

академия  
больших  
данных



mail.ru  
group

# Высокопроизводительные вычисления.

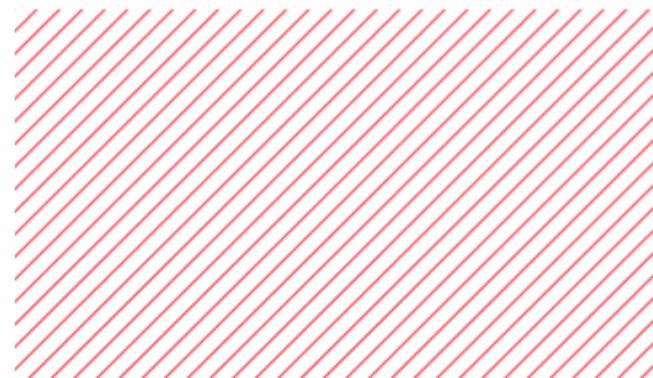
## Лекция 1. Введение

Рыкованов Сергей

PhD, доцент Сколтеха

Матвеев Сергей

к.ф-м. наук, доцент ВМК МГУ



# Логистика и правила

- Лекции / семинары / лабораторные занятия по пятницам 19:00-22:00
- Общение происходит в discord
- Если хотите задать вопрос – нажмите raise hand в Zoom
- Можете писать в личный чат если хотите обсудить материалы или задать вопрос – будет возможность открыть breakout room
- Создайте приватный репозиторий на github MADE2021 - домашние задания по программированию будут приниматься через github

## Рекомендуемая литература:

- Sterling, Anderson, Brodowicz. High Performance Computing. Modern Systems and Practices. Morgan Kaufmann Publishers, 2018
- В.П. Гергель. Высокопроизводительные вычисления для многоядерных многопроцессорных систем. Издательство Нижегородского госуниверситета, 2010
- В.Л. Баденко. Высокопроизводительные вычисления. Учебное пособие. Издательство Политехнического университета, Санкт-Петербург. 2010
- High Performance Computing for Dummies.

## Видео ресурсы:

- Coursera: Введение в параллельное программирование с использованием OpenMP и MPI
- Udacity: Introduction to High Performance Computing

# Предполагаемые навыки и установки

- Знание Linux (Unix) и возможность использования Linux или Unix системы
  - Пользователи Windows: [www.virtualbox.org](http://www.virtualbox.org) или подобный софт
  - Установленный компилятор gcc (желательно последней версии)
  - Установленный openmpi
  - Установленный openmp
  - **Мы предоставим виртуальный кластер, к которому вы сможете подключиться по ssh**
  - Знание C/C++ (уверенное понимание указателей и массивов)
- 
- <https://www.geeksforgeeks.org/pointers-in-c-and-c-set-1-introduction-arithmetic-and-array/>
  - <https://ubuntu.com/tutorials/command-line-for-beginners#1-overview>

# Лекторы



Сергей Рыкованов  
PhD, доцент Сколтеха

2000-2006 МГУ им. Ломоносова, физический факультет  
2006-2009 PhD в университете Людвига Максимилиана  
в Мюнхене (вычислительная физика плазмы)  
2009-2012 научный сотрудник в университете Людвига  
Максимилиана в Мюнхене  
2012-2014 научный сотрудник в лаборатории им.  
Лоуренса в Беркли  
2014-2018 руководитель лаборатории в институте  
Гельмгольца в Йене (Германия)  
2018-... Сколтех

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github: ssstuvz



Сергей Матвеев  
к. ф-м. наук, доцент МГУ

2010 - 2015 МГУ им. М. В. Ломоносова , ВМК  
2014 - техник НИВЦ МГУ  
2015-2018 аспирантура, МГУ им. М. В. Ломоносова  
2015 - 2018 младший научный сотрудник Сколтех  
2019 - по н.в. научный сотрудник ИВМ РАН  
(совместитель)  
2018 – 2021 научный сотрудник Сколтех  
с февраля 2021 доцент ВМК МГУ

[matseralex@gmail.com](mailto:matseralex@gmail.com)  
github: matseralex

# Цели курса

Не бояться огромных суперкомпьютеров.

Уметь писать параллельные программы на современных многоядерных ЦПУ и ГПУ

Научиться использовать большие машины коллективного пользования

Получать удовольствие от учебы

# Программа курса

1. Введение в HPC
2. Терминал, переменные окружения, линковка, Makefile, виртуализация
3. Навыки работы на суперкомпьютере
4. multithreading, OpenMP и др
5. Библиотека MPI для работы на распределенных серверах
6. Multiprocessing и MPI в Python
7. Python code profiling и Numba
8. CUDA, CUDA Libraries examples, основные примитивы
9. CUDA in Python
10. Тренды в HPC, дополнительные главы (parallel I/O, визуализация)

# Баллы за д/з



- Каждое д/з содержит базовую часть и бонусные баллы.
- Итоговые баллы д/з нормируются на стоимость базовой части и получаются проценты успешности очередного д/з.
- Курс не полагается сложным, но информацию о лучших студентах курса мы перешлем кураторам MADE
- Из-за бонусов за конкретные д/з можно набрать >100% (!)
- По итоговым процентам д/з считается среднее -- это финальный балл

Какие домашки? после следующих лекций:

1. Вводная лекция по истории НРС	5-6. Библиотека MPI и MPI4Py
2. Терминал, переменные окружения Makefile	7, 9. Cuda/PyCuda
3. Pthreads, openmp	8. Профилировка и биндинг С/C++/Python **
4. Навыки работы на суперкомпьютере *	** полностью бонусная

# Сегодня: введение, история, общие сведения

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# Four paradigms of modern science

## 1. Experiment



## 2. Theory

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi$$



### Limitations:

- experiments/theory too complicated
- experiments too expensive (car/airplane construction)
- experiments too slow (evolution of galaxies)
- experiments too dangerous (explosives, chemicals, climate)
- experiments not possible at the moment

# Four paradigms of modern science

1. Experiment



2. Theory

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi$$

3. Modeling



Mathematical models  
Numerical methods  
Computers and supercomputers

# Four paradigms of modern science

1. Experiment



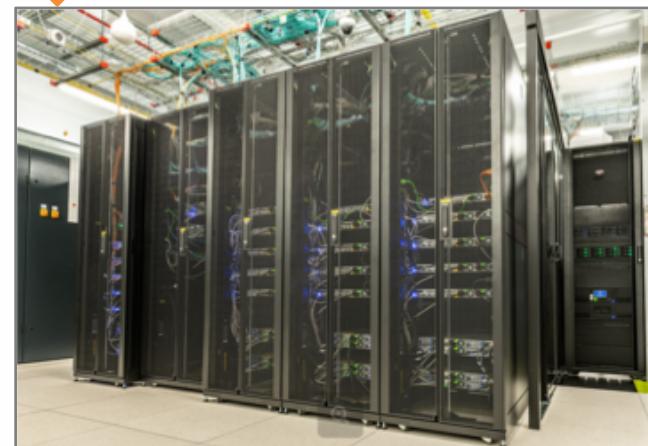
2. Theory

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi$$

3. Modeling



4. Big Data and AI



# High Performance Computing is a strategic necessity

- Main players like USA, China, European Union are investing **billions of dollars** into HPC
- HPC drives scientific discovery (plasma physics, computational chemistry, novel materials, artificial intelligence).
- HPC has entered almost all areas of human activity, for example:
  - new perfumes development
  - automobile tires development
  - entertainment industry, movies, cybersport
  - PayPal saved **~1 billion dollars** detecting online fraud with HPC
- HPC is one of the main drivers of the modern world innovation.

- **Airlines:**
  - System-wide logistics optimization systems on parallel systems.
  - Savings: approx. \$100 million per airline per year.
- **Automotive design:**
  - Major automotive companies use large systems (500+ CPUs) for:
    - CAD-CAM, crash testing, structural integrity and aerodynamics.
    - One company has 500+ CPU parallel system.
  - Savings: approx. \$1 billion per company per year.
- **Semiconductor industry:**
  - Semiconductor firms use large systems (500+ CPUs) for device electronics simulation and logic validation
  - Savings: approx. \$1 billion per company per year.
- **Energy**
  - Computational modeling improved performance of current nuclear power plants, equivalent to building two new power plants.

# The Future of AI is Decentralized

Training GPT-3 reportedly cost \$12 Million for a single training run<sup>1</sup>. Is that really the most efficient way to train a model?



Ala Shaabana Feb 28 · 5 min read



## Green AI

<https://towardsdatascience.com/the-future-of-ai-is-decentralized-848d4931a29a>

<https://arxiv.org/pdf/1907.10597.pdf>

# Экспоненциальный рост данных и необходимость их обработки с помощью машинного обучения и искусственного интеллекта



- Люди с давних времен аккумулировали и каталогизировали информацию (в основном в текстовом формате): книги, справочники, энциклопедии, базы данных и т.п.
- В наше время произошел взрывной рост накопления аудио, видео и фото информации – такая информация существенно сложнее, ее структура плохо поддается анализу, в том числе из-за использования сжатия. Для того, чтобы ее обрабатывать необходимы качественно и количественно намного большие и специализированные вычислительные ресурсы, более сложные алгоритмы и подходы. Информацию уже окрестили «современной нефтью».
  - Тот, кто сможет эффективно обрабатывать большие объемы такой (плохо структурированной) информации, получит неоспоримое преимущество во многих областях науки и бизнеса.
    - В настоящее время между передовыми державами идет борьба за первенство в области высокопроизводительных вычислений для ИИ.

# HPC share compared to the country GDP



24% GDP

38% HPC power



15% GDP

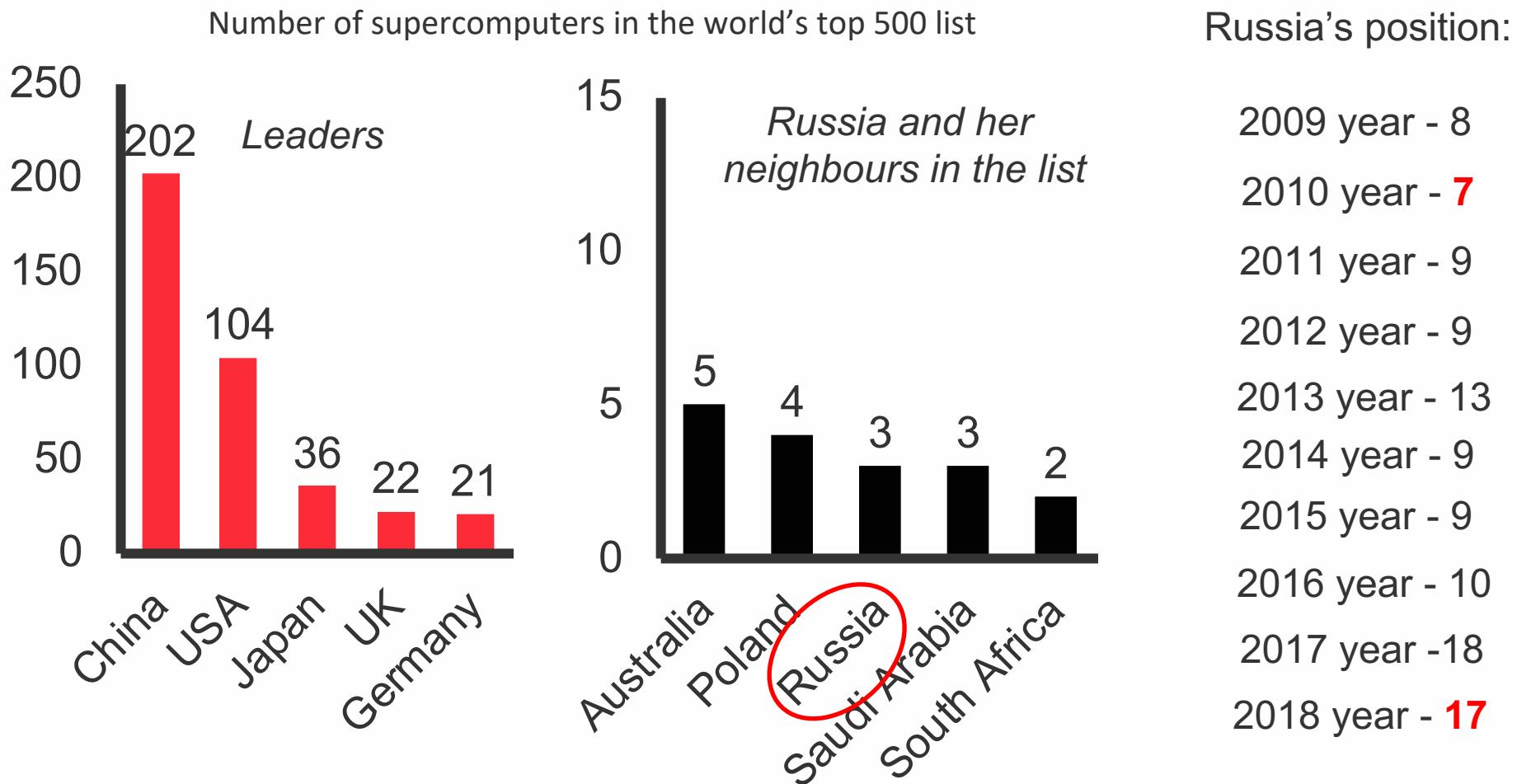
29% HPC power



2% GDP

**0.3% HPC power  
(19th place, Poland – 18th)**

# Russia's position on the global HPC arena



# Units for measuring supercomputer performance

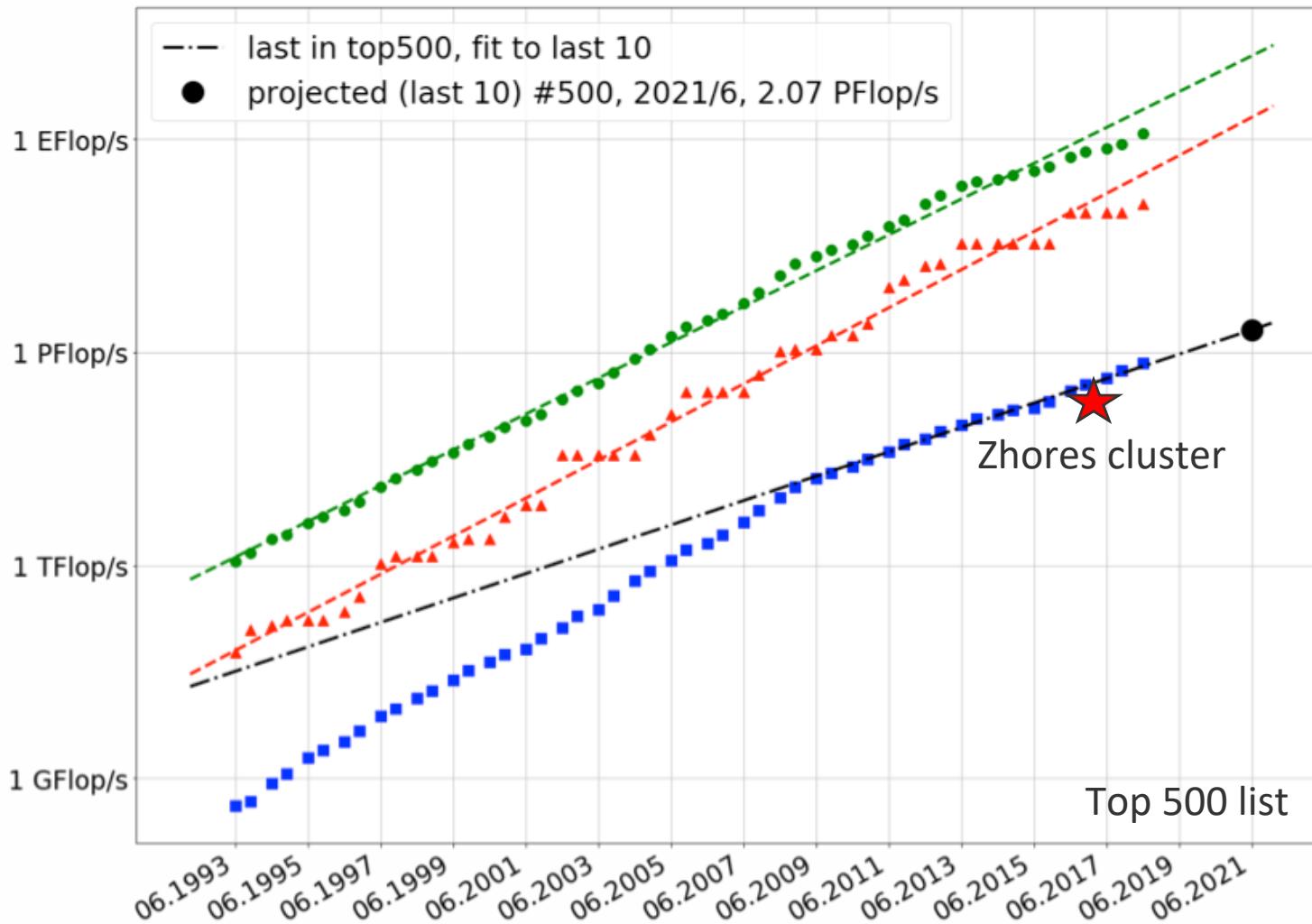
- High Performance Computing (HPC) units are:
  - Flop: floating point operation, usually double precision unless noted
  - Flop/s: floating point operations per second
  - Bytes: size of data (a double precision floating point number is 8 bytes)
- Typical sizes are millions, billions, trillions...

Kilo	$\text{Kflop/s} = 10^3 \text{ flop/sec}$	$\text{Kbyte} = 10^3 \sim 2^{10} = 1024 \text{ bytes (KiB)}$
Mega	$\text{Mflop/s} = 10^6 \text{ flop/sec}$	$\text{Mbyte} = 10^6 \sim 2^{20} \text{ bytes (MiB)}$
Giga	$\text{Gflop/s} = 10^9 \text{ flop/sec}$	$\text{Gbyte} = 10^9 \sim 2^{30} \text{ bytes (GiB)}$
Tera	$\text{Tflop/s} = 10^{12} \text{ flop/sec}$	$\text{Tbyte} = 10^{12} \sim 2^{40} \text{ bytes (TiB)}$
Peta	$\text{Pflop/s} = 10^{15} \text{ flop/sec}$	$\text{Pbyte} = 10^{15} \sim 2^{50} \text{ bytes (PiB)}$
Exa	$\text{Eflop/s} = 10^{18} \text{ flop/sec}$	$\text{Ebyte} = 10^{18} \sim 2^{60} \text{ bytes (EiB)}$
Zetta	$\text{Zflop/s} = 10^{21} \text{ flop/sec}$	$\text{Zbyte} = 10^{21} \sim 2^{70} \text{ bytes (ZiB)}$
Yotta	$\text{Yflop/s} = 10^{24} \text{ flop/sec}$	$\text{Ybyte} = 10^{24} \sim 2^{80} \text{ bytes (YiB)}$

- Current fastest (public) machines are petaflop systems
  - Up-to-date list at [www.top500.org](http://www.top500.org)

$\sim 10 \text{ Mflop/Watt}$

# Top 500 – list of most powerful supercomputers



Currently only 3 Russian supercomputers are in the list

# Top 500 – list of most powerful supercomputers

Operating system Family System Share

● Linux

100%

2020

Operating system Family System Share

- Linux
- Unix
- Mixed
- Windows
- BSD Based

93.8%

1995

Accelerator/Co-Processor System Share

- NVIDIA Tesla P100
- NVIDIA Tesla V100
- NVIDIA Tesla K80
- NVIDIA Tesla K20x
- NVIDIA Tesla V100 SXM2
- NVIDIA Tesla K40
- NVIDIA Tesla P100...
- NVIDIA Volta GV100
- Intel Xeon Phi 5120D
- Intel Xeon Phi 5110P
- Others

11.4%

42.9%

29.3%

Vendors Performance Share

- Lenovo
- Inspur
- Sugon
- Cray Inc.
- HPE
- Bull
- Fujitsu
- Huawei
- Dell EMC
- IBM
- Others

25.5%

16.6%

6.7%

5.5%

13.1%

13.6%

7.4%

## System Performance

- Peak performance of 200 petaflops for modeling & simulation
- Peak of 3.3 ExaOps for data analytics and artificial intelligence

## Each node has

- 2 IBM POWER9 processors
- 6 NVIDIA Tesla V100 GPUs
- 608 GB of fast memory
- 1.6 TB of NVMe memory

## The system includes

- 4608 nodes
- Dual-rail Mellanox EDR InfiniBand network
- 250 PB IBM Spectrum Scale file system transferring data at 2.5 TB/s



# Russia in Top 500

3 entries found.

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
61	<b>Christofari</b> - NVIDIA DGX-2, Xeon Platinum 8168 24C 2.7GHz, Mellanox InfiniBand EDR, NVIDIA Tesla V100, Nvidia SberCloud Russia	99,600	6,669.0	8,789.8	
199	<b>Lomonosov 2</b> - T-Platform A-Class Cluster, Xeon E5-2697v3 14C 2.6GHz, Intel Xeon Gold 6126, Infiniband FDR, Nvidia K40m/P-100, T-Platforms Moscow State University - Research Computing Center Russia	64,384	2,478.0	4,946.8	
240	<b>MTS GROM</b> - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100 40GB, Infiniband, Nvidia #CloudMTS Russia	19,840	2,258.0	3,011.8	

# Functioning of a single compute node

- *Von Neumann Principle*

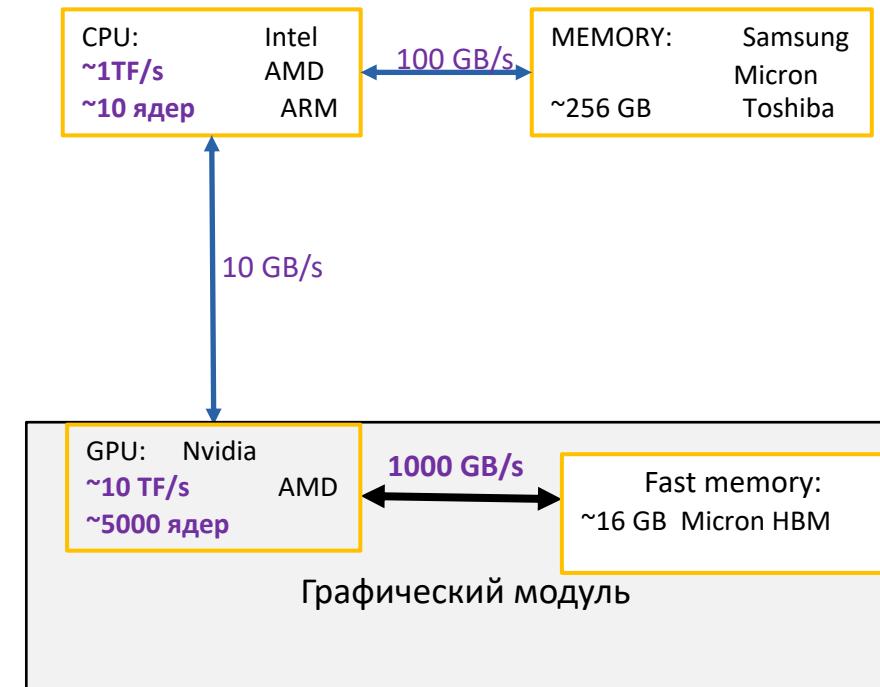
- CPU loads data from memory, operates on it and puts the result back to memory: classical PC
- Bottleneck is memory transfer CPU-memory which limits the computation speed



- *Specialized accelerator*

- Applications need to be rewritten
- Example: GPU computing (CUDA, OpenCL);
- “Fast” memory inside the GPU;
- Memory volume is bounded

(V100: 16 ГБ)



Memory hierarchy

# Measuring the cluster performance

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- Benchmark for performance measurement (LINPACK):  $Ax = b$   
where  $A$  is an  $N \times N$  matrix,  $N$  is large ( $10^6$ )  
Performance: benchmark –  $R_{\max}$ ; theoretical or peak –  $R_{\text{peak}}$

Системы на ключевых местах в списке ТОП-500

No	Cluster	Country	Rmax [Pflop/s]	Rpeak [Pflop/s]	Power [MW]
1	Summit - IBM	USA	122,3	187,6	8,8
2	Sunway TaihuLight	China	93	125,4	15,3
...	...	...			
500	CSCS Cray	Switzerland	0,7	0,84	0,3
...	...	...			
...	Zhores - Dell	Russia, Skoltech	0,5	0,8	0,1

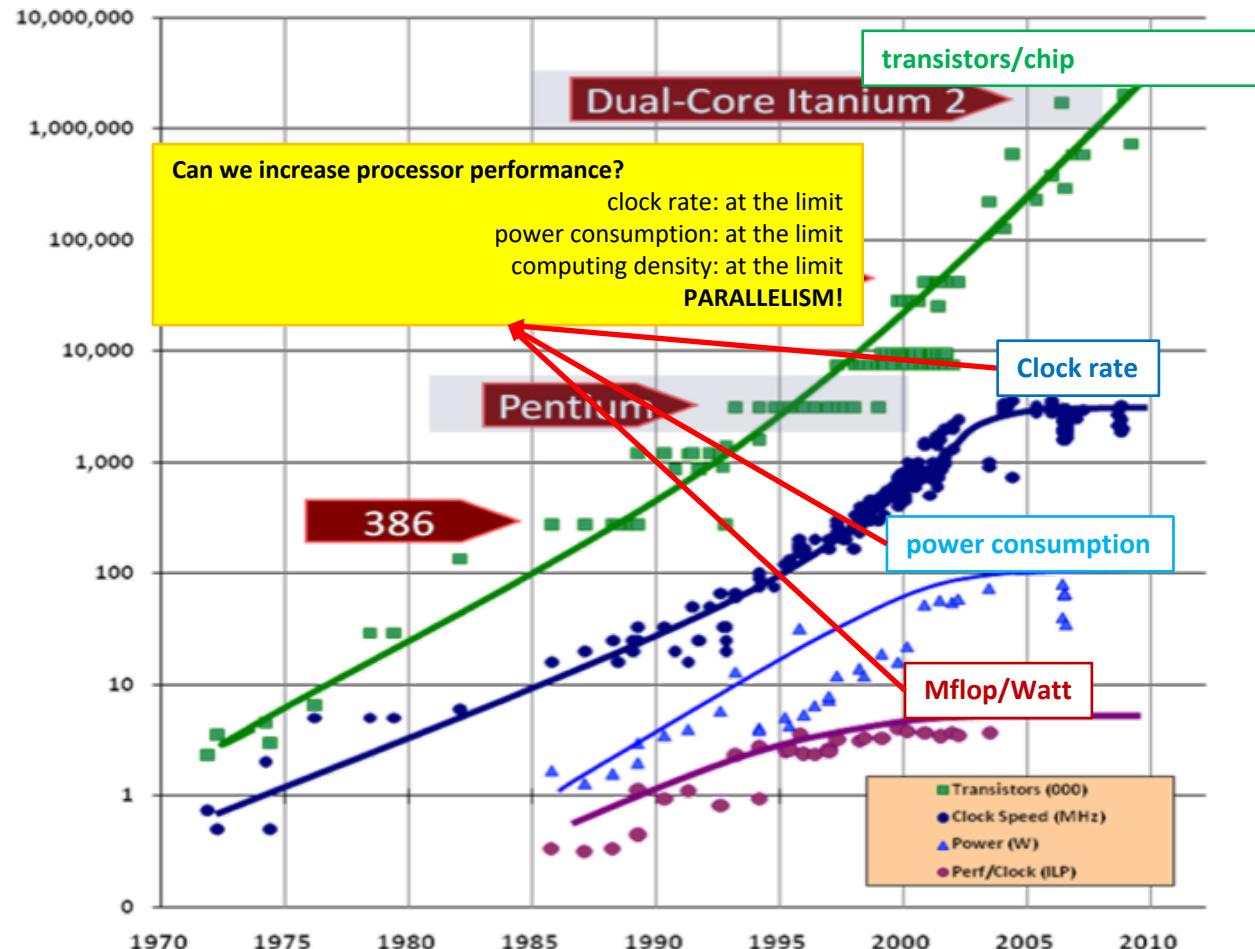
# Factors influencing the performance

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- **Technology of semiconductors**
  - CMOS technology;
  - Decreasing the size of the semiconductor structures leads to better performance:  
size, energy consumption, clock rate, price
- **Compute node architecture**
  - Connection of CPUs and GPUs to memory, memory bandwidth, interconnect bandwidth
- **Infrastructure architecture**
  - Energy efficiency;
  - Cooling efficiency (influences the clock rate)
  - Computational density (less path for the signal to take)

# Processor technology overview

Scale	Year Intro
130 nm – 2001	
90 nm – 2004	
65 nm – 2006	
45 nm – 2008	
32 nm – 2010	
22 nm – 2012	
14 nm – 2014	
10 nm – 2017 (-19 Intel)	
7 nm – 2019 AMD (Roma)	
5 nm – ~2020 (???)	



*all*

(since 2005)

# Why the ~~Fastest~~ Computers are Parallel Computers

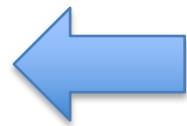
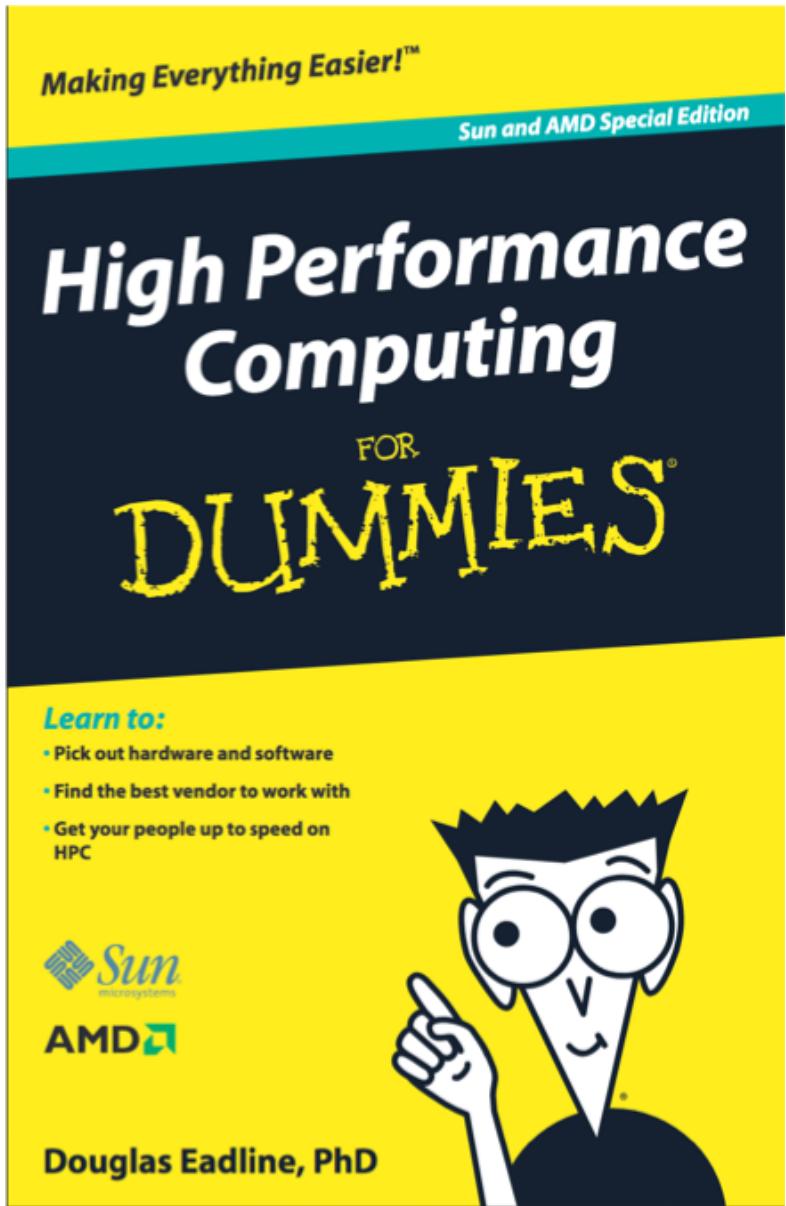
Including laptops and cell phones

Think parallel!

# Moore's Law revisited

- Number of cores per chip can double every 2 years
- Clock rate will not increase (probably it will decrease)
- Systems with millions of concurrent threads (GPUs)
- Inter-chip parallelism (MPI) or intra-chip parallelism (OpenMP)

# What is a supercomputer and HPC?



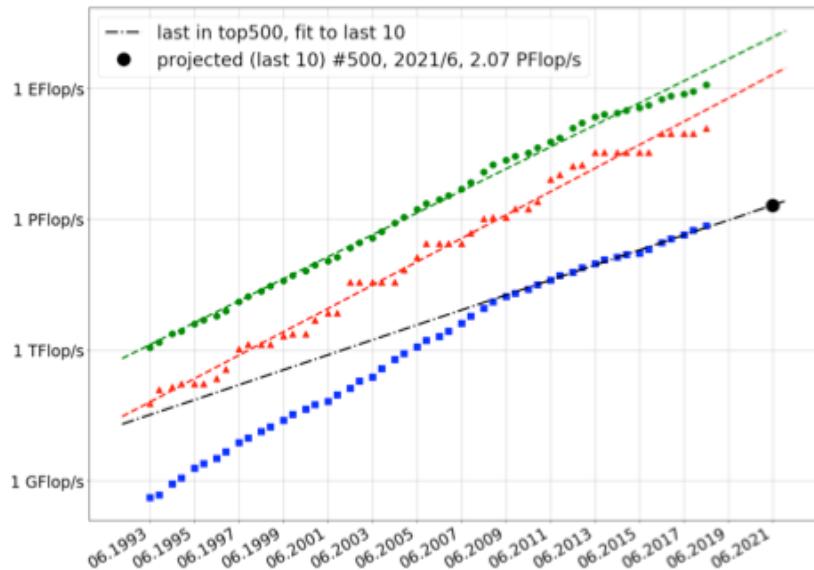
Highly recommended book  
(google for pdf)

# What is a supercomputer and HPC?

**HPC is aggregation of computing power well beyond your typical laptop/desktop.**

Definition is relativistic (relative in space-time)

Relative in time:



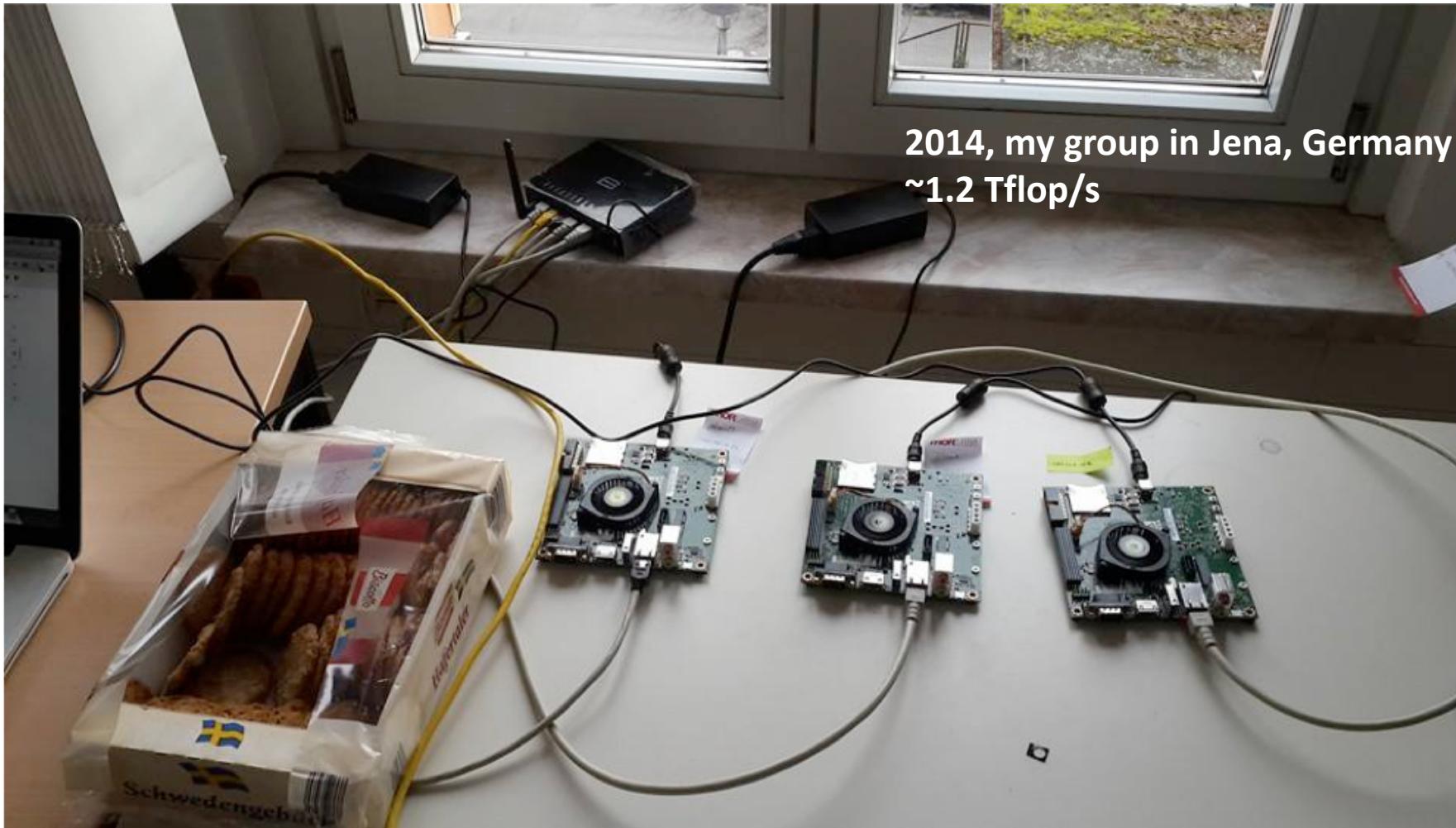
Your laptop was top 100 in the world in 1990s

Relative in space:



You can't put >1000kg computer on-board of autonomous vehicles

# What is a supercomputer and HPC?



# What is a supercomputer and HPC?



# Visionary quotes about computers and HPC

**Thomas Watson (chairman of IBM), 1943:**

*“I think there is a world market for maybe five computers.”*

**Ken Olson (chairman of DEC), 1977:**

*“There is no reason for any individual to have a computer in his home.”*

**Bill Gates, 1981:**

*“640K ought to be enough for anybody”*

**Popular mechanics 1949:**

*«Where a calculator on the ENIAC is equipped with 18,000 vacuum tubes and weighs 30 tons, computers in the future may have only 1,000 vacuum tubes and weigh only 1.5 tons.»*

# History of HPC

Abacus, 5 BC



17th century, Pascaline (1642)



Leibniz's Stepped reckoner (1671)



# History of HPC

19th century

Arithmometer, Charles de Calmar (1820)



Punched card for weaving (1801)

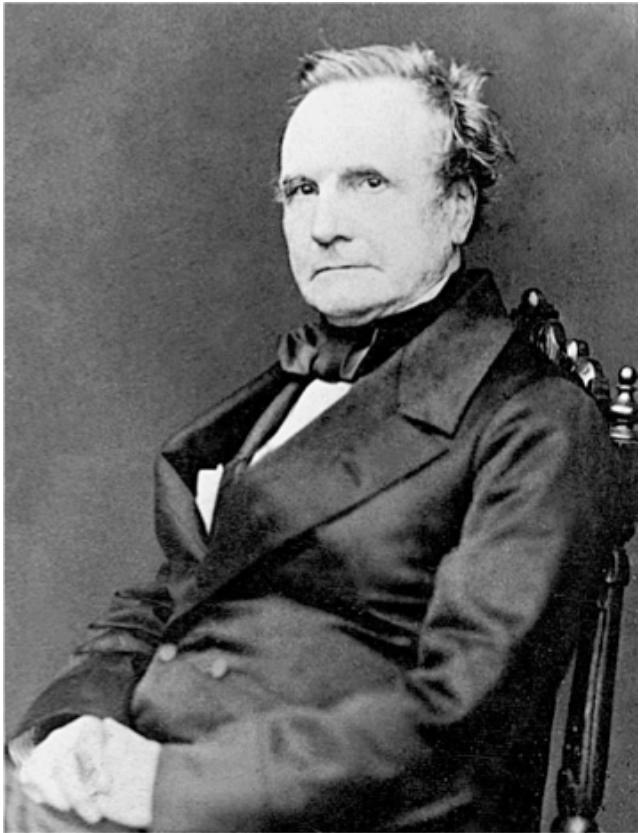


Punched card + calculator,  
Herman Hollerith (1890)



# History of HPC

## 19th century



Charles Babbage, concept of  
fully automated calculation by  
mechanical means



Ada Lovelace, first programmer,  
first algorithm

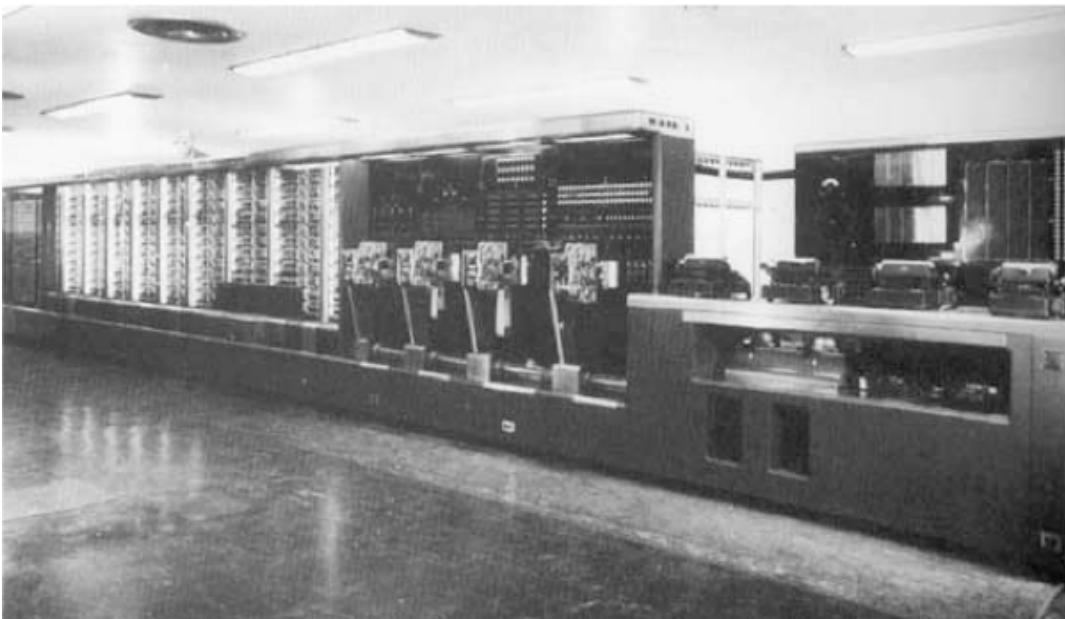
Punched card for weaving (1801)



# History of HPC



Konrad Zuse 1938, Z1 – first programmable mechanical computer



Harvard Mark I

9/9

0800 Anchor started  
1000 " stopped - anchor ✓ { 1.2700 9.032 847 025  
13' 06" (032) MP - MC 1.432 16000 9.037 846 785, connect  
032 PRO 2 2.130 476 465  
connect 2.130 676 315  
Relays 6-2 in 032 failed switch signal test  
In Relays - 16, no test.  
Relays changed

1100 Started Cosine Tape (Sine check)  
1525 Started Multi Adder Test.

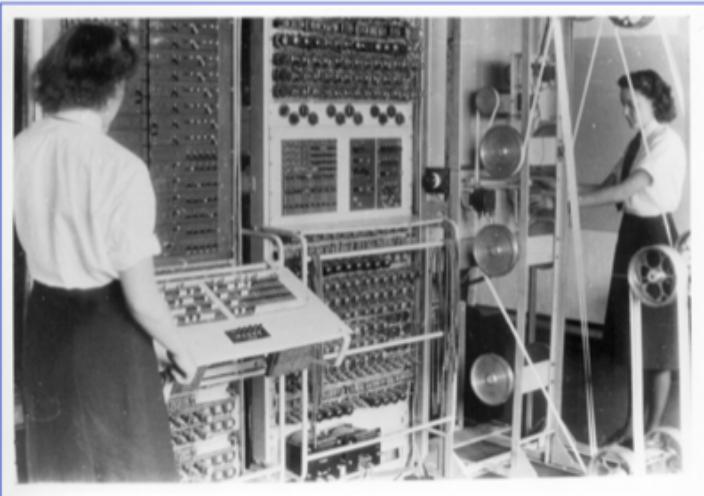
1545 Relay #70 Panel F  
(moth) in relay.

1600 First actual case of bug being found.  
1700 Antennae started.  
1700 closed down.

Paging  
214-  
Aug 31 1943

# History of HPC

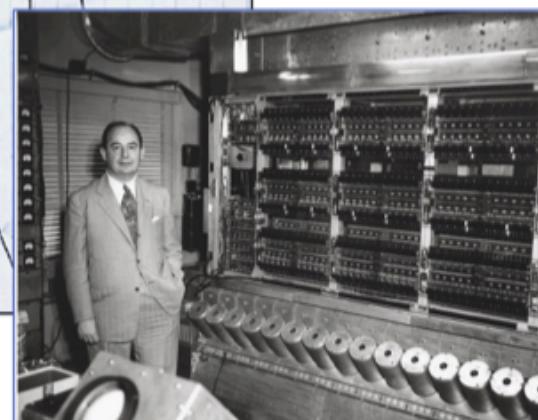
- **Electronic computing developed to meet military needs in WWII**
  - Colossus, Bletchley Park, 1943 ... code breaking, dedicated function
  - ENIAC, U. Pennsylvania, 1945 ... ballistics tables, plugboard programming
  - Von Neumann
    - Initiated 1946 at Institute for Advanced Studies (IAS)
    - Vacuum tubes, oscilloscopes, assembly language ... many operational challenges
    - But momentous – flexible stored program, reliability architecture, hydrogen bomb
    - IAS, Princeton, 1951
    - MANIAC, LANL, 1952
    - ORACLE, ORNL, 1953



Women's Royal Naval Service operating Colossus during World War II

Orders Set of word (16 bits) to 2 words, code value CA = Current address									
Address	Memory	Operation	Shift	+	1	0	1	0	1
1	0	1	0	1	0	1	0	1	0
(10-12)	100000	(0-12)	0-12	(0-12)	(0-12)	12			
(13-16)									
17									

First line of code written for the von Neumann Digital Computing Project



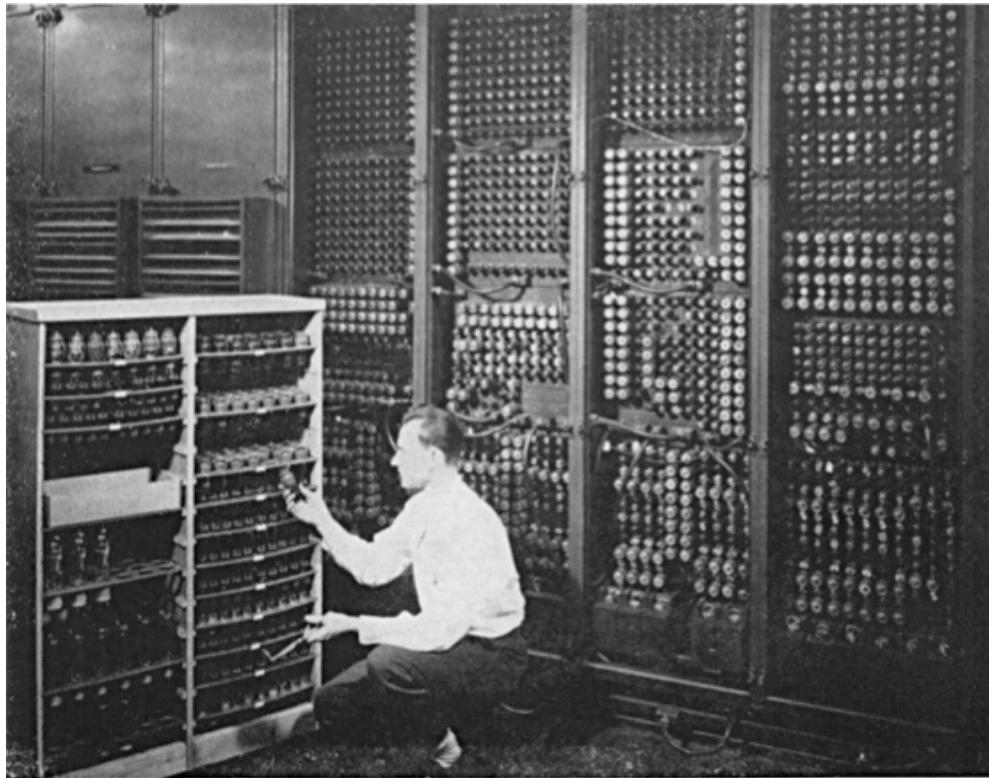
von Neumann with the IAS machine

# History of HPC



Cray-1, 1976, specialized supercomputer  
133 MFlops

# Высокопроизводительные системы СССР



1948 МЭСМ, Лебедев

- 1948, МЭСМ, Лебедев
- с 1952 серия БЭСМ
- БЭСМ 6 выпуск до 1987 года, в работе до 1995 года
- серия «Эльбрус» в разработке до 90х
- 1968 – «гибель» отечественного компьютеростроение – решение о создании серии «РЯД» – клонирование IBM (ЕС)
- 50е-60е проекты сети ВЦ (**ЕГСВЦ**) → ОГАС (аналог ARPANET)
- Инновационные проекты: Сетунь (тернарная логика)

<https://www.ferra.ru/review/computers/ussr-pc-evolution.htm>

<https://www.the-village.ru/city/modern-architecture/171409-kak-v-sssr-stroili-doma-dlya-kompyuterov>

# Советские дома для суперкомпьютеров



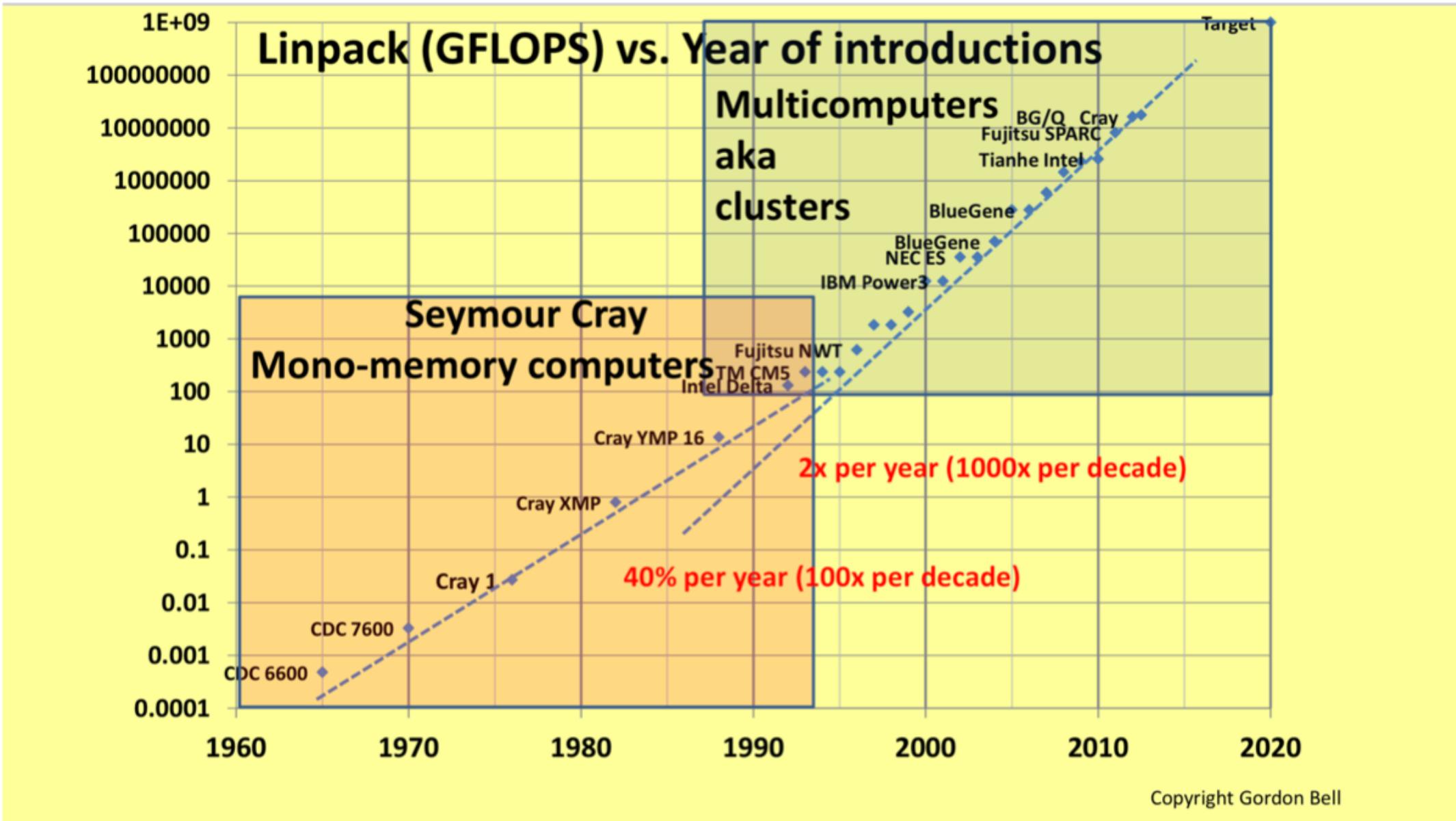
Вычислительный центр ГосПлана СССР (1970) – проспект ак. Сахарова 12

# History of HPC



Scalable „Beowulf“ cluster made of similar compute nodes interconnected between each other.

1994, NASA (Thomas Sterling)



# Flagship supercomputer “Zhores” for AI, Big data and HPC

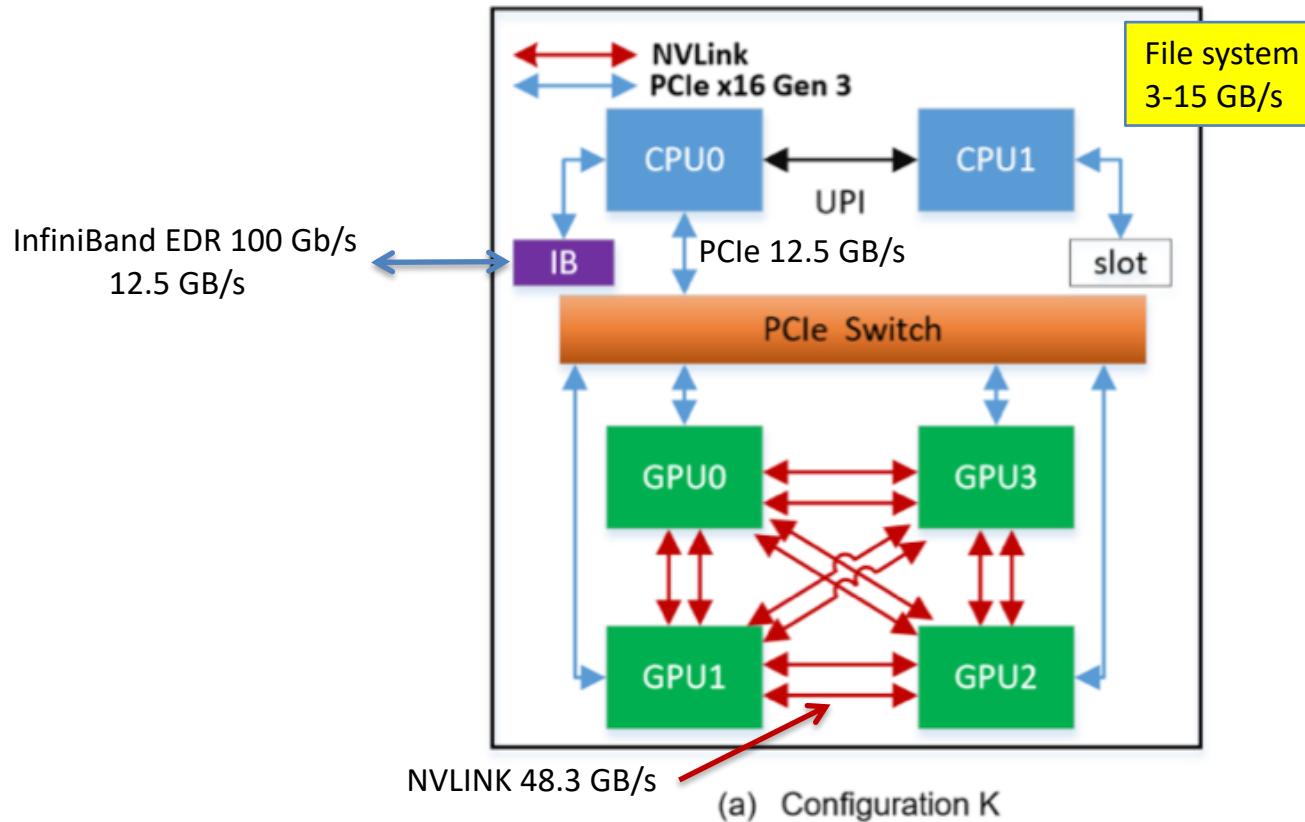
Hybrid energy-efficient architecture

- 74 compute nodes
- 26 nodes with powerful graphic cards Nvidia Tesla V100 (NVLink + RDMA)
- tensor cores for deep learning;
- 90 kWatt power consumption;
- 1PFlops peak performance;
- 0.5 Pbytes storage system
- #8 in Russia
- was installed by our own small team



*«Zhores» is a unique for Russia supercomputer capable of solving a wide range of interdisciplinary problems in machine learning, data science and mathematical modeling in such areas as: biomedicine, image classification, Digital Pharma, Photonics, predictive maintenance, new X- and gamma-ray sources*

# Main power is in the GPU nodes



<b>Platform</b>	PowerEdge C4140 (configuration K and M)
<b>CPU</b>	2xCPU Intel 6140 (18c, 2.3 GHz)
<b>Memory</b>	384 GB DDR4 @ 2666MHz
<b>GPU</b>	NVidia Tesla V100 SXM2 (16 Gb @ 900 GB/s)

# Parallel intuition

- Examples of parallelism in real world?

# Parallel intuition

## How to really understand concurrency.



# Building a house



Say, we have 4 workers building a house

Construction will be faster than if it would be done by 1 worker

After each floor, workers have to synchronize

Connect their parts - communication

Can't build 7th floor before 3rd

# Amdahl's law

Speed-up of a parallel program/work:

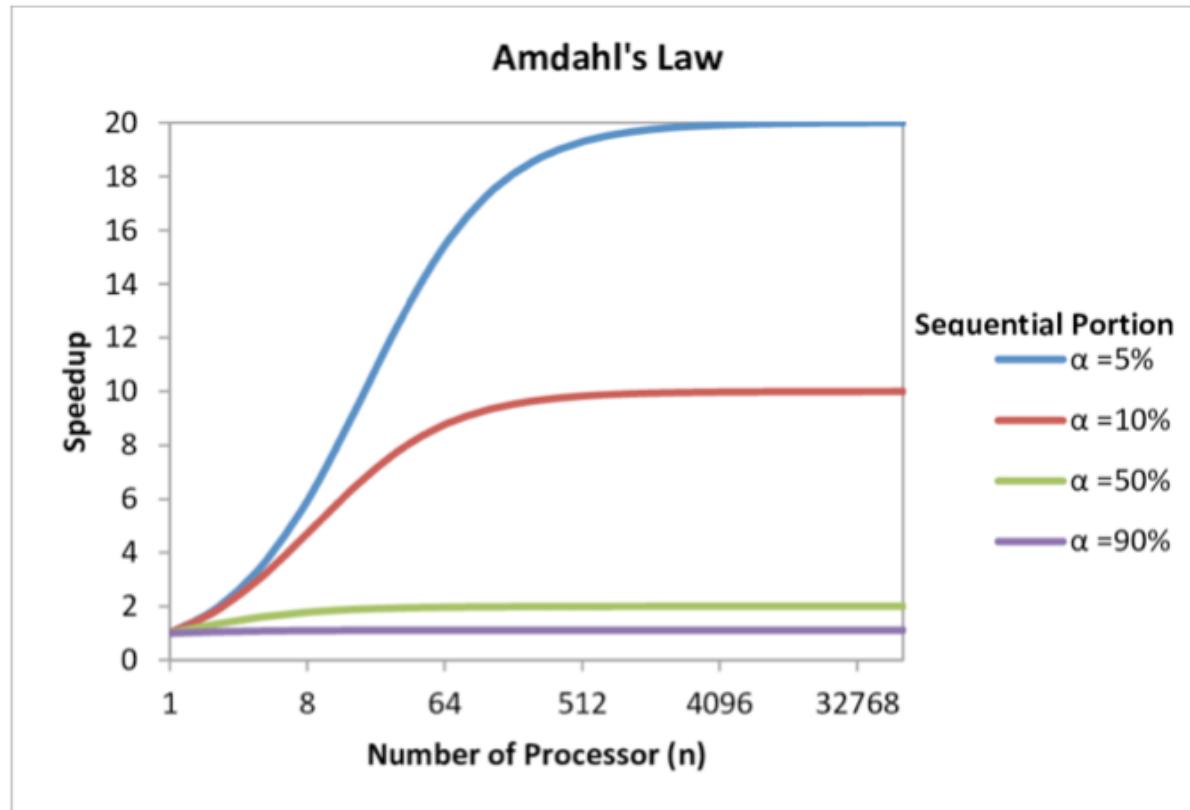
$$Speedup = \frac{1}{(1 - p) + p/N}$$

p – is a fraction of the work that can be done in parallel

N – number of parallel workers



# Amdahl's law implication



$$Speedup = \frac{1}{(1 - p) + p/N}$$

N	p=0.5	p=0.9	p=0.99
10	1.82	5.26	9.17
100	1.98	9.17	50.25
1000	1.99	9.91	90.99
10000	1.99	9.91	99.02
100000	1.99	9.99	99.9

For 90x speedup on 100 processors sequential part can only be 0.1%

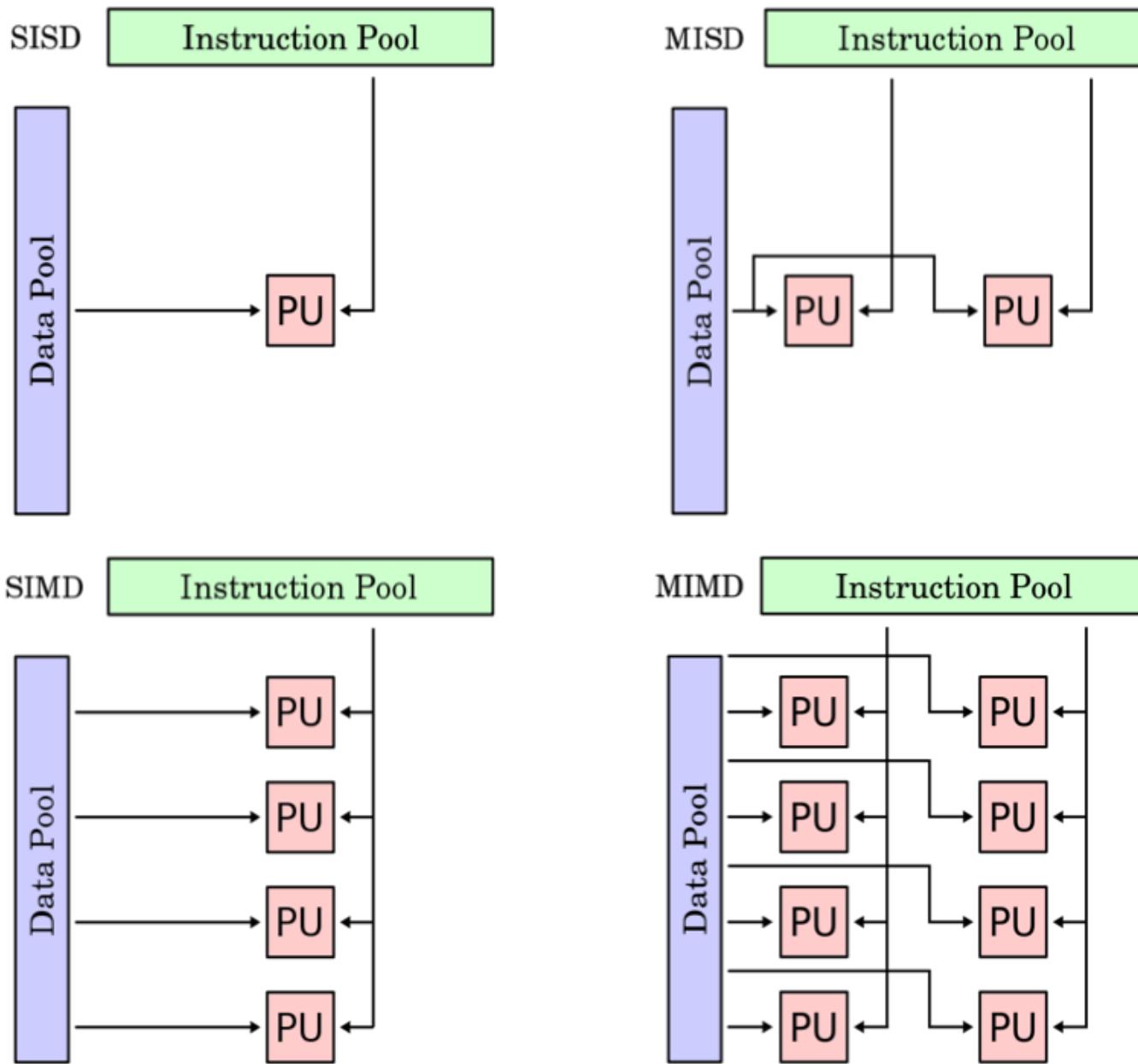
## 2 PITFALLS

- Expecting  $x N$  performance on  $N$  workers for a poorly parallelized code
- Expecting low energy usage on low resource utilization: servers draw up to 2/3 of power while running on 10% load

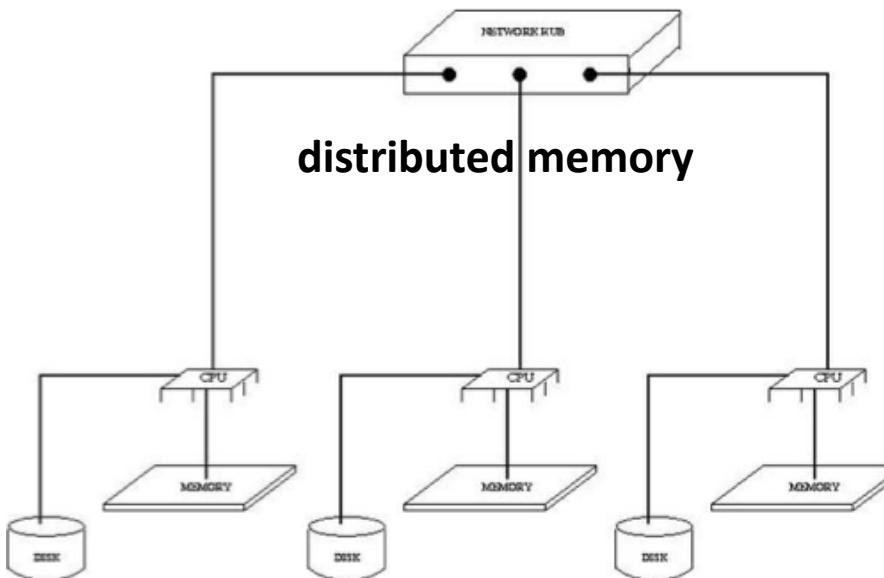
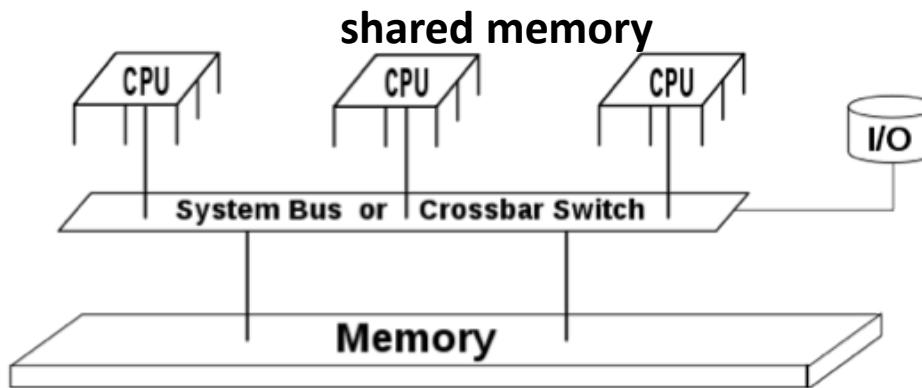
# Why writing parallel programs is hard?

- Finding enough parallelism (Amdahl's law)
- Locality –moving data costs more than arithmetics
- Load balance
- Coordination and synchronization: data sharing safety
- Tuning / debugging / profiling

# Flynn's taxonomy



# Shared memory and distributed memory



# Ways to work parallel

1. Scientific software (Matlab, Mathematica, ANSYS, OpenFoam, Tensorflow, PyTorch, etc)  
Актуальная задача – Neural Architecture Search (i.e. for mobile devices <https://www.mdpi.com/2073-431X/10/8/104>)
2. Libraries (Math Kernel Library, CuDNN, CuBlas, Thrust, Boost)
3. Parallel instruments (OpenMP, MPI, Cuda, OpenCL)

# Types of parallelism in computing

1. Task parallelism (multi-core CPUs) – different tasks or instructions can be done concurrently
2. Data parallelism (GPUs) – same instruction can be done on multiple data concurrently

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1. Task parallelism (multi-core CPUs) – different tasks or instructions can be done concurrently
2. Data parallelism (GPUs) – same instruction can be done on multiple data concurrently

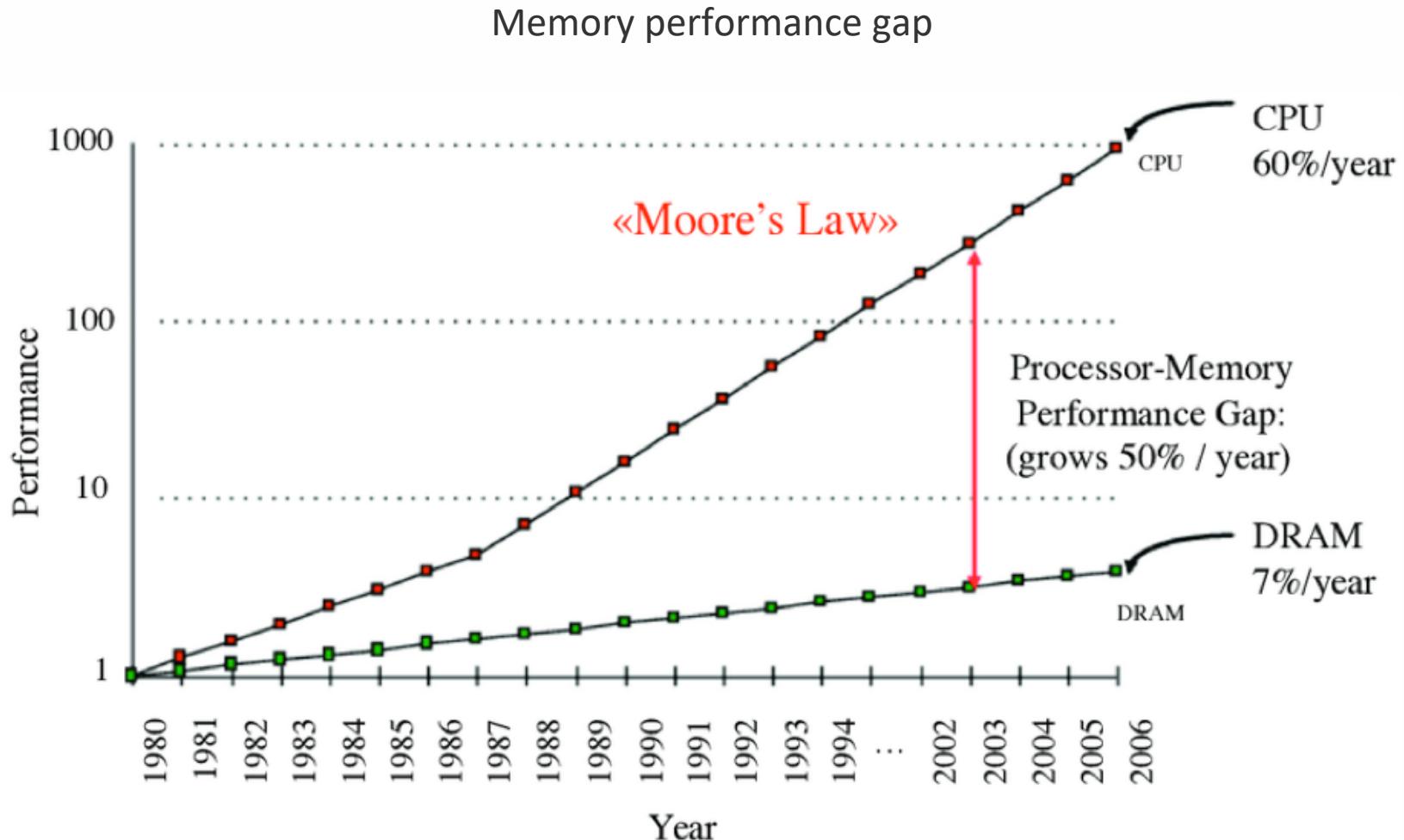
## Types of parallel tasks:

1. Embarrassingly parallel tasks (aka "farming") – no communication between workers  
*bitcoin mining, solving integral with a parameter for 1e6 parameters, running simulation for different input parameters (different initial conditions)*
2. Compute-intensive tasks  
*main time is spent on computing, low level of communication, i.e. numerical photonics or plasma physics simulations*
3. Data-intensive tasks  
*main time is spent on data transfer (big data, operations with file system, databases)*

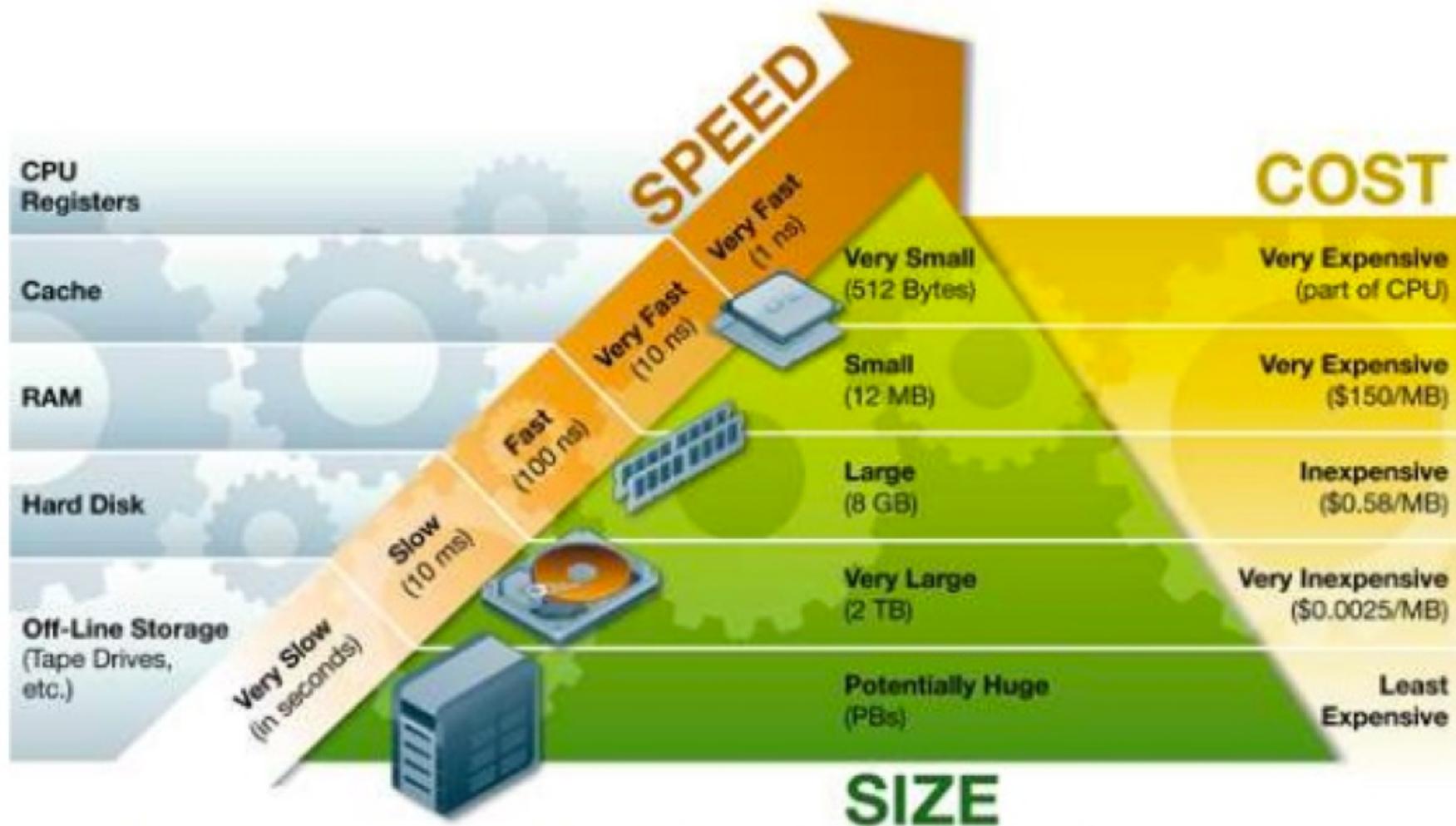


# 1. Перемножение матриц, иерархия памяти

# Отставание производительности памяти



# Иерархия памяти в компьютере



Source: [http://www.ts.avnet.com/uk/products\\_and\\_solutions/storage/hierarchy.html](http://www.ts.avnet.com/uk/products_and_solutions/storage/hierarchy.html)

# «Найвное» перемножение матриц

$$\begin{matrix} c_{00} & c_{01} & c_{02} \\ c_{10} & c_{11} & c_{12} \\ c_{20} & c_{21} & c_{22} \end{matrix} = \begin{matrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{matrix} \times \begin{matrix} b_{00} & b_{01} & b_{02} \\ b_{10} & b_{11} & b_{12} \\ b_{20} & b_{21} & b_{22} \end{matrix}$$

NxN matrices: A, B, C

$N \gg 1$

$C = A * B$

$$C_{ij} = \sum_{n=0}^{N-1} a_{in} * b_{nj}$$

```
for i from 0 to N-1:  
    for j from 0 to N-1:  
        for n from 0 to N-1:  
  
            C[i][j] += A[i][n] * B[n][j]
```

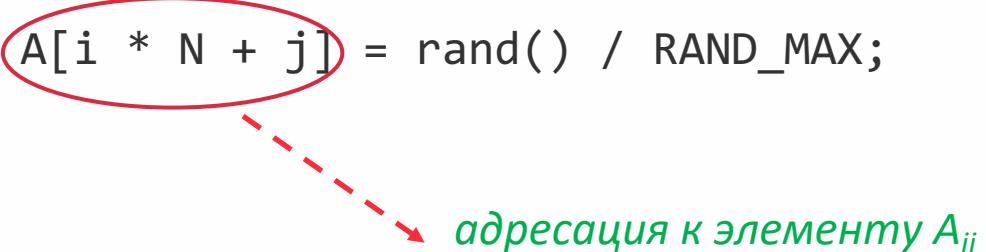
# Основные элементы кода: аллокация памяти и адресация

```
double *A, *B, *C;  
A = (double *) malloc(N * N * sizeof(double));  
B = (double *) malloc(N * N * sizeof(double));  
C = (double *) malloc(N * N * sizeof(double));  
free(A); free(B); free(C);
```



матрица  $N \times N$

```
void RandomMatrix(double * A, size_t N)  
{  
    srand(time(NULL));  
    for (int i = 0; i < N; i++)  
    {  
        for (int j = 0; j < N; j++)  
        {  
            A[i * N + j] = rand() / RAND_MAX;  
        }  
    }  
}
```



адресация к элементу  $A_{ij}$

# Основные элементы кода: matmul и измерение времени

*matmul:*

```
for (i = 0; i < N; i++)
    for(j = 0; j < N; j++)
        for(k = 0; k < N; k++)
            C[i * N + j] = C[i * N + j] + A[i * N + k] * B[k * N + j];
```

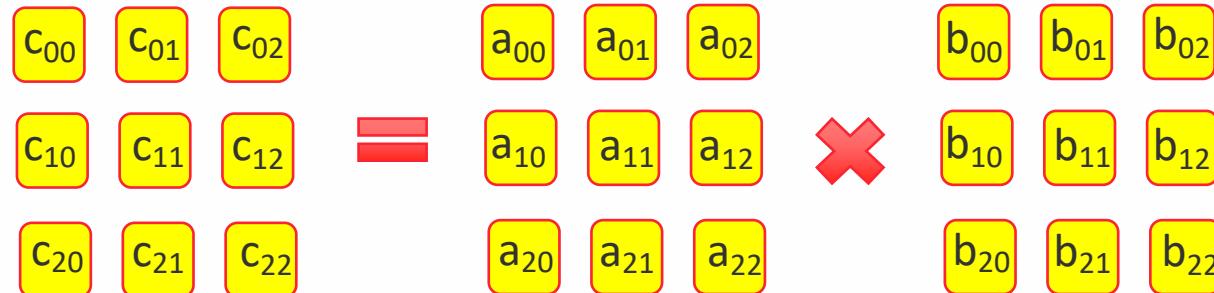
```
struct timeval start, end;
double r_time = 0.0;
gettimeofday(&start, NULL);
... работа
... еще работа
gettimeofday(&end, NULL);
r_time = end.tv_sec - start.tv_sec + ((double)(end.tv_usec - start.tv_usec)) / 1000000;
```



секунды

микросекунды

другие опции с разным разрешением: `clock()`; `clock_gettime()`



```

for i from 0 to N-1:
    for j from 0 to N-1:
        for n from 0 to N-1:

            C[i][j] += A[i][n] * B[n][j]

```

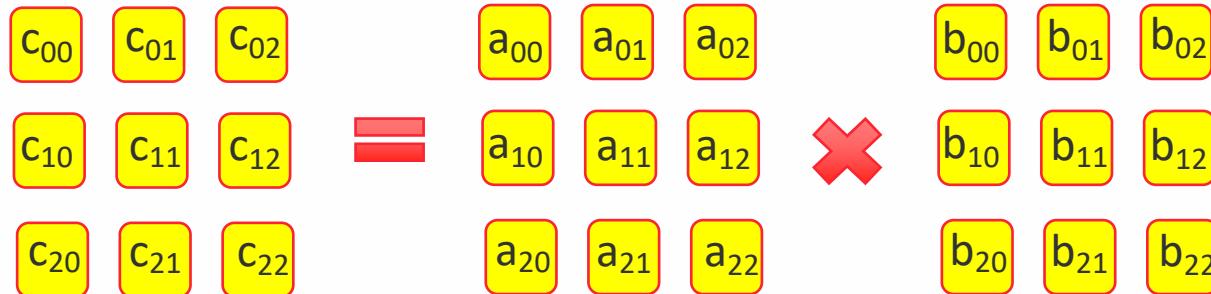
Registers



Cache L1



**RAM**

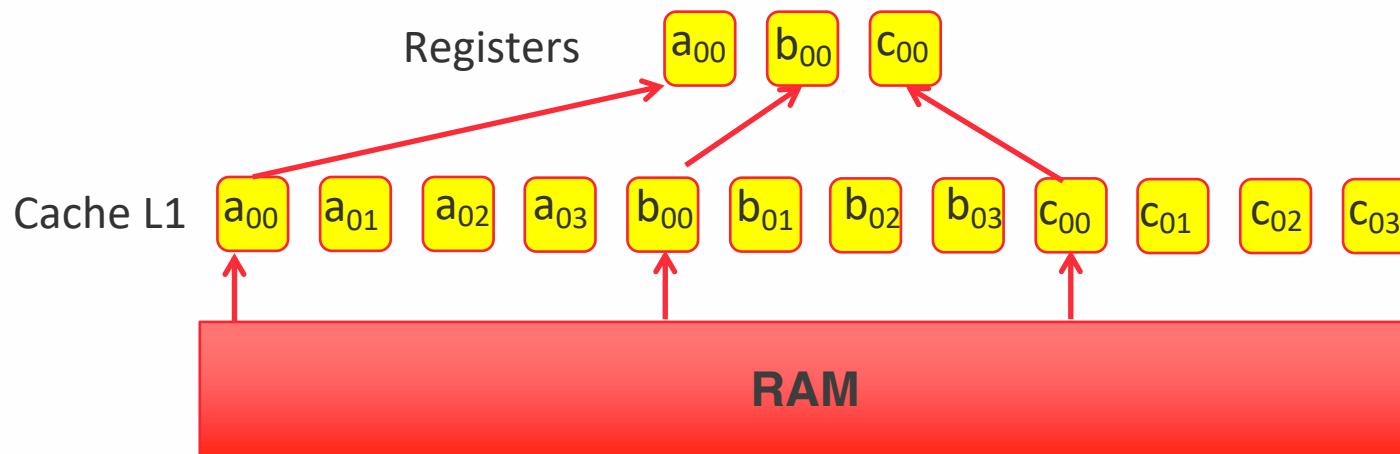


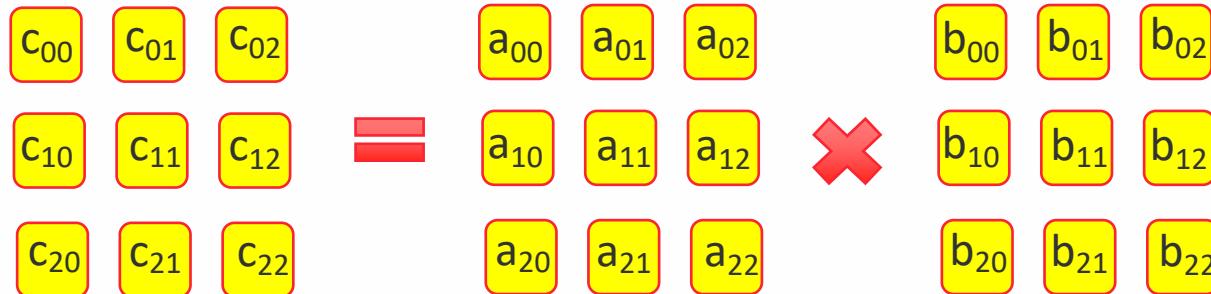
```

for i from 0 to N-1:
    for j from 0 to N-1:
        for n from 0 to N-1:
            C[i][j] += A[i][n]*B[n][j]
    
```

```

i=0
j=0
n=0
C[0][0] += A[0][0]*B[0][0]
    
```



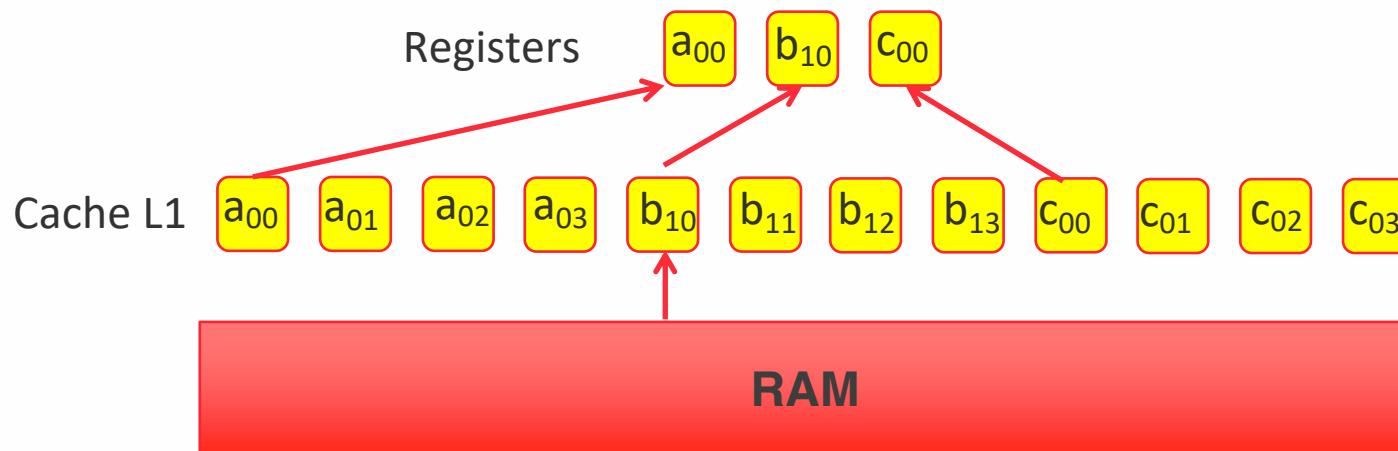


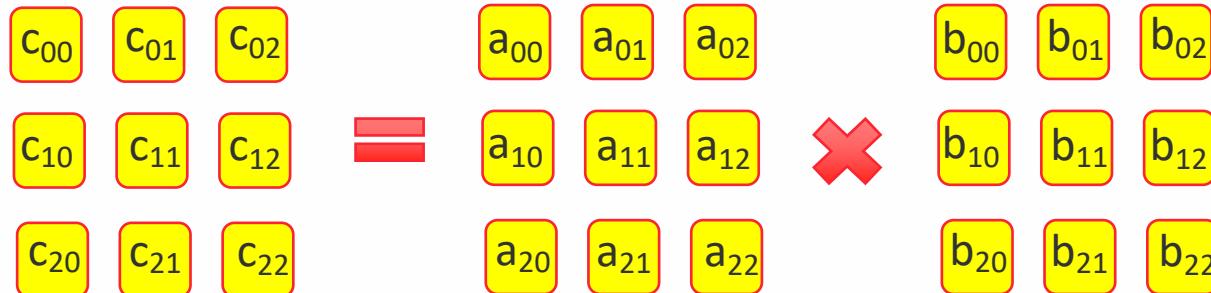
```

for i from 0 to N-1:
    for j from 0 to N-1:
        for n from 0 to N-1:
            C[i][j] += A[i][n]*B[n][j]
    
```

```

i=0
j=0
n=1
C[0][0] += A[0][1]*B[1][0]
    
```



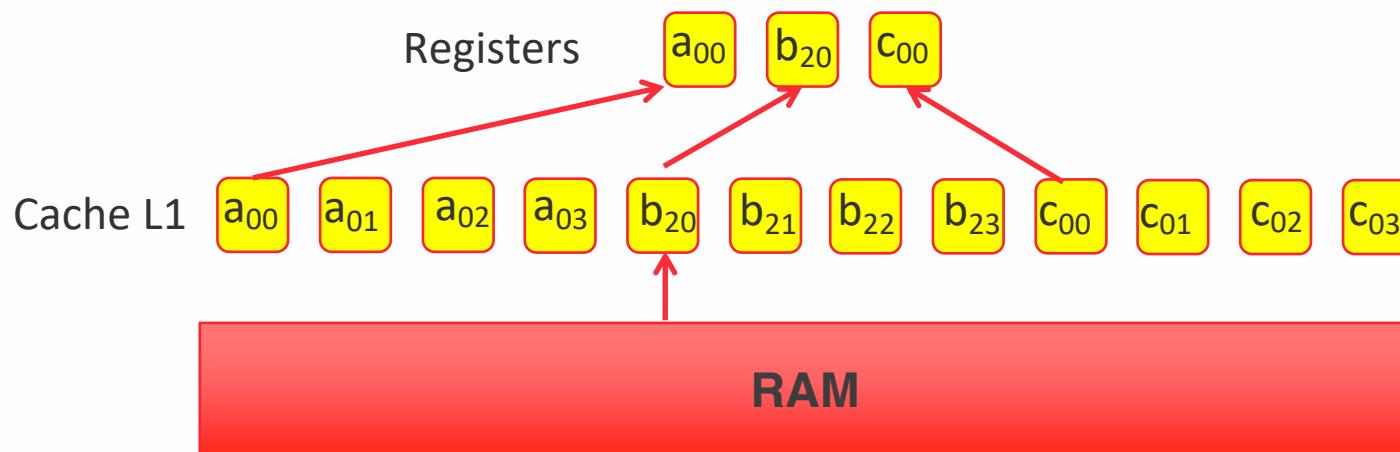


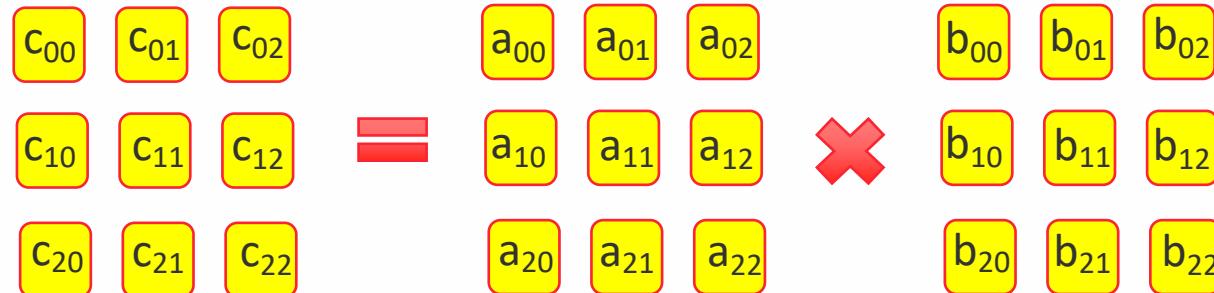
```

for i from 0 to N-1:
    for j from 0 to N-1:
        for n from 0 to N-1:
            C[i][j] += A[i][n]*B[n][j]
    
```

```

i=0
j=0
n=2
C[0][0] += A[0][2]*B[2][0]
    
```





```

for n from 0 to N-1:
    for i from 0 to N-1:
        for j from 0 to N-1:

            C[i][j] += A[i][n]*B[n][j]

```

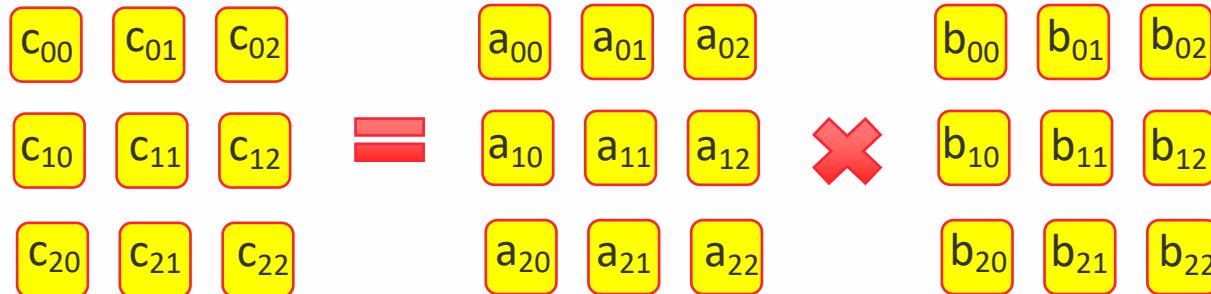
Registers



Cache L1



**RAM**

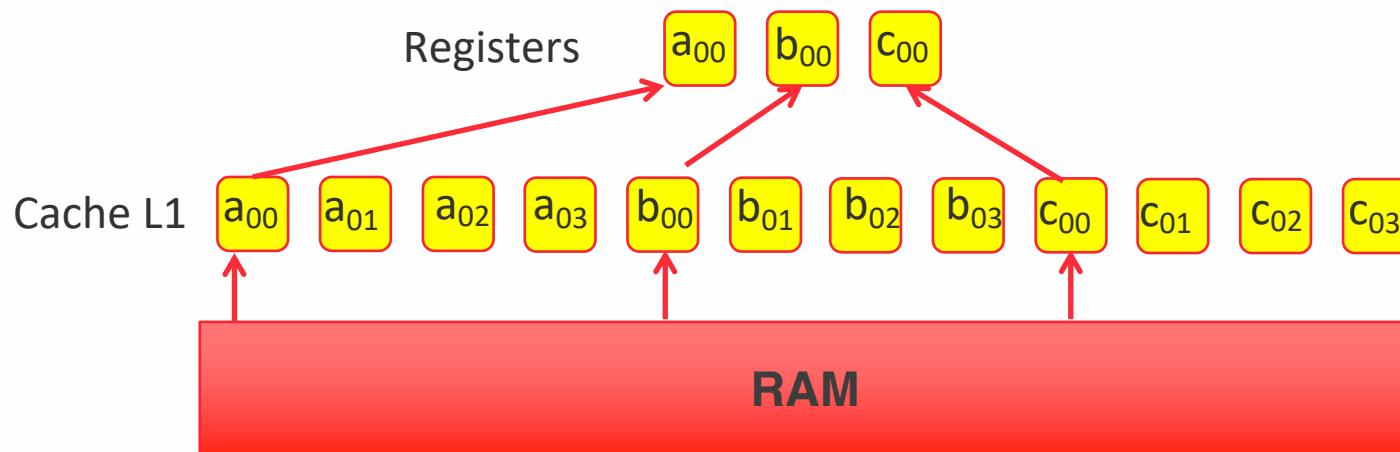


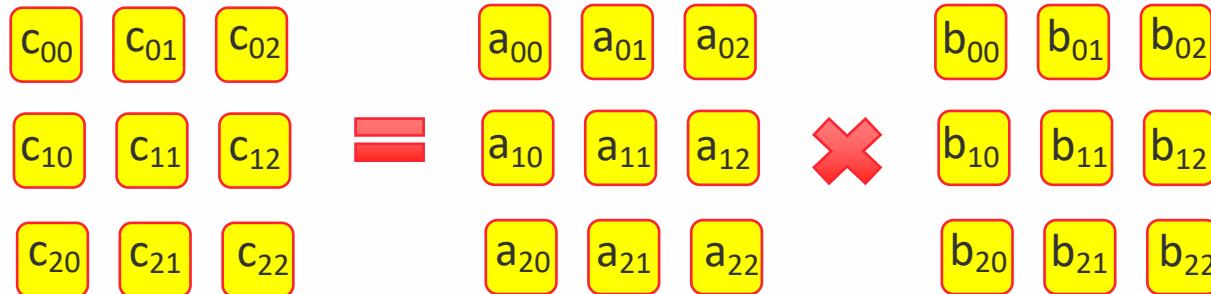
```

for n from 0 to N-1:
    for i from 0 to N-1:
        for j from 0 to N-1:
            C[i][j] += A[i][n]*B[n][j]
    
```

```

n=0
i=0
j=0
C[0][0] += A[0][0]*B[0][0]
    
```



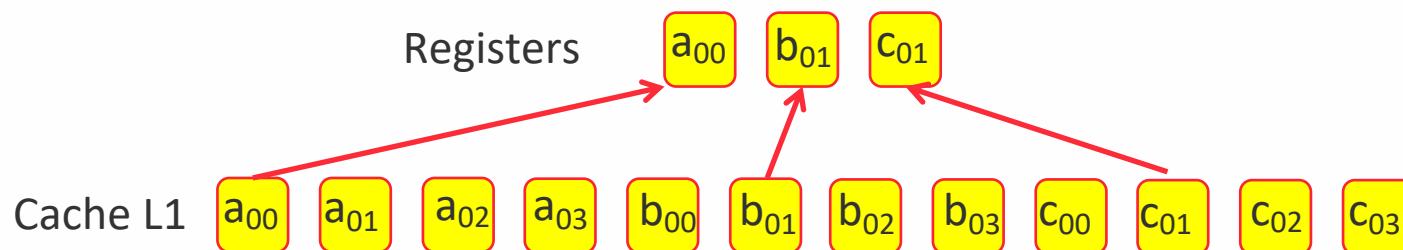


```

for n from 0 to N-1:
    for i from 0 to N-1:
        for j from 0 to N-1:
            C[i][j] += A[i][n]*B[n][j]
    
```

```

n=0
i=0
j=1
C[0][1] += A[0][0]*B[0][1]
    
```





# Выводы к первой лекции

---

1. Высокопроизводительные вычисления активно развиваются и приносят ощутимый экономический эффект
2. Видна тенденция на соединение ИИ и высокопроизводительных вычислений
3. Виден запрос от индустрии на HPC и Green AI
4. Разнообразные вычислительные платформы требуют разнообразных приемов HPC

# д/з 1



- 50% На основании данных рейтинга top500 спрогнозировать производительность компьютера №1 в 2025
- 50% оцените какой процент всего производимого на Земле электричества потребляют все компьютеры из top500 (на основании открытых данных top500.org)
- 10% Бонус: Улучшить производительность программы с реализацией алгоритма матричного умножения

Какие домашки? после следующих лекций:

1. Вводная лекция по истории НРС	5-6. Библиотека MPI и MPI4Py
2. Терминал, переменные окружения Makefile	7, 9. Cuda/PyCuda
3. Pthreads, openmp	8. Профилировка и биндинг С/C++/Python **
4. Навыки работы на суперкомпьютере *	** полностью бонусная