MAX

DRIVING THE EXASCALE TRANSITION

H2020 EUROPEAN CENTRE OF EXCELLENCE _ EU GRANT # 676598

Facing the exascale challenge

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- What are the trends in the supercomputing world?
- What are the perspective of the software in this context?
- What are the opportunities offered by the supercomputing scenario?

Or.. Shortly: ok, exaflops are coming… what to do with them?

Top500 – November 2017

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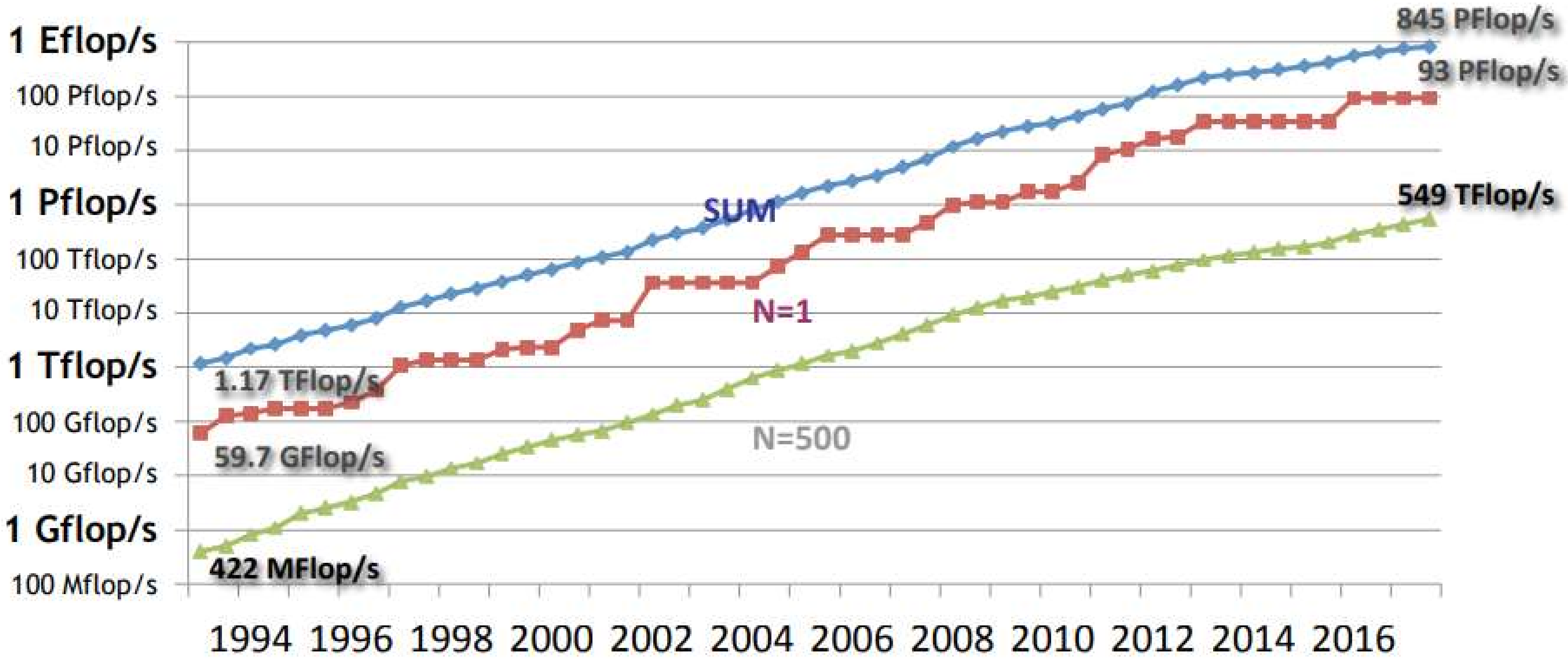
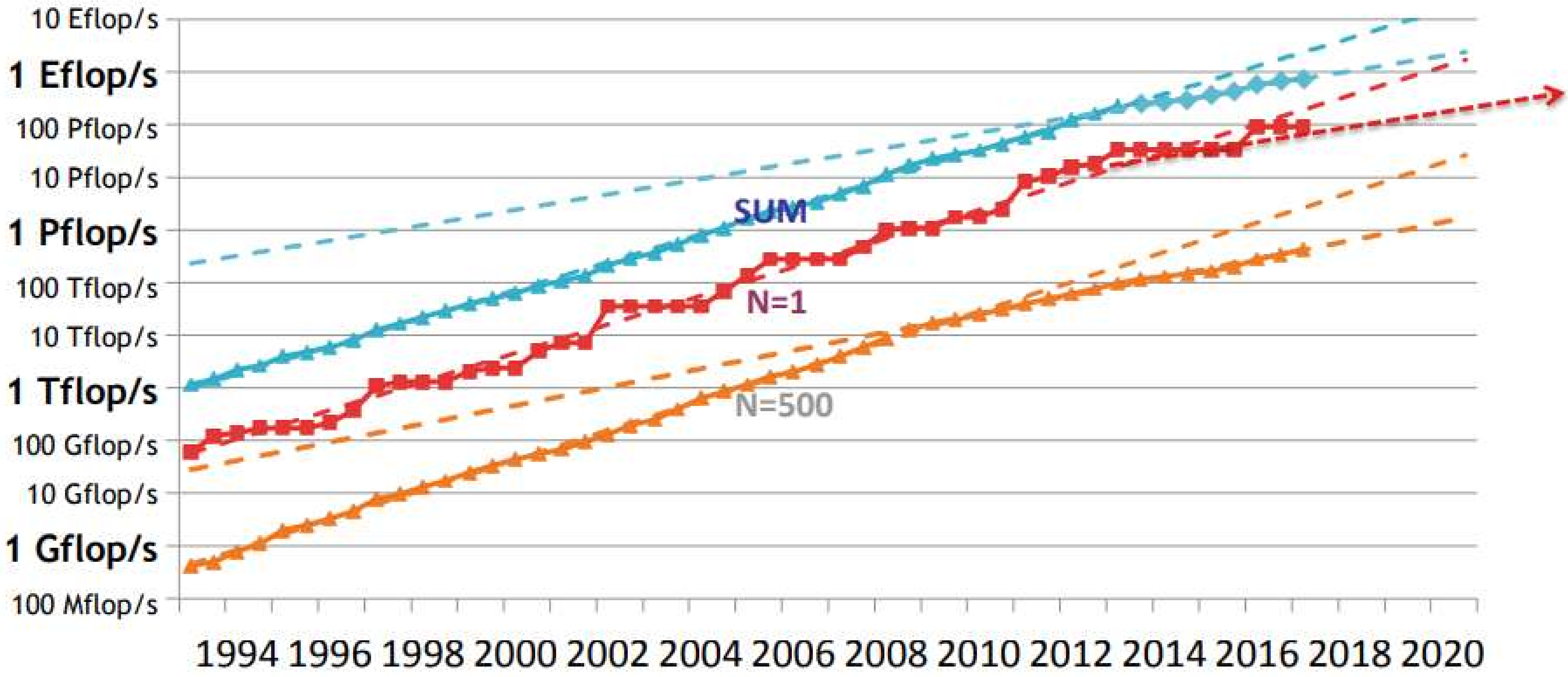
#	Site	Manufacturer	Computer	Country	Cores	Rmax (Pflops)	Power [MW]
1	National Supercomputing Center in Wuxi	NRCPC	Sunway TaihuLight NRCPC Sunway SW26010, 260C 1.45GHz	China	10,649,600	93.0	15.4
2	National University of Defense Technology	NUDT	Tianhe-2 NUDT TH-IVB-FEP, Xeon 12C 2.2GHz, IntelXeon Phi	China	3,120,000	33.9	17.8
3	Swiss National Supercomputing Centre (CSCS)	Cray	Piz Daint Cray XC50, Xeon E5 12C 2.6GHz, Aries, NVIDIA Tesla P100	Switzerland	361,760	19.6	2.27
4	Japan Agency for Marine-Earth Science and Technology	ExaScaler	Gyoukou ZettaScaler-2.2 HPC System, Xeon 16C 1.3GHz, IB-EDR, PEZY-SC2 700Mhz	Japan	19,860,000	19.1	1.35
5	Oak Ridge National Laboratory	Cray	Titan Cray XK7, Opteron 16C 2.2GHz, Gemini, NVIDIA K20x	USA	560,640	17.6	8.21
6	Lawrence Livermore National Laboratory	IBM	Sequoia BlueGene/Q, Power BQC 16C 1.6GHz, Custom	USA	1,572,864	17.2	7.89
7	Los Alamos NL / Sandia NL	Cray	Trinity Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries	USA	979,968	14.1	3.84
8	Lawrence Berkeley National Laboratory	Cray	Cori Cray XC40, Intel Xeons Phi 7250 68C 1.4 GHz, Aries	USA	622,336	14.0	3.94
9	JCAHPC Joint Center for Advanced HPC	Fujitsu	Oakforest-PACS PRIMERGY CX1640 M1, Intel Xeons Phi 7250 68C 1.4 GHz, OmniPath	Japan	556,104	13.6	2.72
10	RIKEN Advanced Institute for Computational Science	Fujitsu	K Computer SPARC64 VIIIfx 2.0GHz, Tofu Interconnect	Japan	795,024	10.5	12.7

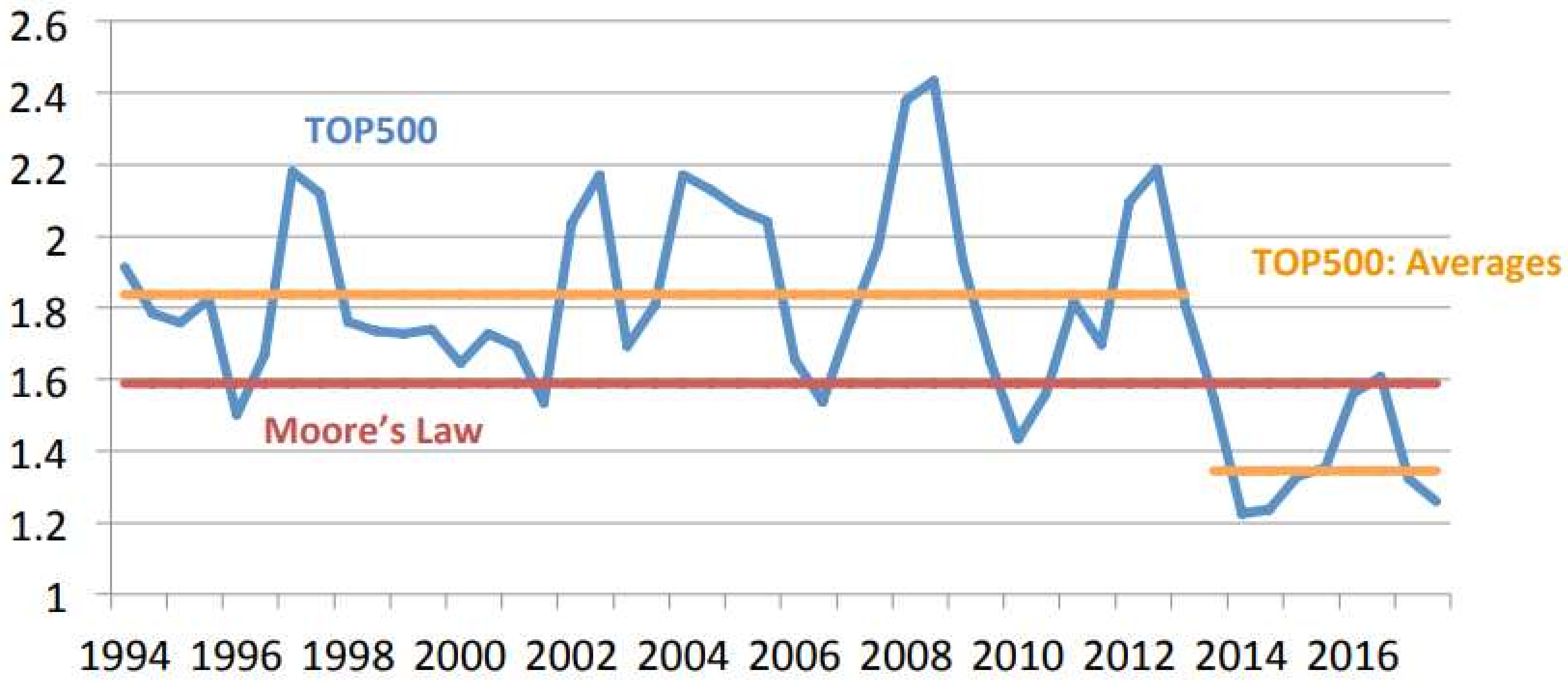
Top500 Performance development



Top500 Projected performance



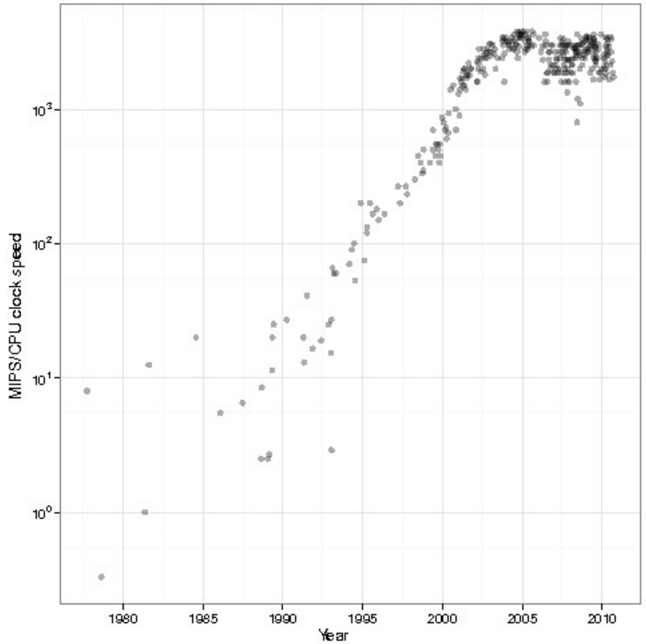
Verifying the Moore's law



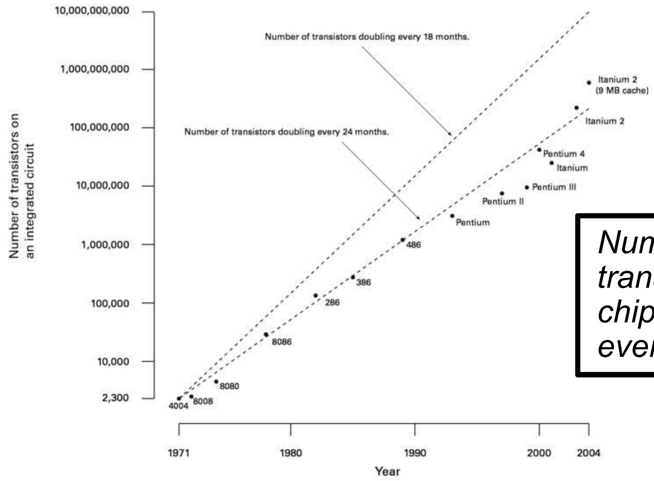
HPC Trends

Moore's Law

Dennard scaling law (downscaling)



The core frequency and performance do not grow following the Moore's law any longer	Increase the number of cores to maintain the architectures evolution on the Moore's law



Number of transistors per chip double every 24 month

Amdahl's law

maximum speedup tends to
1 / (1 − *P*)
P= parallel fraction

The upper limit for the scalability of parallel applications is determined by the fraction of the overall execution time spent in non-parallel operations.

HPC Trends

Peak Performance	Exaflops 10^18	Moore law
FPU Performance	Gigaflops 10^9	Dennard law
Number of FPUs	10^9	Moore + Dennard
App. Parallelism	serial fraction 1/10^9	Amdahl's law
System TCO	Power >10^6 Watt	Moore + Dennard

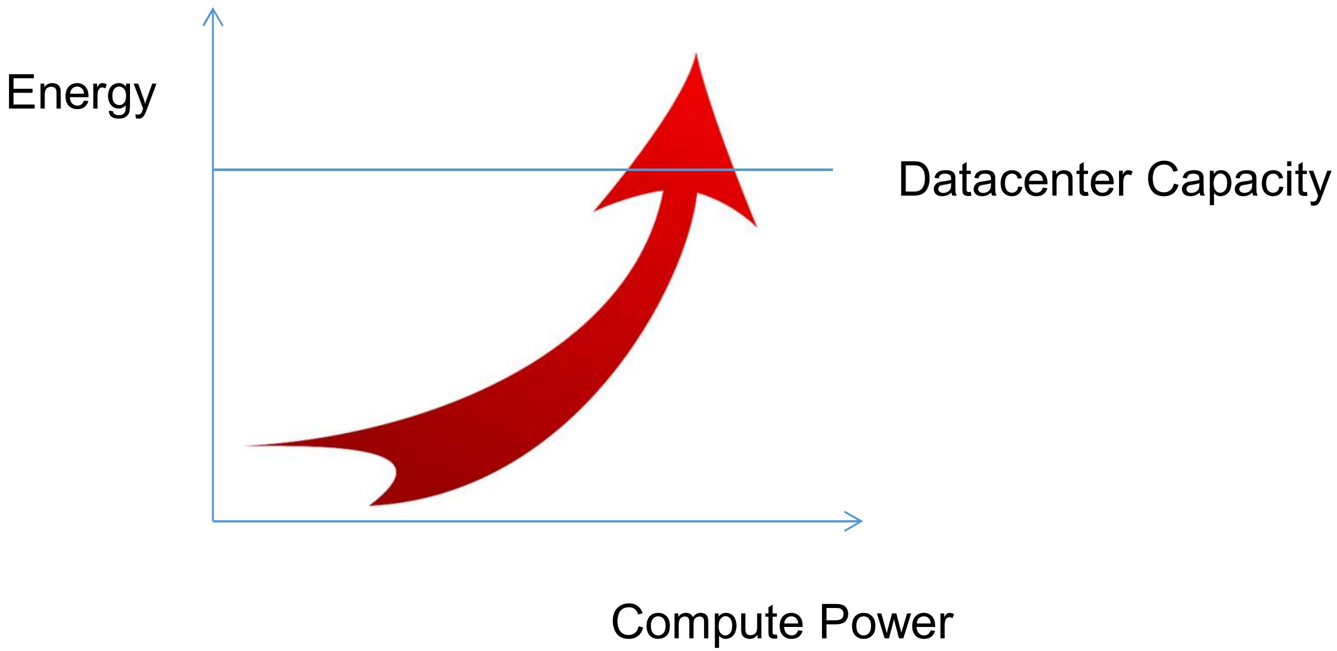
opportunity

challenge

Energy trends

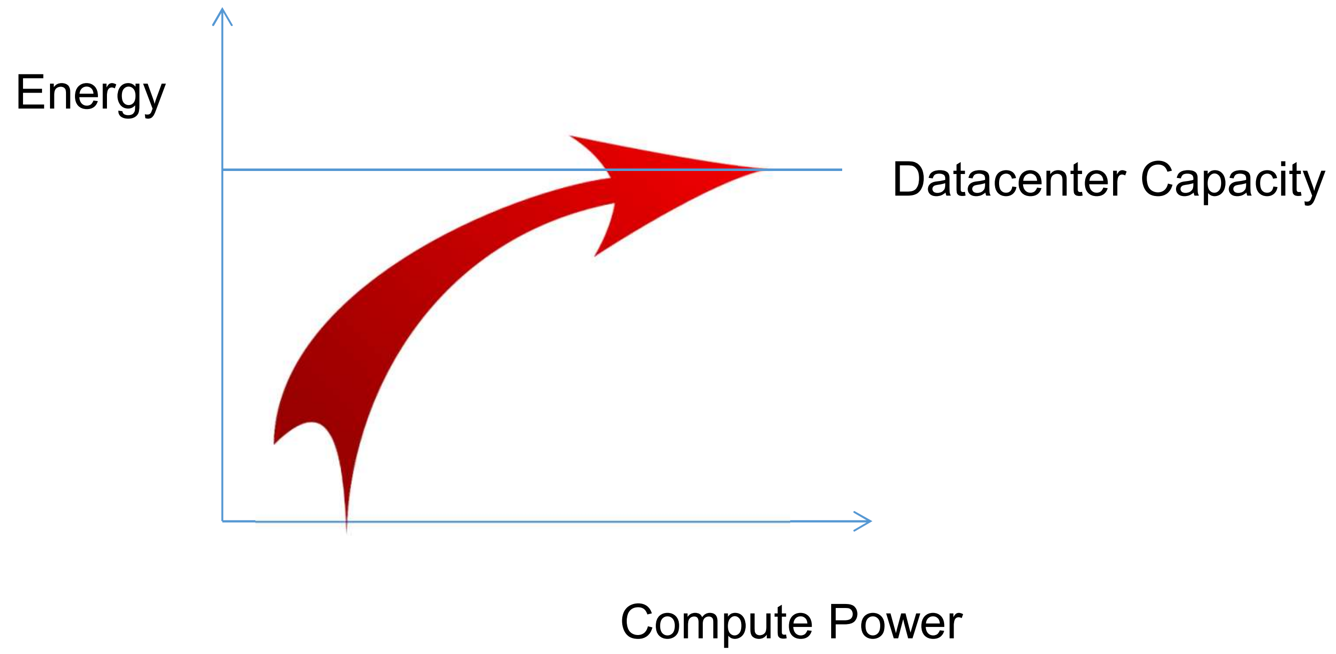
“traditional” RISC and CISC chips are designed for maximum performance for all possible workloads

A lot of silicon to maximize single thread performace

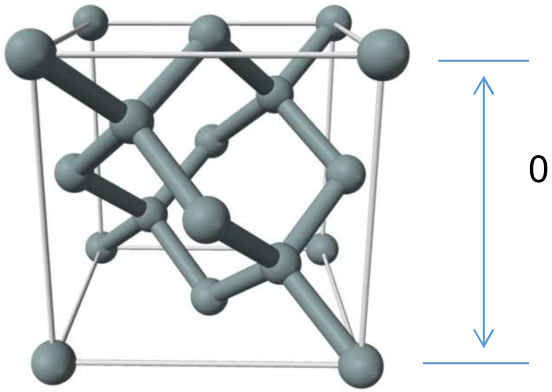


Change of paradigm

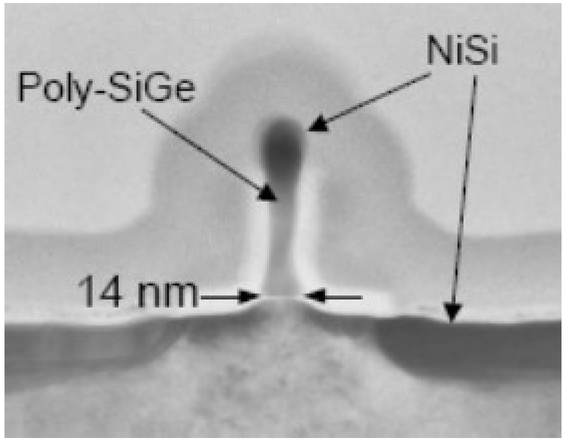
New chips designed for maximum performance in a small set of workloads → Simple functional units, poor single thread performance, but maximum throughput



The silicon lattice



Si lattice



50 atoms!

There will be still 4~6 cycles (or technology generations) left until
we reach 11 ~ 5.5 nm technologies, at which we will reach downscaling limit, in some year between 2020-30 (H. Iwai, IWJT2008).

Paradigm and co-design

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Identify latency and throughput sub/module/class

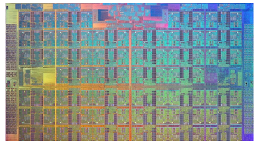
App workflow

- latency
- throughput
- comm
- latency
- throughput

→ Re-factor

- Latency code
- Throughput code

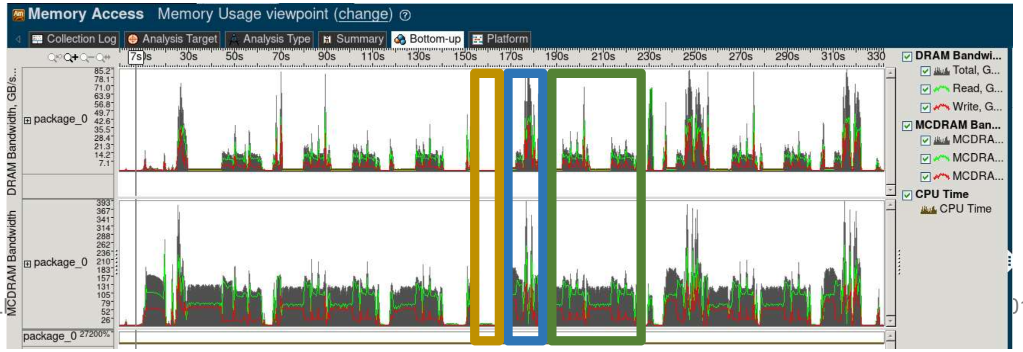
→ Map to HW



knl

host

Heterogeneus



One size do not fit all

10^9 FPU to leverage

Best algo for 1FPU /= best algo for 10^9FPU

Implement the best algo for each scale

e.g. 2 FFT and data distribution in QE 6.2

Autotuning

Choose the best at runtime

How to keep the pace

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- Modularization: easy to modernize codes and it enables interoperability
- Adopt best practises of software engineering
  - The code should remain flexible and easily portable to different architectures
- Expose parallelism: MPI tasks, OpenMP threads, data locality, etc. etc.

Why we should do that?

- ~~Exascale~~ Extreme scale computing can enable new science
- It is important to not discard the opportunities opened by the computational landscape
- Not only in terms of strong scalability, but also for high-throughput research (material screening, ensemble simulations, etc.)

Some examples from PRACE

15th Project Access Call – Awarded Projects

Wednesday 4 October 2017

Results of the 15th Call for Proposals for Project Access.

Projects from the following research areas:

- Biochemistry, Bioinformatics and Life sciences (4)
- Chemical Sciences and Materials (18)
- Earth System Sciences (2)
- Engineering(8)
- Fundamental Constituents of Matter (8)
- Mathematics and Computer Sciences (0)
- Universe Sciences (6)

Biochemistry, Bioinformatics and Life sciences (4)

Electronic and optical properties of high-performance monolayer and multilayer materials

Project Title: Electronic and optical properties of high-performance monolayer and multilayer materials
Project Leader: Nicola Marzari
Resource Awarded: 30 million core hours on Marconi – KNL

BioTitan – Ab initio molecular dynamics of biomolecular adsorption on fully hydrated TiO2-water interfaces

Project Title: BioTitan – Ab initio molecular dynamics of biomolecular adsorption on fully hydrated TiO2-water interfaces
Project Leader: Alexander Lyubartsev
Resource Awarded: 50.2 million core hours on MareNostrum

High-throughput simulations of transistors based on 2-D materials

Project Title: High-throughput simulations of transistors based on 2-D materials
Project Leader: Mathieu Luisier
Resource Awarded: 71 million core hours on Piz Daint

Looking overseas

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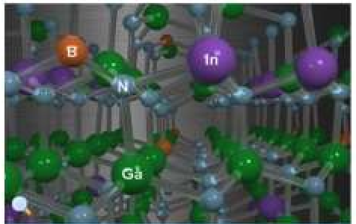
NERSC RESOURCES HELP PREDICT NEW MATERIAL FOR HIGH-POWER, HIGH-EFFICIENCY LEDS

Atomistic calculations find that adding boron to indium-gallium nitride increases the efficiency of LEDs

NOVEMBER 21, 2017
Contact: Andrew McAllister, Univ. of Michigan, mcala@umich.edu; Emmanouil Kioupakis, kioup@umich.edu, 734-764-3321

High-power white LEDs face the same problem that Michigan Stadium faces on game day — too many people in too small of a space. Of course, there are no people inside of an LED. But there *are* many electrons that need to avoid each other and minimize their collisions to keep the LED efficiency high. Using predictive atomistic calculations and high-performance supercomputers at the National Energy Research Scientific Computing Center (NERSC), researchers Logan Williams and Emmanouil Kioupakis at the University of Michigan found that incorporating the element boron into the widely



Crystal structure of a BInGaN alloy. Image: Michael Waters and Logan Williams, University of Michigan

NERSC PI: Emmanouil Kioupakis
Lead Institution: University of Michigan
Project Title: Electronic and Optical Properties of Novel Photovoltaic and Thermoelectric Materials from First Principles
DOE Program Office: BES—Materials Sciences and Engineering
Journal Citation: L. Williams, E. Kioupakis, "BInGaN alloys nearly lattice-matched to GaN for high-power high-efficiency visible LEDs," *Applied Physics Letters* 111, 211107, November 2017. doi: 10.1063/1.4997601

What we will see in the next days

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- Material science codes!
- What are the techniques, the algorithms, the solutions implemented on some material science softwares
- Some examples of large scale exploitation of supercomputers
- Feel free to ask, to discuss: this is not a tutorial, this is a workshop!

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The logo of your institution

The agenda

Monday 4		
9-9.30	Reception and introduction	F. Affinito
9.30-10.30	HPC trends towards exascale and material science challenges	F. Affinito
11.00-12.30	Yambo(1)	A. Marini
14.00-15.30	Yambo(2)	A. Ferretti
16.00-17.30	Introduction to CINECA HPC infrastructure	A. Marani
Tuesday 5		
9.30-10.30	Quantum ESPRESSO: introduction to the code and parallelization schema	P. Bonfà
11.00-12.30	Quantum ESPRESSO: HPC exploitation, a test case	S. De Gironcoli
14.00-15.30	GPU acceleration of plane-wave codes using SIRIUS library	A. Kozhenikov
16.00-17.30	QE-GPU: an experience of porting to GPUs	Anoop Kaithalikunnel
Wednesday 6		
9.30-10.30	The AiiDA platform for computational materials science	A. Marrazzo
11.00-12.30	AiiDA from a user's perspective: HPC and HTC stories	A. Marrazzo
14.00-15.30	Opportunities from Accurate and Efficient Density Functional Theory Calculations for Large Systems	L. Genovese
16.00-17.30	Electronic structure calculations in HPC framework: Solutions for profiling, load-balancing and post-processing	L. Genovese