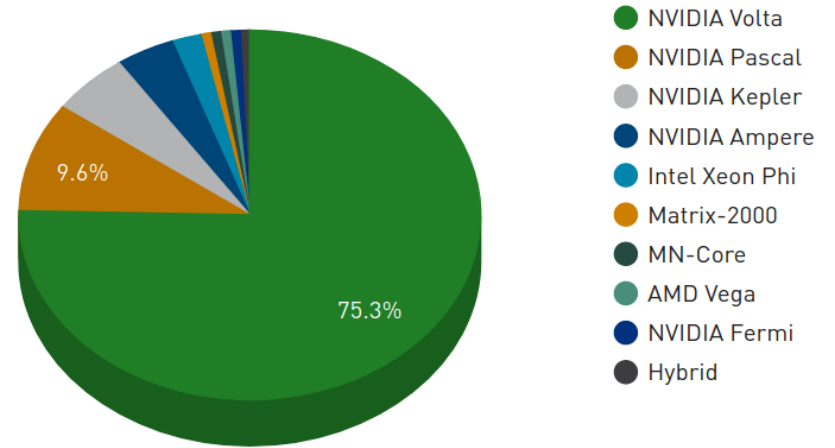


# TOP500 - Accelerators/Coprocessors

Accelerator/CP Family - Systems Share



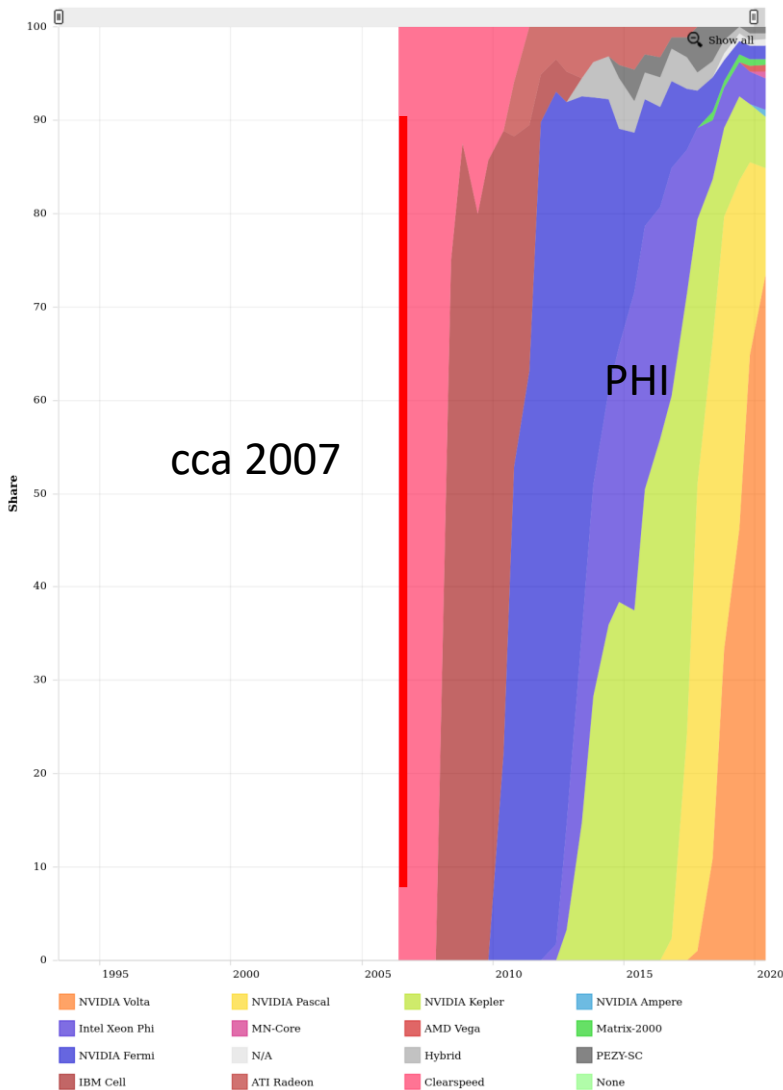
Accelerator/CP Family System Share 2020



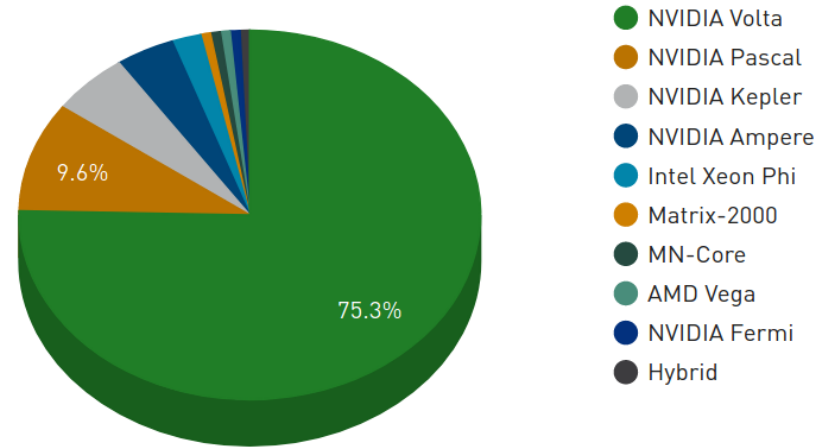
- NVIDIA Volta
- NVIDIA Pascal
- NVIDIA Kepler
- NVIDIA Ampere
- Intel Xeon Phi
- Matrix-2000
- MN-Core
- AMD Vega
- NVIDIA Fermi
- Hybrid

# TOP500 - Accelerators/Coprocessors

Accelerator/CP Family - Systems Share



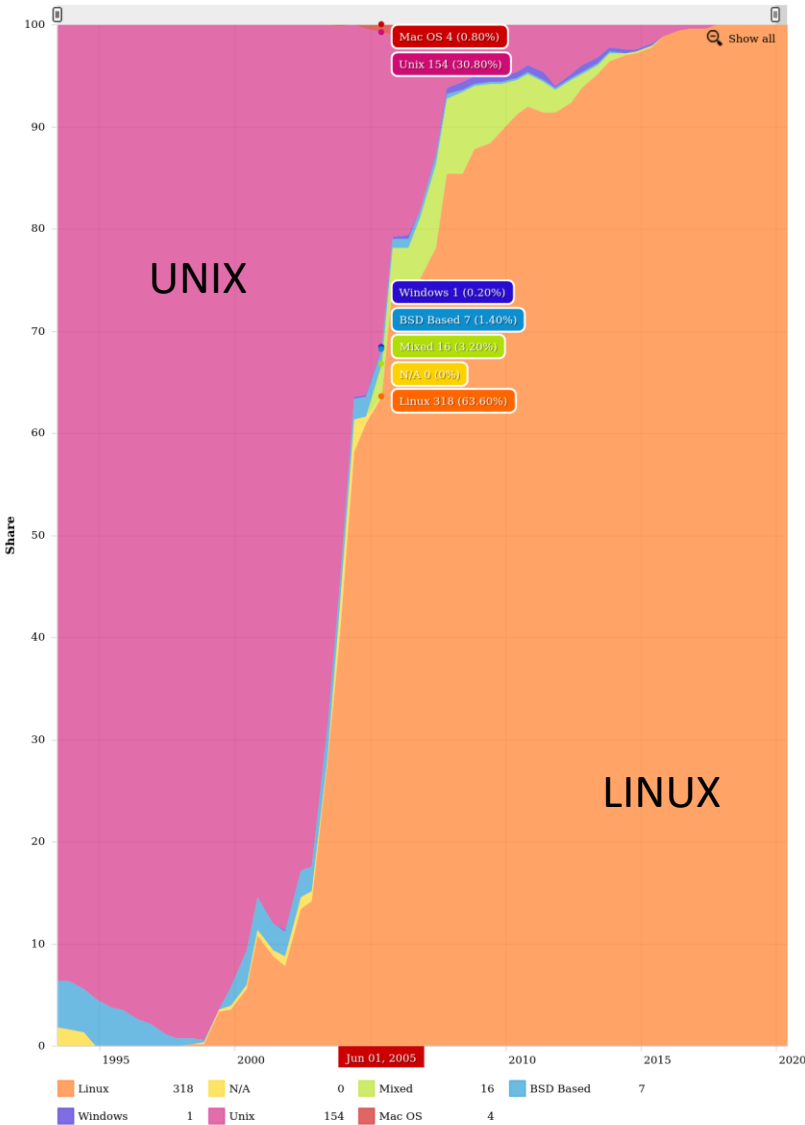
Accelerator/CP Family System Share 2020



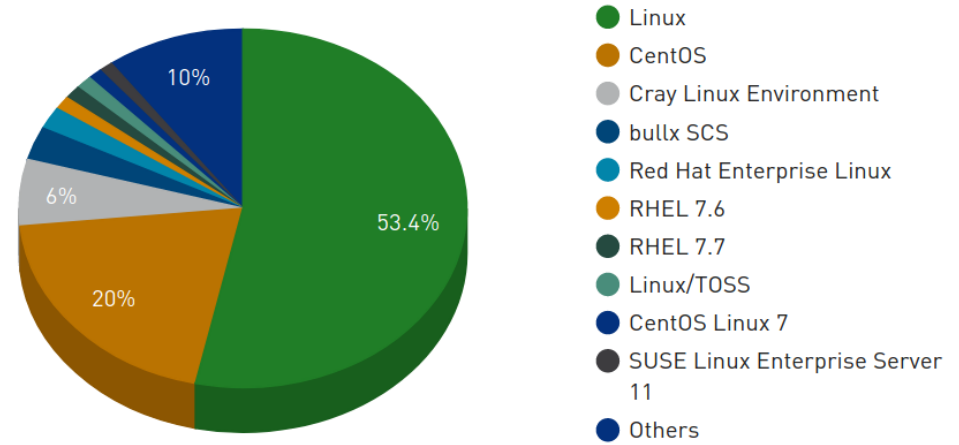
**Practical:**  
MD simulation on GPU

# TOP500 - OS

Operating system Family - Systems Share



Operating System System Share 2020



**MetaCentrum** (Debian)  
**CERIT-SC** (CentOS)  
**IT4I** (CentOS)  
**WOLF** (Ubuntu)

# For your interest

**K - computer, 3rd place, 2012**

<http://www.youtube.com/watch?v=UJPslu9OaTc>

*play video*

**TITAN, 1st place, 2012**

<https://www.youtube.com/watch?v=AdylAE1lgg0>

**Sunway TaihuLight, 1st place, 2017**

<https://www.youtube.com/watch?v=t0HDwE3mGP0>

# Exercise 1

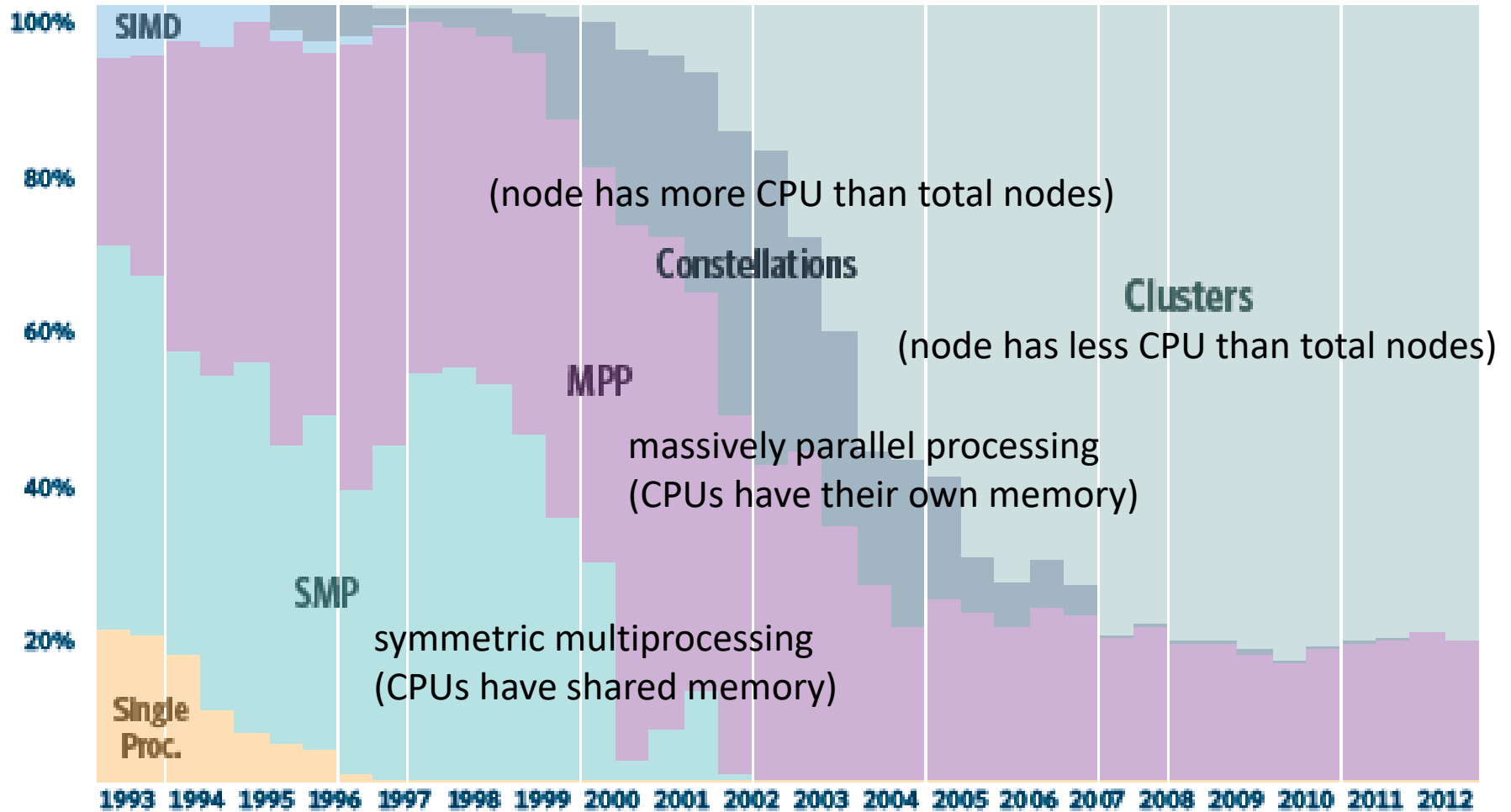
1. What does the FLOPS unit state?
2. What is the name of the fastest supercomputer listed in the TOP500 ranking? What is its power and energy consumption? What type of CPU does it use?
3. What position did the TITAN supercomputer, which was in the first position in the TOP500 ranking in 2012, move to? Has its HW configuration been changed?
4. In 2014, the average energy consumption per capita in the Czech Republic was 1,400 kWh. How many people would cover their annual energy consumption consumed by the world's most powerful computer according to the TOP500 ranking?
5. Estimate what will electrical energy in the supercomputer convert to and in what percentage.
6. What are the names of supercomputers in IT4I?
7. What do they consist of (list key technologies)?
8. What rung are the TOP500 rankings?
9. What processor do you have in your mobile phone? How many times is it more powerful than a supercomputer Cray2 from 1985? [not necessary for protocol]

# TOP500 1995-2012

older but clearer graphs...

# TOP500 - Topology

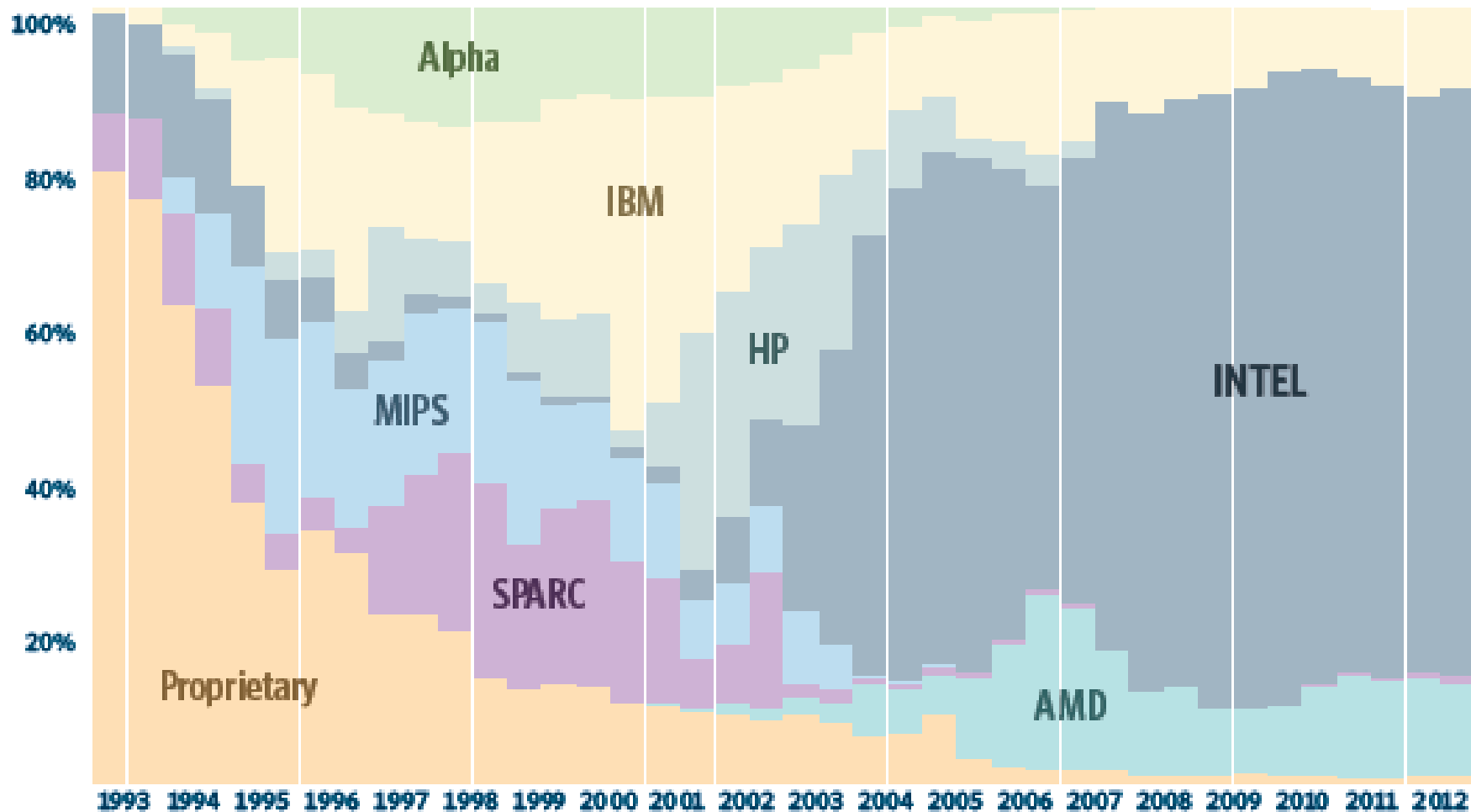
## ARCHITECTURES





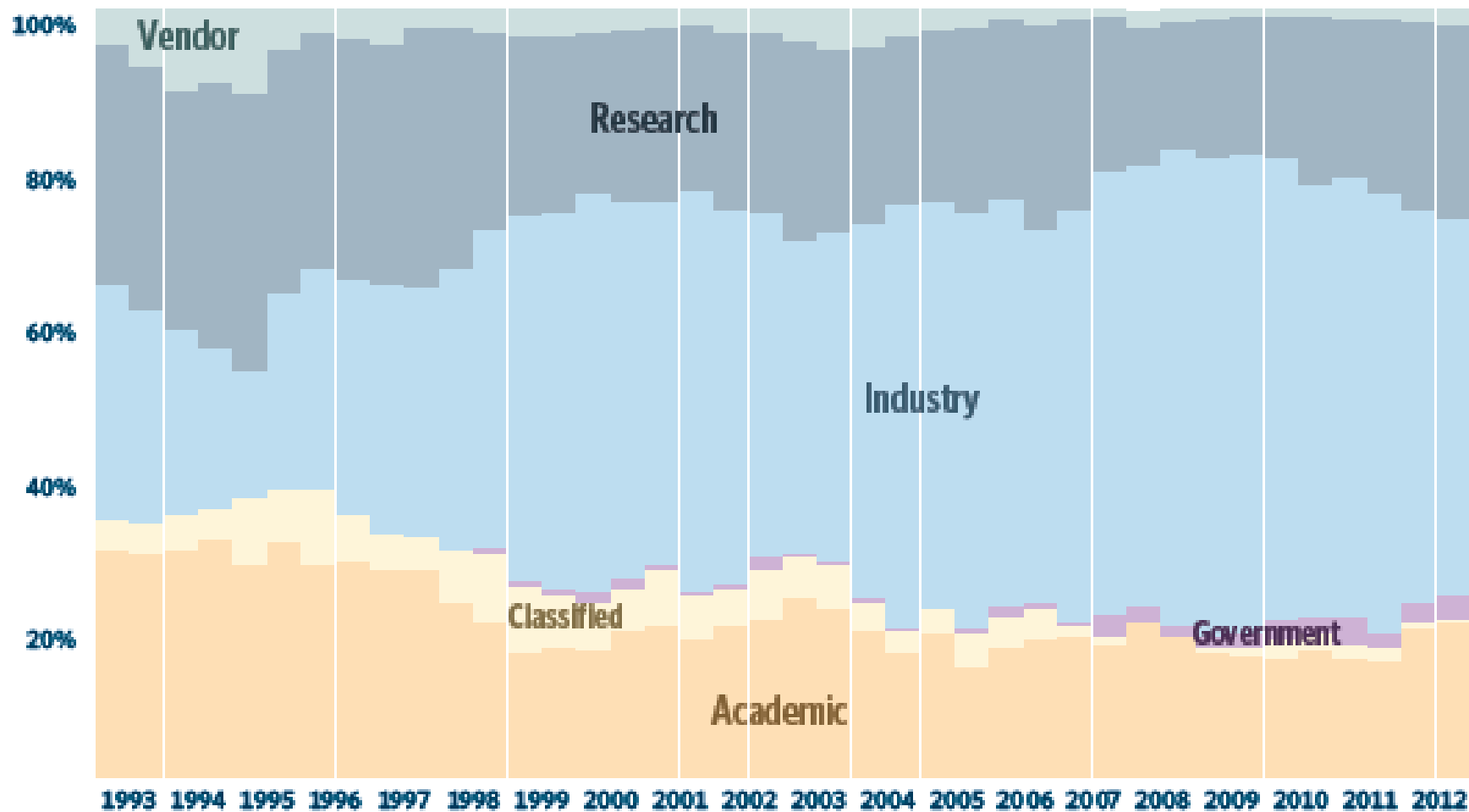
# TOP500 - CPU architecture

## CHIP TECHNOLOGY



# TOP500 - Type of use

## INSTALLATION TYPE



# TOP500 - Accelerators/Coprocessors

## ACCELERATORS/CO-PROCESSORS

