High Performance Computing Directions:
The Drive to ExaScale Computing

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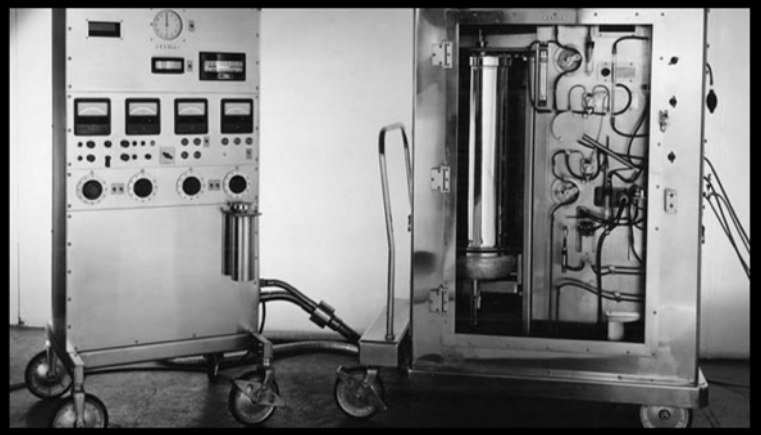
IBM Research Makes World's Smallest Movie Using Atoms

http://www-03.ibm.com/press/us/en/pressrelease/40970.wss

A History of Innovation

1950s… 1960s… 1970s…

1950s: Fighting Polio with Punch Cards



1953: A Heart on Wheels

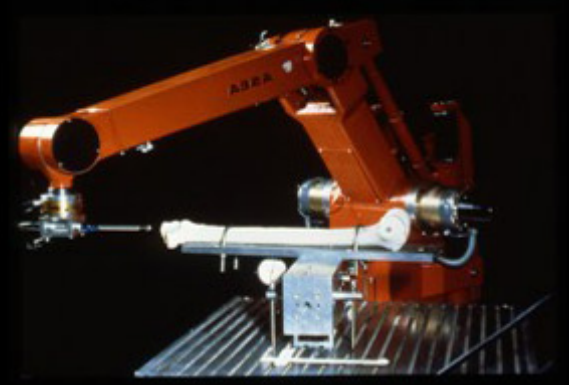
1960s: Taking on Leukemia with Blood Cell Separator

1976: IBM & World Health Organization Map Smallpox Outbreaks

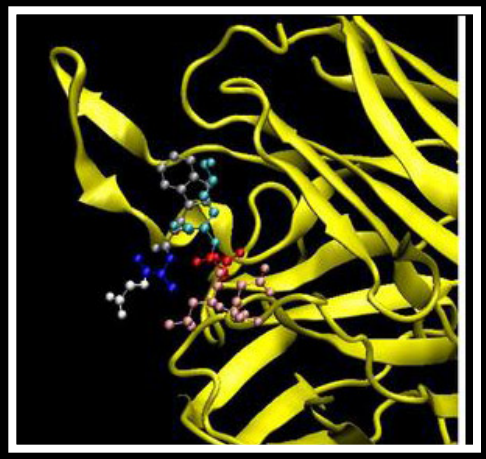
A History of Innovation

1990s… 2000s… 2010s…

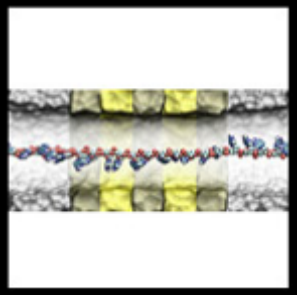
1990s: 3D Medical Imaging
IBM & Univ. of Washington



1992: Surgical Robot
IBM & Univ. of California



2008: IBM & Univ. of Edinburgh
Fight Spread of HIV



2010: IBM & Roche: DNA Sequencing

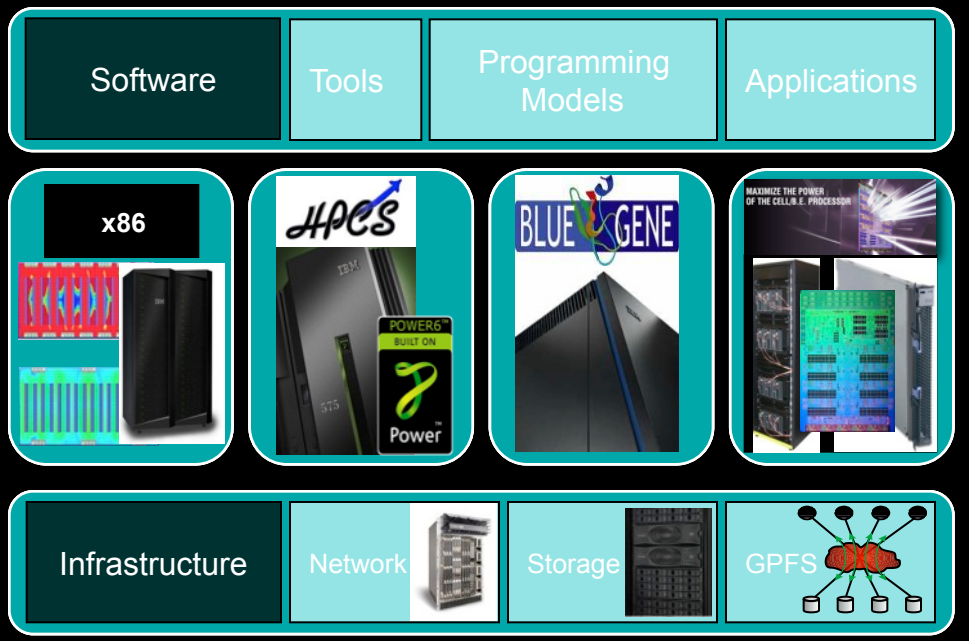
2011: IBM & Singapore's Institute of Bioengineering and Nanotechnology: Using Semiconductor Nanotechnology to Fight Bacteria

IBM Deep Computing

…deriving scientific and business value from information

- **Experience & Expertise**

- **Solutions & Platforms**



IBM Research

Science vs Industry | Theoretical vs Applied Science

IBM Research - Zurich
Member of a global research community

Lab overview

IBM has maintained a research laboratory in Switzerland since 1956, located on its own campus in Rüschlikon near Zurich since 1962. As the European branch of IBM Research, the mission of the IBM Research - Zurich lab — in addition to pursuing cutting-edge research for tomorrow's information technology — is to cultivate close relationships with academic and industrial partners, be one of the premier places to work for world-class researchers, to promote women in IT and science, and to help drive Europe's innovation agenda.

Internal and external collaboration

Worldwide interaction and collaboration with internal partners in research, development, industry sectors, and with IBM customers play a vital role in the laboratory's activities. At the same time, IBM researchers are active members of the international scientific community by participating in seminars, conferences, and professional associations in a variety of functions. IBM Research - Zurich is also involved in many joint projects with universities throughout Europe, in research programs established by the European Union and the Swiss government, and in cooperation agreements with research institutes of industrial partners.

Members of IBM Research - Zurich

IBM Research - Zurich employs a steady stream of postdoctoral fellows, PhD candidates, and summer students who pass through the laboratory. More than 30 nationalities, primarily from European countries, are represented among the research staff members, including such specialists as computer scientists, mathematicians, electrical engineers, physicists, and chemists. They often work together on an interdisciplinary basis.

Nanotechnology Center

→ IBM Research and ETH Zurich team up to establish ultramodern facility

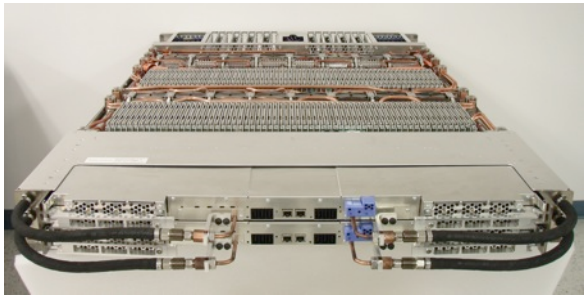
Download

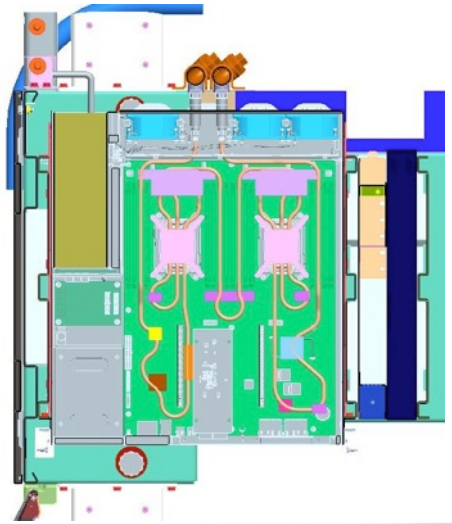
IBM Research brochure

IBM Research - Zurich leaflet

Breakthrough Technology

…state of the art tools for Grand Challenges



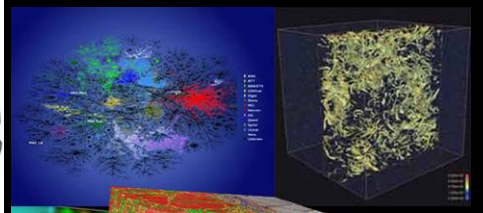


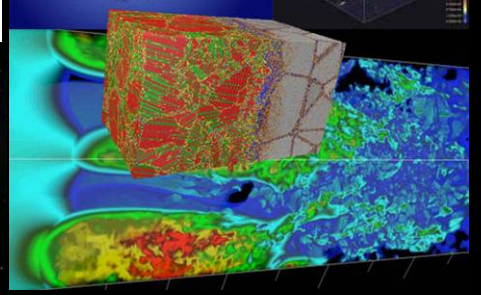
Breakthrough Technology

…the only way to deliver required performance

Breakthrough Science

- Role of simulations in Research
- Explosion of data for study
- Time to discovery / innovation
- **...there are still lots of questions!**

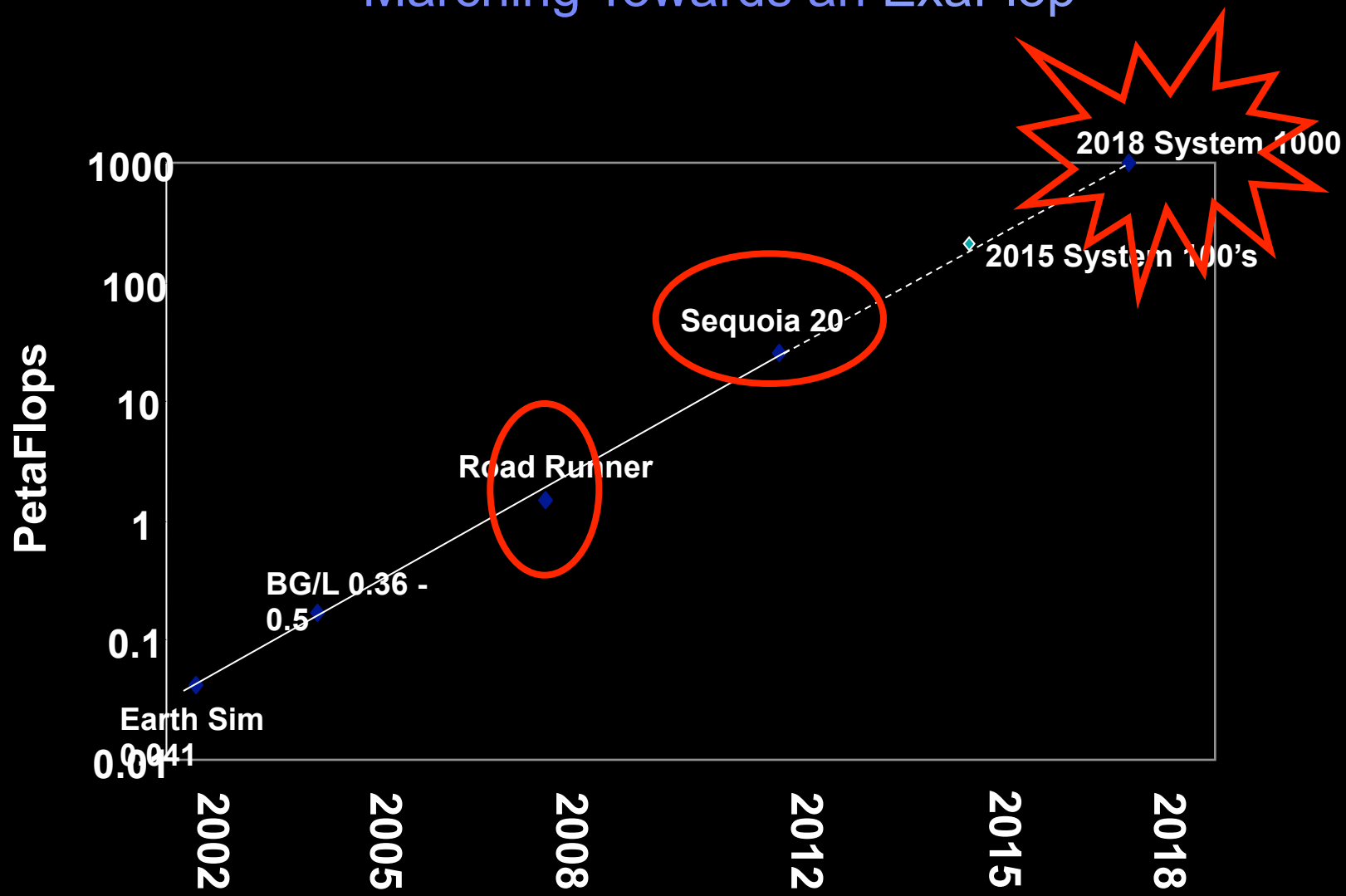


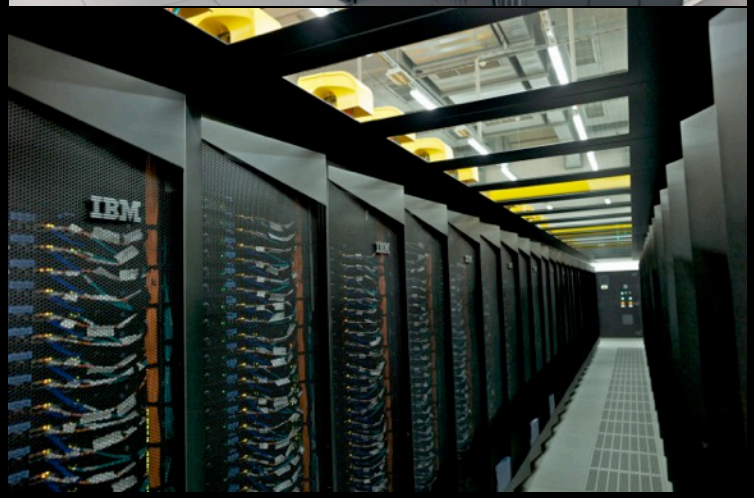


Technological Limitations

- Science is ahead of technology
- Systems are becoming complex
- No escape from parallelism
- **...it will only become weirder!**

Marching Towards an ExaFlop





IBM's Supercomputing Chops

TOP500 list of the world's fastest supercomputers

#1 SEQUOIA IBM POWER (LLNL)

16+ petaflops of performance

Could provide a 10-fold improvement in the prediction of earthquakes and safe evacuation routes

1.55x faster and **2.49x** more energy efficient[1]

#3 MIRA IBM POWER (ANL)

8+ petaflops of performance

More than 5 billion computing hours will be available to researchers on Mira every year

Could develop new materials to stretch the charge on an electric car battery up to **500 miles**

#4 SuperMUC (LRZ)

3 petaflops

Completely water cooled making it **40%** more efficient[2]

Captured energy from SuperMUC is reused to heat campus buildings, providing **$1.25 million** in energy savings per year.

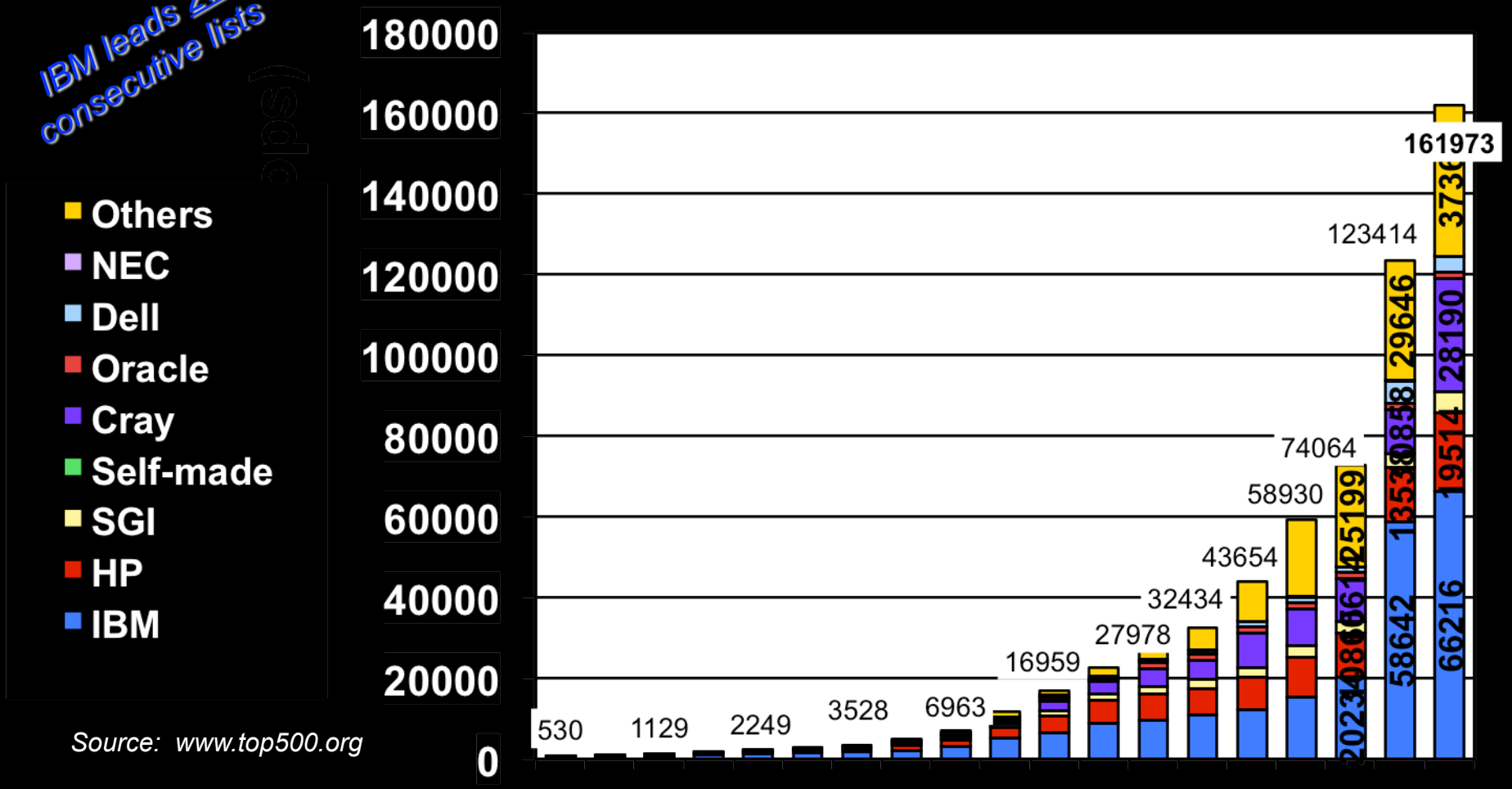
One petaflop runs a quadrillion or 10^{15} instructions per second.

[1] Compared to the next fastest supercomputer in the world.
[2] Compared to an air cooled machine.
Lawrence Livermore National Lab (LLNL), Argonne National Lab (ANL), Leibniz Supercomputing Centre (LRZ)

IBM continues longstanding leadership in total installed aggregate floating point throughput with 40.9% of total installed performance.

TOP500 Installed Aggregate Throughput

IBM leads 27 consecutive lists

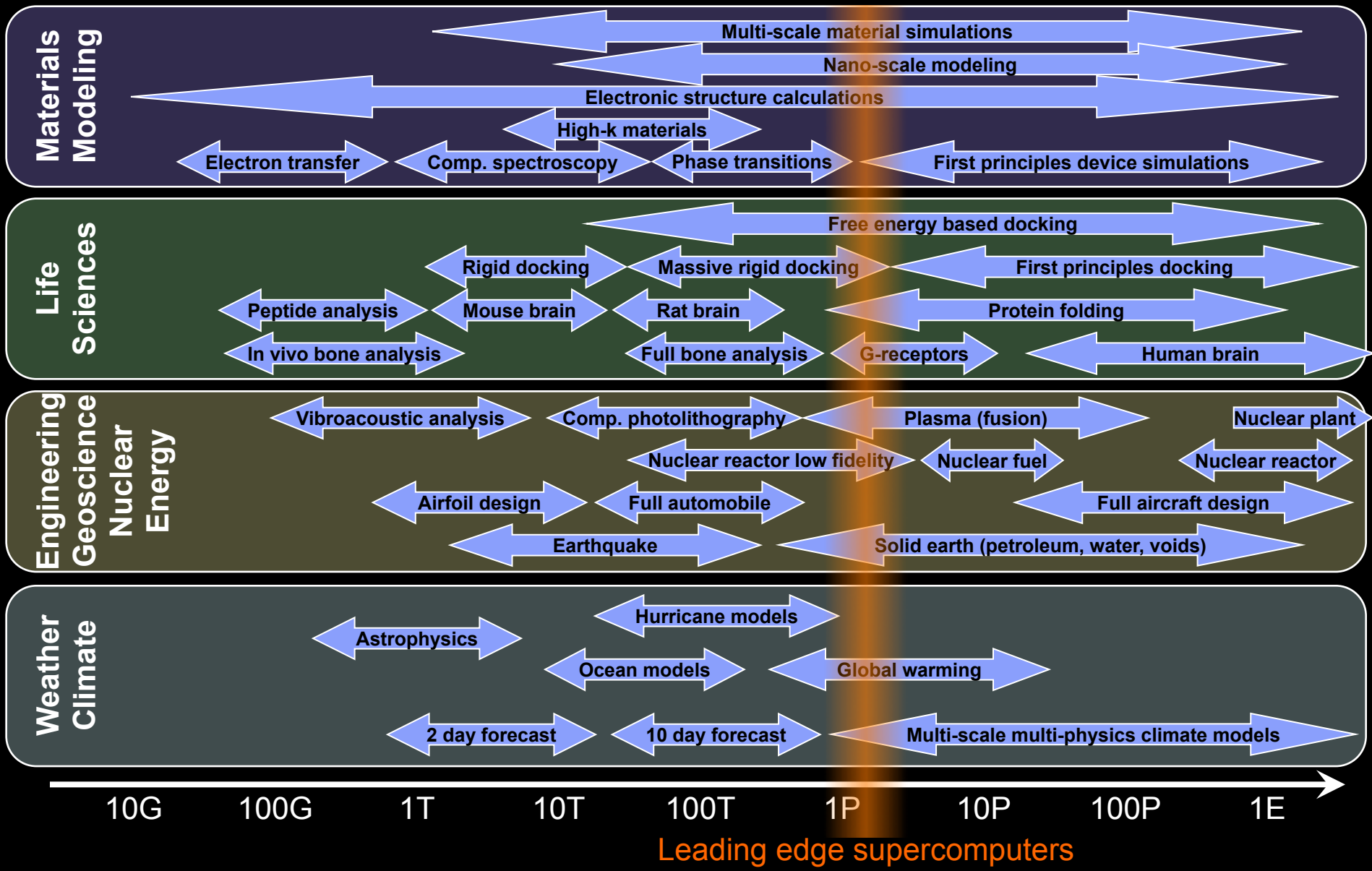


Source: www.top500.org

HPC Applications at their scale

IBM

…too much is never enough



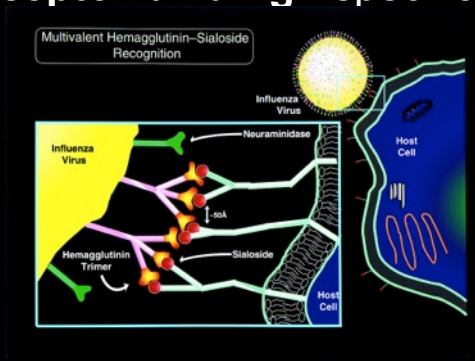
Grand Challenges: Influenza

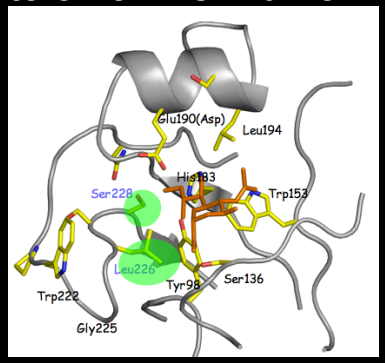
Anticipate virulent genetic changes in the **Influenza** virus that will enable preparation of effective vaccines and therapeutics in advance of those changes

Computational modeling of mutations in proteins H5 and H3

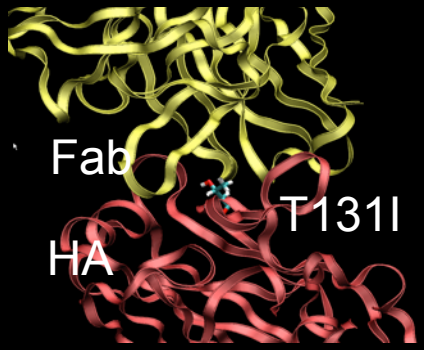
Predict biological consequence of mutations

Receptor binding - specificity to avian vs. human host





Antibody binding
- escape from (vaccine) antibody neutralization



Predicted Mutations: Receptor Binding

H5 HA mutation	α-2,3- (avian)			α-2,6- (human)		
	ΔG_b	ΔG_f	$\Delta\Delta G$	ΔG_b	ΔG_f	$\Delta\Delta G$
V135S	5.68 (0.58)	4.56 (0.4)	1.12 (0.7)	3.87 (0.12)	4.47 (0.15)	-0.60 (0.19)
A138S	4.39 (0.1)	4.52 (0.58)	-0.13 (0.59)	4.25 (0.22)	4.66 (0.24)	-0.41 (0.32)
V135S+	9.48	8.64	0.84	7.85	10.41	-2.56 (73)

Prediction of Ab Escape Mutants

Mutation	Calc. ΔΔG (kcal/mol)	Expt. ΔΔG (kcal/mol)	Mutation	Calc. ΔΔG (kcal/mol)	Expt. ΔΔG (kcal/mol)
T131I	5.20 ± 0.94	5.0	T131F	5.68 ± 1.48	
T131G	-3.72 ± 0.69		T131W	7.46 ± 1.91	
T131A	-2.81 ± 0.91		T131L	3.15 ± 1.19	
T131C	0.117 ± 1.24		T131H	3.84 ± 1.17	
T131V	2.58 ± 0.89		T131Y	6.01 ± 1.31	
T131M	0.57 ± 1.63		T131N	2.92 ± 1.16	
T131Q	1.22 ± 1.20				
T131S	-0.48 ± 1.57		S157L	4.10 ± 1.69	3.7

Grand Challenge: Automotive Safety

Computer simulations have reduced the number of physical crash tests by about 85%

So we now know the effect of crashes on Dummies… which enables us to infer the effects on people

What if we could simulate the effect of a crash on the anatomy and physiology of real human beings?

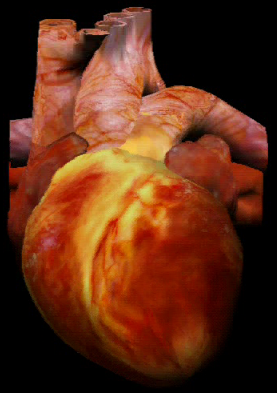
Grand Challenge: Simulating the Human Body

Mathematical models of the heart will enable better therapies for heart disease..

...but modeling the heart requires bridging between organ level & molecular level

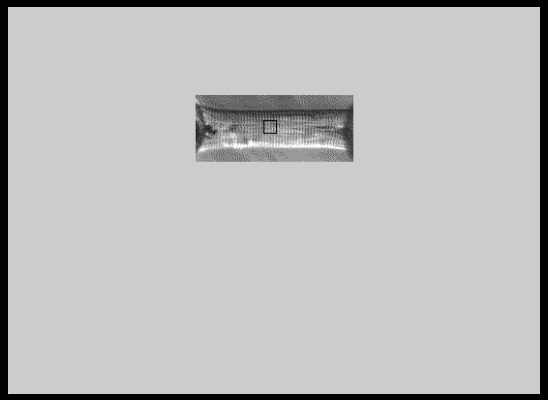
Organ level

Seconds



Reconstruction and simulation of the whole heart

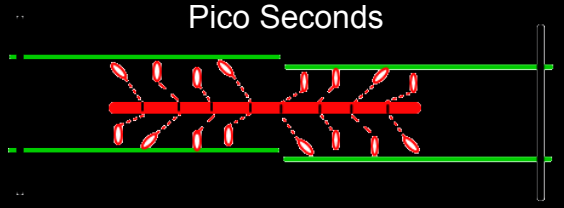
Cell level



In each cell of the heart, a lattice of sarcomeres produce contraction on every heart beat.

Molecular level

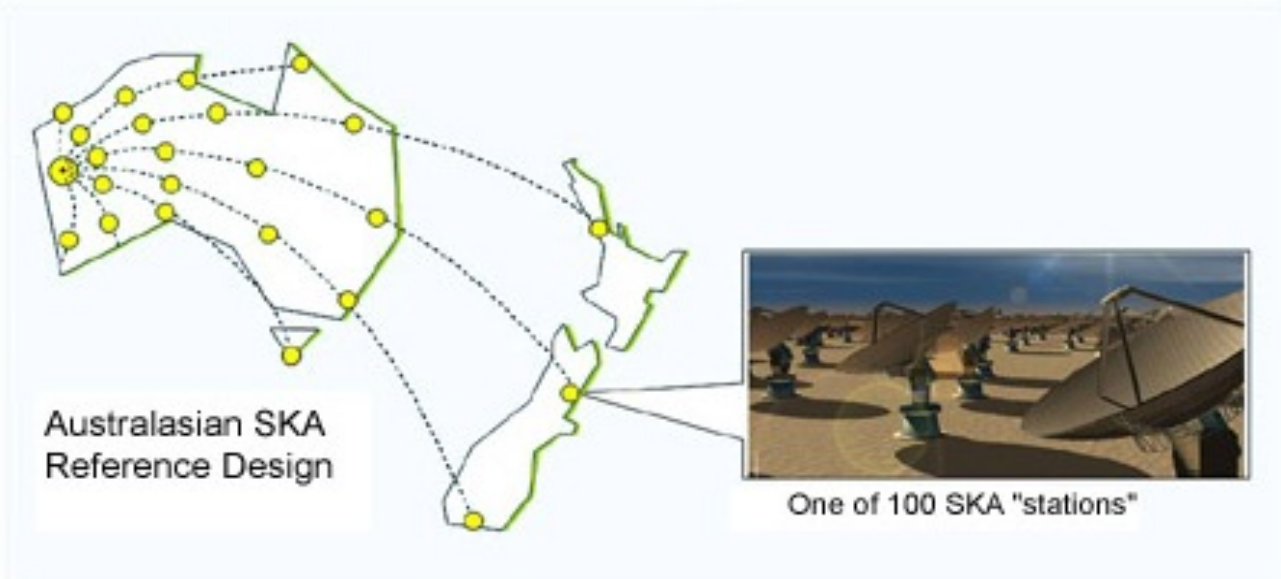
Pico Seconds



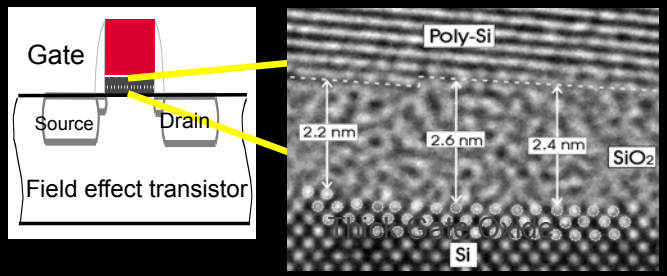
Sarcomere contracts by cyclical interactions of myosin on thick filament (red) and actin in thin filament (green).

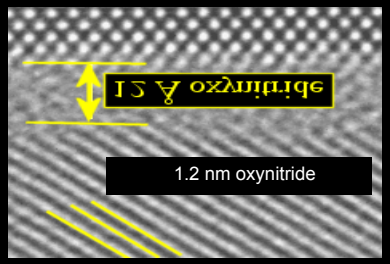
Grand Challenge: Square Kilometer Array (SKA)

- SKA is an ambitious project to build worlds largest Radio Telescope (and scientific instrument)
- Will comprise of ~5000 12m radio telescopes spread across ~5000km all synchronised to create 1 virtual telescope with a collecting area equivalent of 1sq km (massive sensor network)
- Will require exaflop signal processing/compute, petabit/s networking and exabyte storage capability.
- Solving SKA challenges support sensor network evolution



Grand Challenge: Power Efficient Computing





Scaled Gate Oxide

Today's most energy efficient computers @ 1 Exaflop = **~2GWatts @ $1/Year/Watt =**

$2 Billion/Year

IBM's Target:

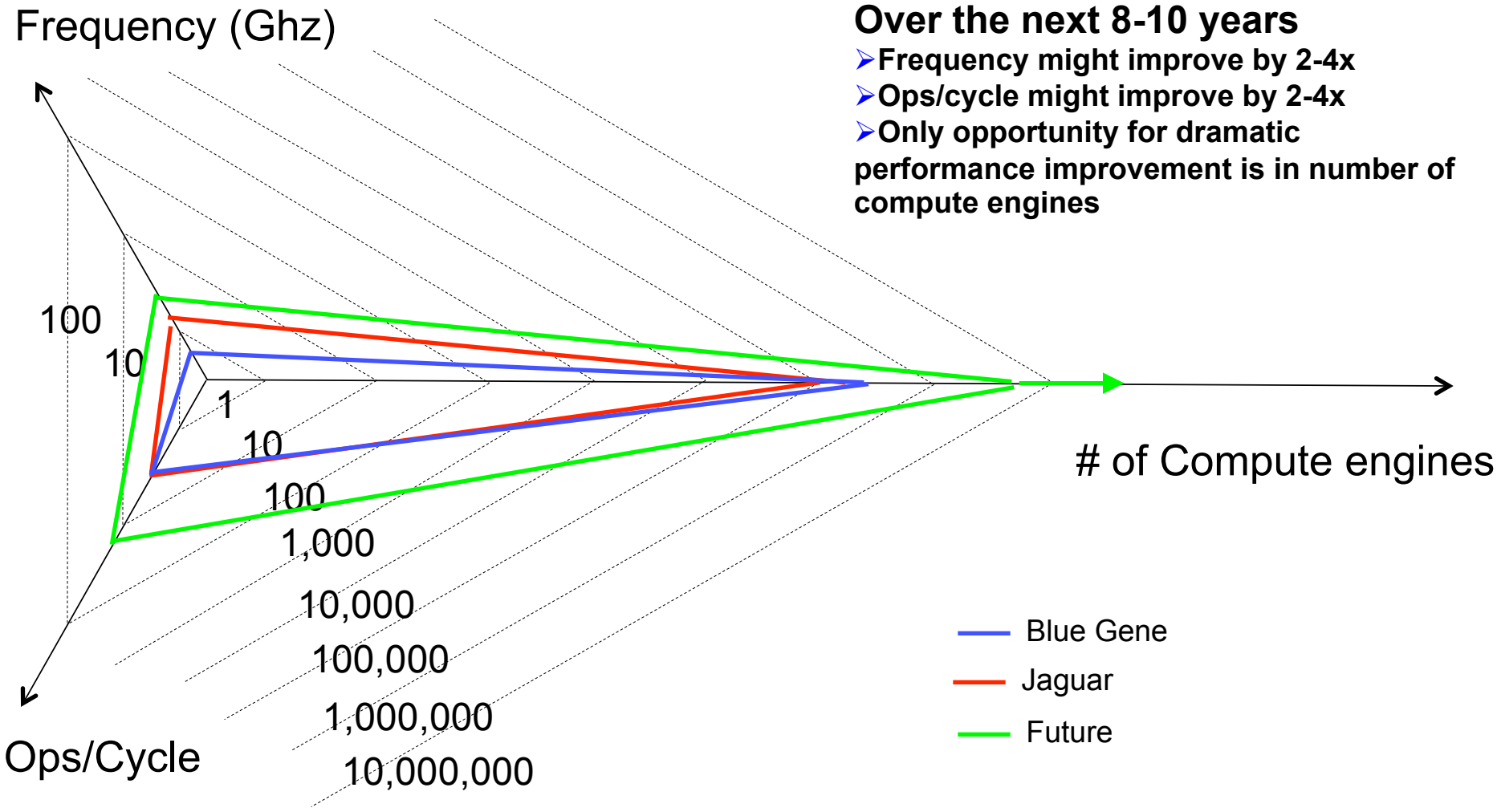
1ExaFlop =~20MWatts

The Green500 List

Listed below are the June 2012 The Green500's energy-efficient supercomputers ranked from 1 to 100.

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	2,100.88	DOE/NNSA/LLNL	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	41.10
2	2,100.88	IBM Thomas J. Watson Research Center	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	41.10
3	2,100.86	DOE/SC/Argonne National Laboratory	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	82.20
4	2,100.86	DOE/SC/Argonne National Laboratory	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	82.20
5	2,100.86	Rensselaer Polytechnic Institute	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	82.20
6	2,100.86	University of Rochester	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	82.20
7	2,100.86	IBM Thomas J. Watson Research Center	BlueGene/Q, Power BQC 16C 1.60 GHz, Custom	82.20
8	2,099.56	University of Edinburgh	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	493.10
9	2,099.50	Science and Technology Facilities Council - Daresbury Laboratory	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	575.30
10	2,099.46	Forschungszentrum Juelich (FZJ)	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	657.50
11	2,099.39	CINECA	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	821.90
12	2,099.14	High Energy Accelerator Research Organization /KEK	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	246.60
13	2,099.14	EDF R&D	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	328.80
14	2,099.14	IDRIS/GENCI	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	328.80
15	2,099.14	Victorian Life Sciences Computation Initiative	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	328.80
16	2,099.14	IBM - Rochester	BlueGene/Q, Power BQC 16C 1.60 GHz, Custom	164.40
17	2,099.14	IBM - Rochester	BlueGene/Q, Power BQC 16C 1.60 GHz, Custom	164.40
18	2,099.14	DOE/NNSA/LLNL	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	164.40
19	2,069.04	DOE/SC/Argonne National Laboratory	BlueGene/Q, Power BQC 16C 1.60GHz, Custom	3,945.00
20	2,069.04	DOE/NNSA/LLNL	BlueGene/Q, Power BQC 16C 1.60 GHz, Custom	7,890.00

Scalability



Over the next 8-10 years

- **Frequency might improve by 2-4x**
- **Ops/cycle might improve by 2-4x**
- **Only opportunity for dramatic performance improvement is in number of compute engines**

High Performance Computing Goes Mainstream

High-powered technical computing increasingly is used to solve practical problems in manufacturing, life sciences, oil and gas, and other industries, but many companies still aren't fully tapping its potential.

Over **70%** of members of the National Center for Manufacturing Sciences (NCMS) believe increased adoption of advanced computing would lead to **competitive advantages**.[1]

Only **6%** of the estimated 285,000 small to medium manufacturers in the US are fully taking advantage of **technical computing** today.[2]

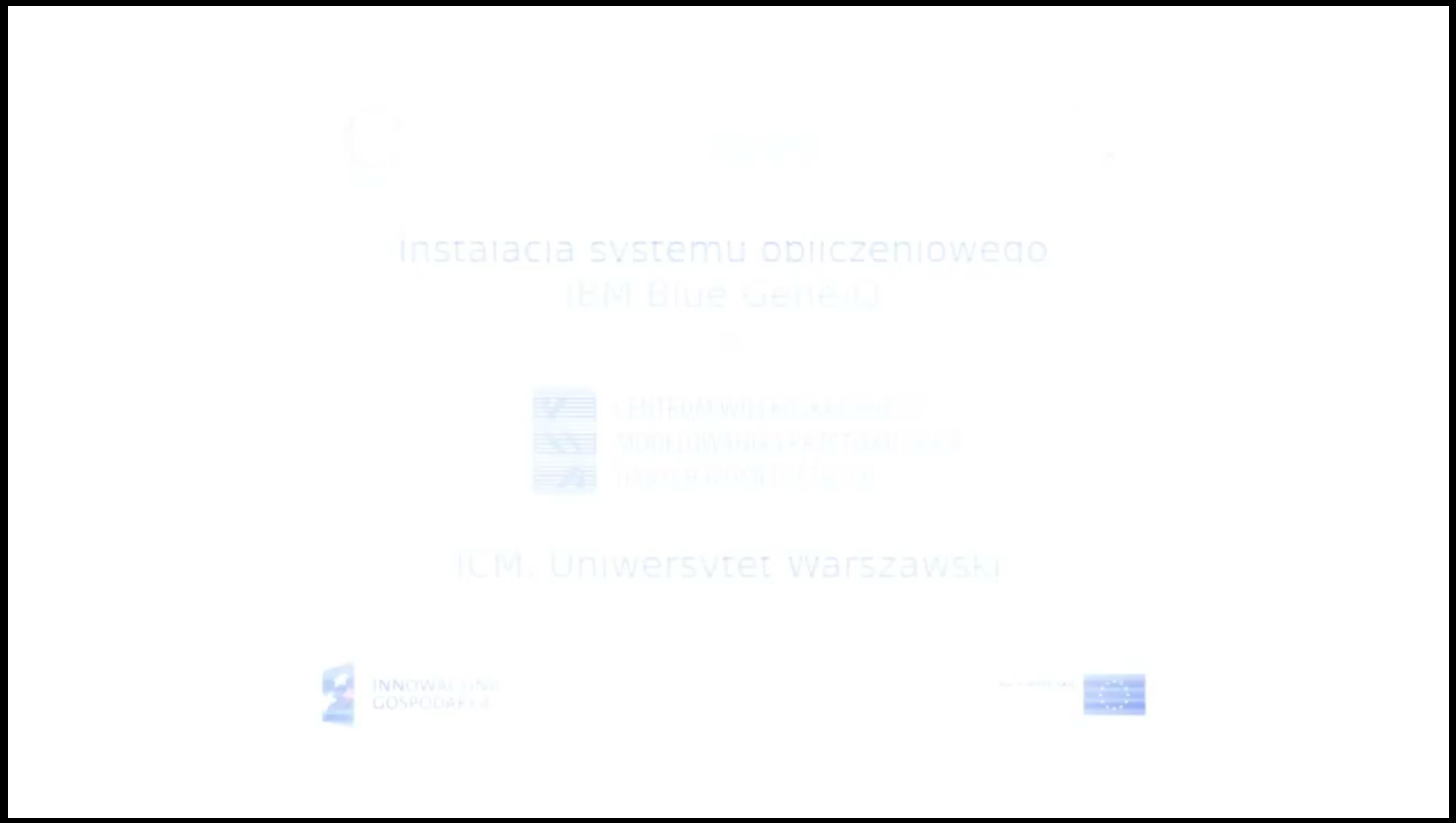
Technical computing achievments

The Boeing Company aims to use simulations to redesign the vertical tail of a commercial jet, potentially saving **$300 million** in fuel costs annually.

Using IBM technical computing, **Vestas Wind Systems** reduced their wind turbine placement analysis from weeks to less than **one hour.**

Red Bull Racing used IBM technical computing software to simulate new car designs and achieved a **20% increase** in performance and throughput, coming up with a design that reduces their cars' drag on the track.

ICM's New Blue Gene Supercomputer Supports The Largest Biomedical Research Initiative In Poland



interdyscyplinarne centrum modelowania matematycznego i komputerowego

News room > News releases >

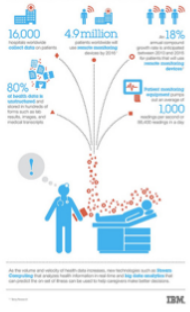
ICM's New Blue Gene Supercomputer Supports The Largest Biomedical Research Initiative In Poland

Nostromo to bridge the gap between bench and practice
The supercomputer will gather and process biomedical Big Data

News release | Contact(s) information
Related XML feeds | Related resources

WARSAW, Poland - 04 Apr 2013: IBM (NYSE: IBM) Blue Gene/Q, the most powerful single architecture supercomputer in Poland, has been chosen by The Interdisciplinary Centre for Mathematical and Computational Modeling, University of Warsaw (ICM) of Poland to support the country's largest biomedical and biotechnological research initiative called, "Centre for Pre-clinical Research and Technology (CePT)." More than 500 life sciences and biomedical researchers, physicians and students, from a consortium led by The Medical University of Warsaw (WUM) and consisting of three universities and seven research centers of the Polish Academy of Sciences, will use the supercomputer and its supporting e-infrastructure to gain further insight into chronic diseases.

Big Data in Healthcare: Tapping New Insight to Save Lives



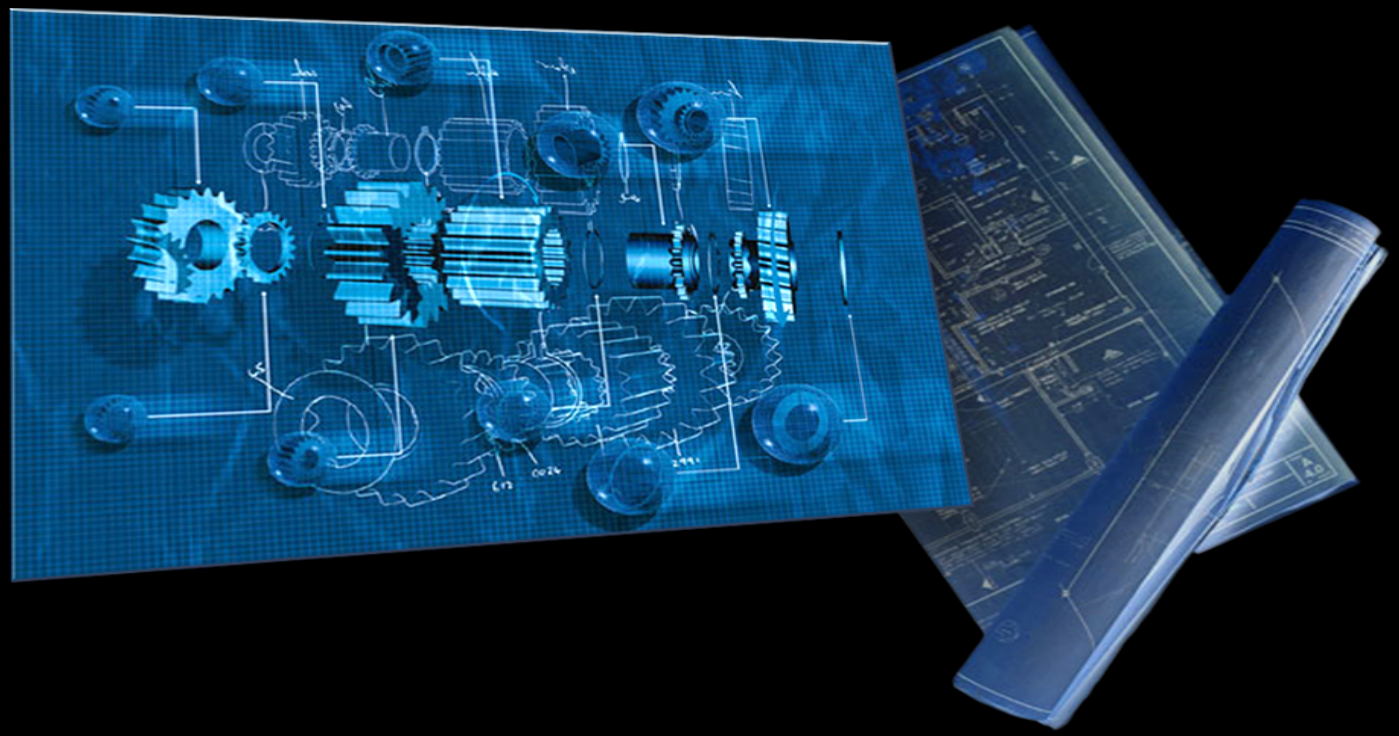
"CePT, a EUR 100 million project, aims to support Poland's transition towards more preventive and patient-centric healthcare," said Dr. Robert Sot, Director of CePT, Warsaw University. "The project will allow the medical community to provide a more holistic approach and open collaboration for the development of innovative treatments and drugs that will improve patients' quality of life over the long term."

CePT Centre for Preclinical Research and Technology

http://www-03.ibm.com/press/us/en/pressrelease/40788.wss

IBM's vision for HPC

Leverage technology, science, management and innovation to make major improvements in business and society – in the very way the world works



Thank You!