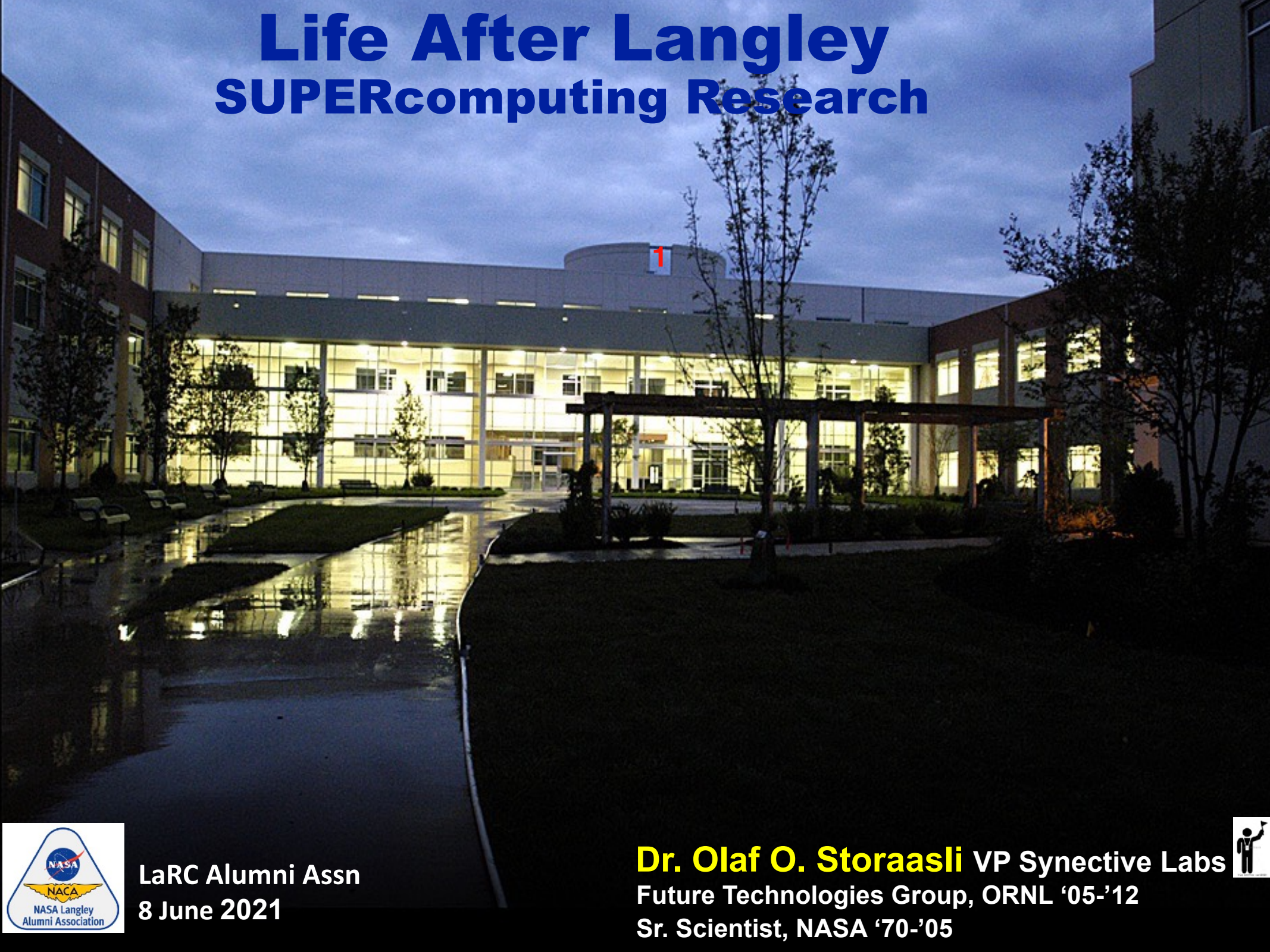


Life After Langley

SUPERcomputing Research



LaRC Alumni Assn
8 June 2021

Dr. Olaf O. Storaasli VP Synective Labs
Future Technologies Group, ORNL '05-'12
Sr. Scientist, NASA '70-'05



Prairies => VA => TN



Saskatoon



NASA



Parallel Computing

Supercomputers are efficient because they work on multiple problems simultaneously, a process known as "parallel computing." What if you had to complete a long and difficult task like building a house? Working alone, you could only complete one task at a time. But if a crew worked on the house, one team could shingle the roof while another installed drywall, and so on.



ORNL

NASA Langley Research Center, Hampton VA



Katherine Johnson CRF

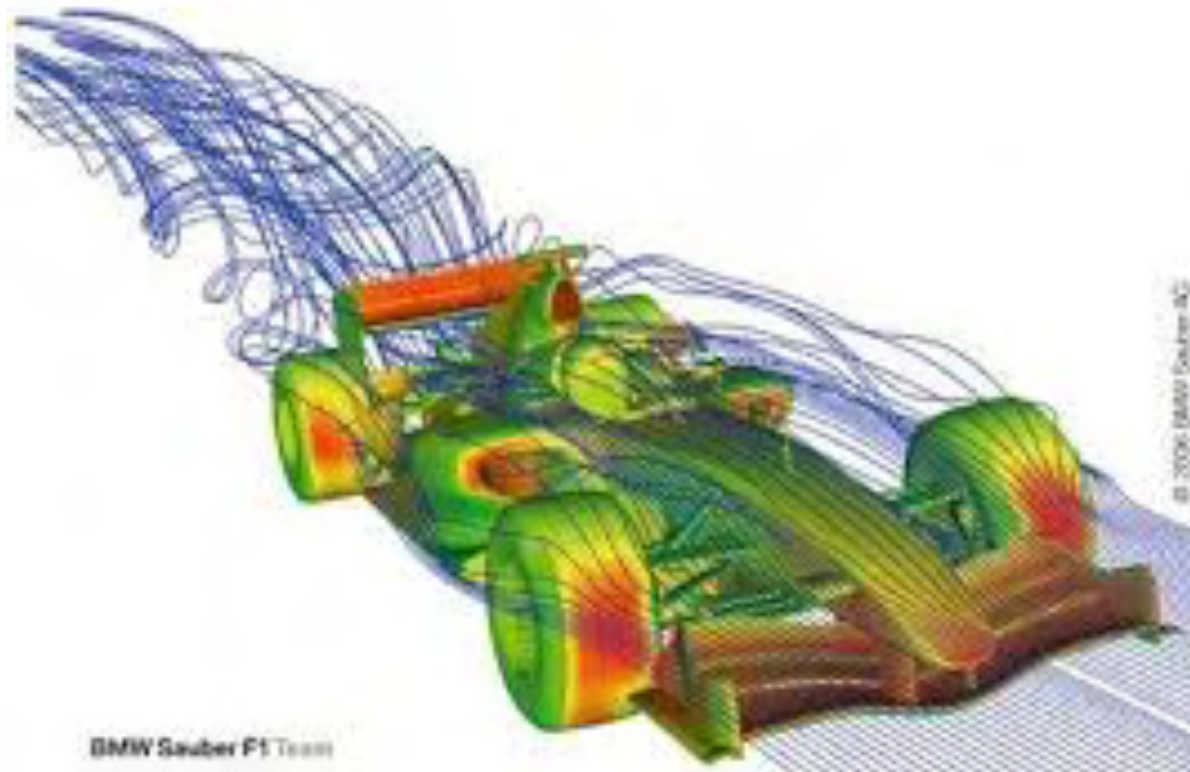
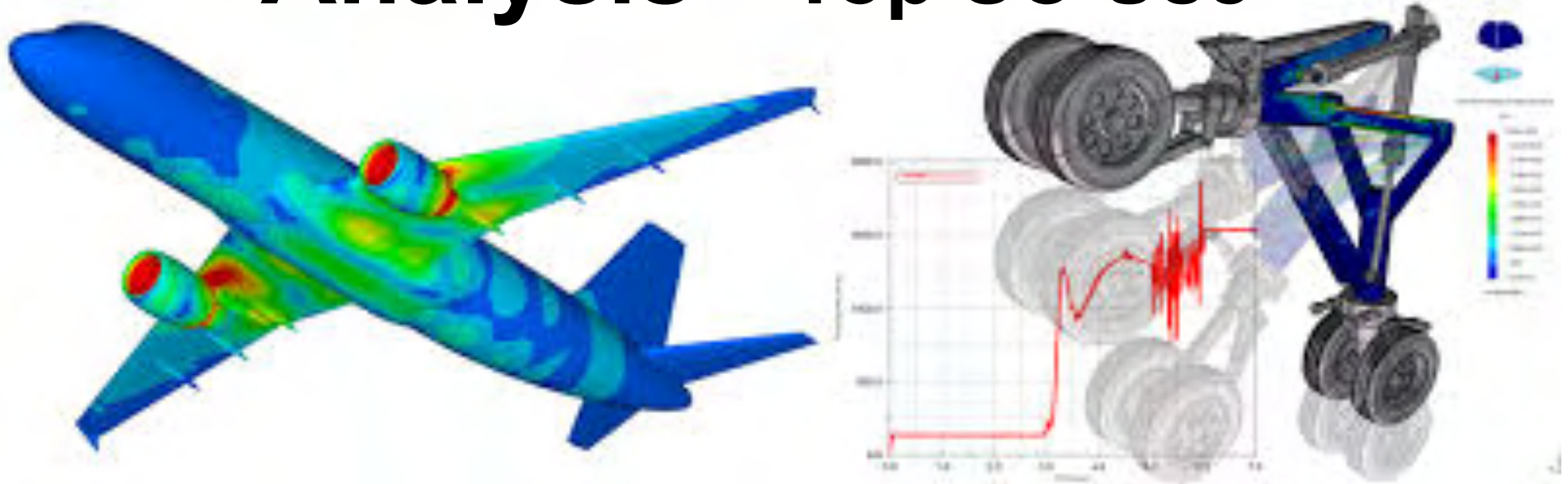


NASA Career '70-'05

FE Analysis-*Viking*-IPAD-CAD/CAM-*FEM*-*Shuttle*-GFA
Thompson-GPS (SWYA)-*FPGA* HyperComputer-*RSC*



Analysis - Top SC Use



Nastran
Dyna
Ansys
Abaqus
Star
Foam



NASA Viking 1st Mars Landings

Many Langley engineers “pulled it off”



Mel Anderson - Aeroshell

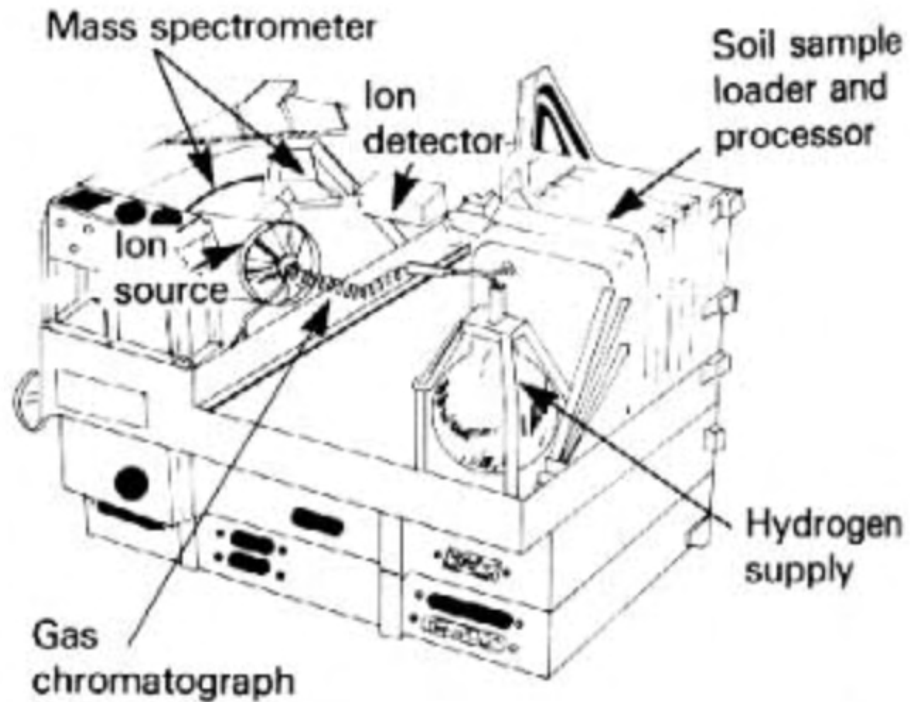


Dick Snyder & Olaf - Lander



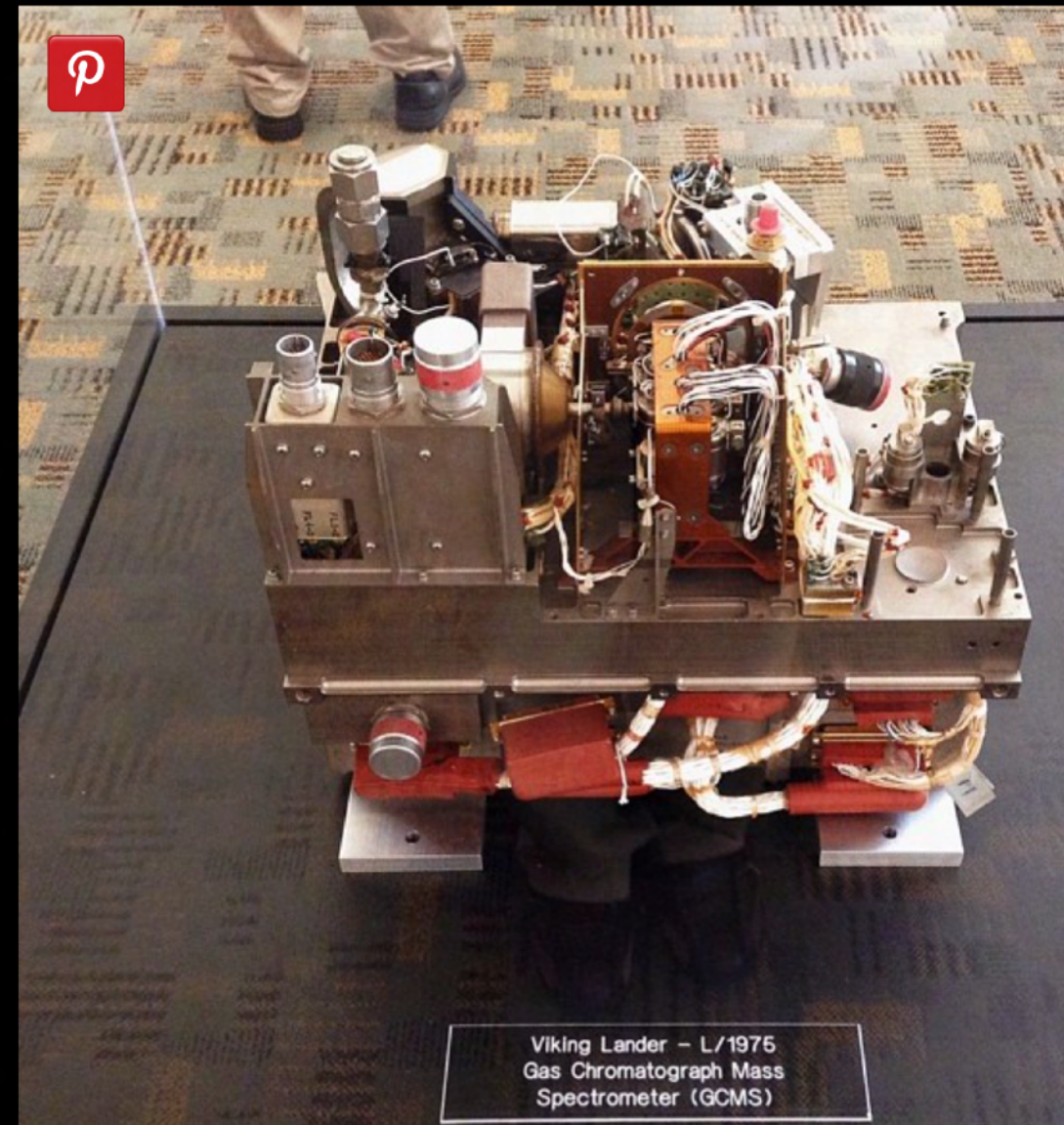
Viking Lander GCMS “box”

LaRC Tiger Team redesign, build & test



VIKING LANDER GCMS – 2014-06-17 23:52:48

BY ED SPRAKE | PUBLISHED JUN 18 2014



Space Shuttle (pre/post Challenger)

- Wing/tail structural analysis
- Solid Rocket Booster Redesign

L-89-14315

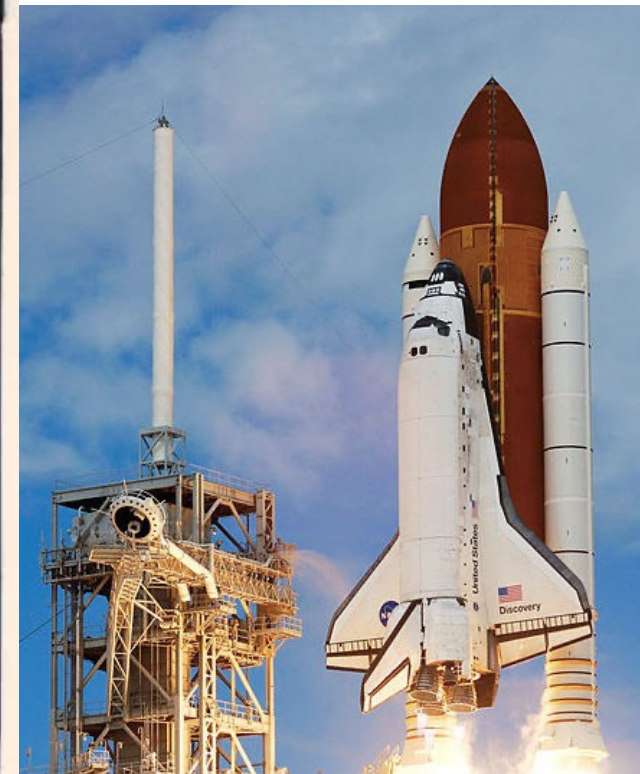
Shuttle SRB Analysis Wins Cray Gigaflop Award



54,870
Equations

14 hrs	VAX	} 60
1.1 hrs	Cray 2	
14 min	(vector)	
13 sec	Cray 2	}
6 sec	Cray Y-MP	

pvsolve



US Supercomputer Lead

How? MC, GPU, FPGA, Cell?

Manhattan Project X10 -> ORNL

Gas Centrifuge, Y12, S50, K25



2



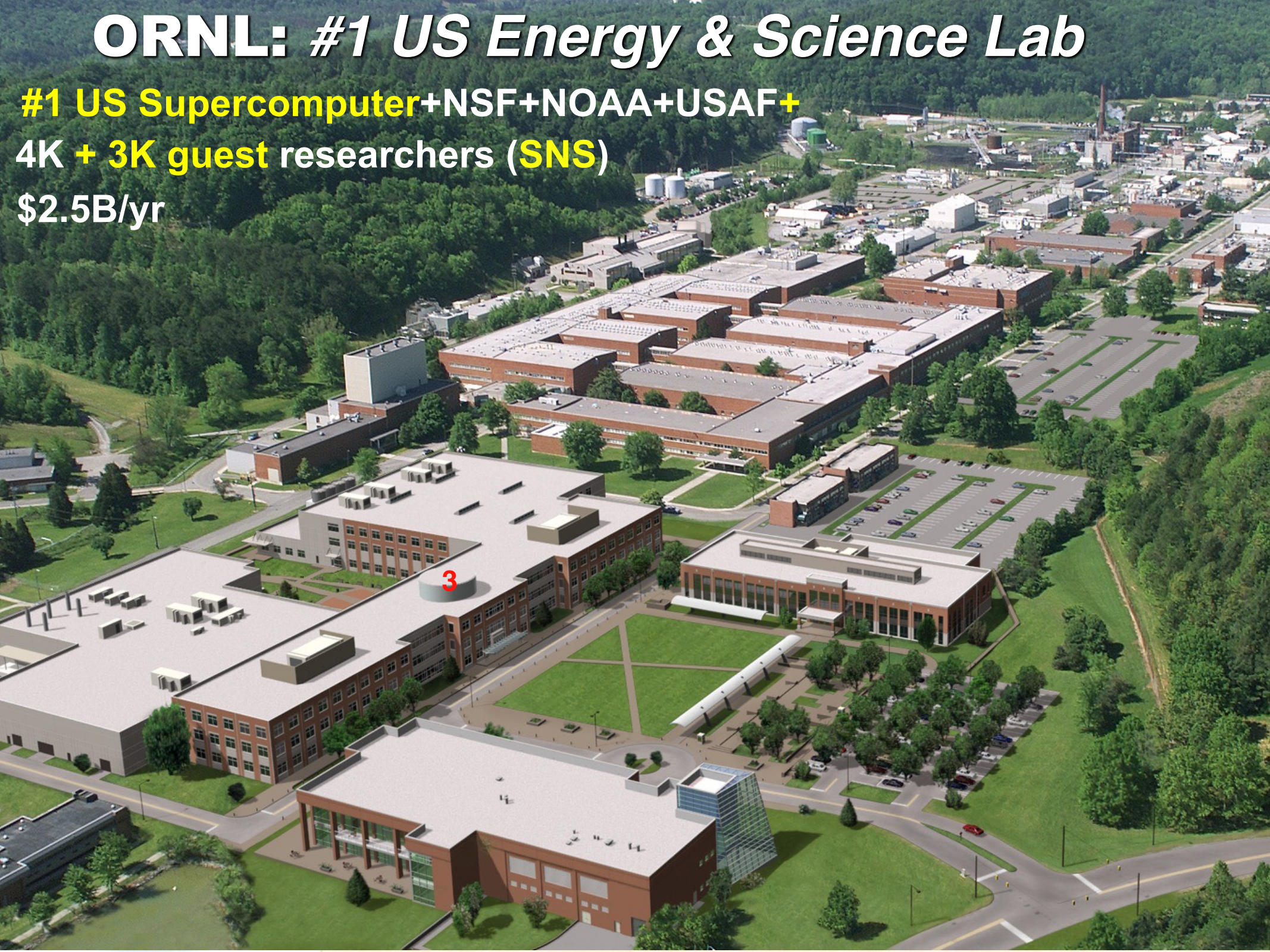
X10: 1st Pilot Pu Reactor => PNL

Y12 *Ernest Lawrence + uncle built Calutrons to enrich U*



ORNL: #1 US Energy & Science Lab

#1 US Supercomputer+NSF+NOAA+USAF+
4K + 3K guest researchers (SNS)
\$2.5B/yr



Change LaRC => DOE

GOGO vs. GOCO (JPL)

Security Physical & Cyber

TOP SECRET

EXPORT CONTROLS



Rewards Freedom, Pubs/Talks/Travel(Intl)

Research respect: ORNL-US-SCworld

+50%\$, 6wk vac, 3Xretire, ClubORNL

Colleagues* PhDs, Natl/Intl, Teams

Cyber leads, young, Seminars

*** LANL, LLNL, LBL, ANL, UT, DARPA, NSA, SC**

*Future
Technologies
Group*



DOE Security

Redo NASA Conf/Secret/TS => L/Q/SCI*Fs
Bldg control, TS+SCI monthly training

Why? US Nuke (U) Depository+Codes
Store/Produce/Control/Lend U to DOD+
TS ORNL Dir+4 SCI-trained 3hrs for OS talk

TS Cyber Security: air gap @Secret Site

Control code, talk, notes, phones, cameras, USB
How to write TS code?

***Sensitive Compartmented Information**

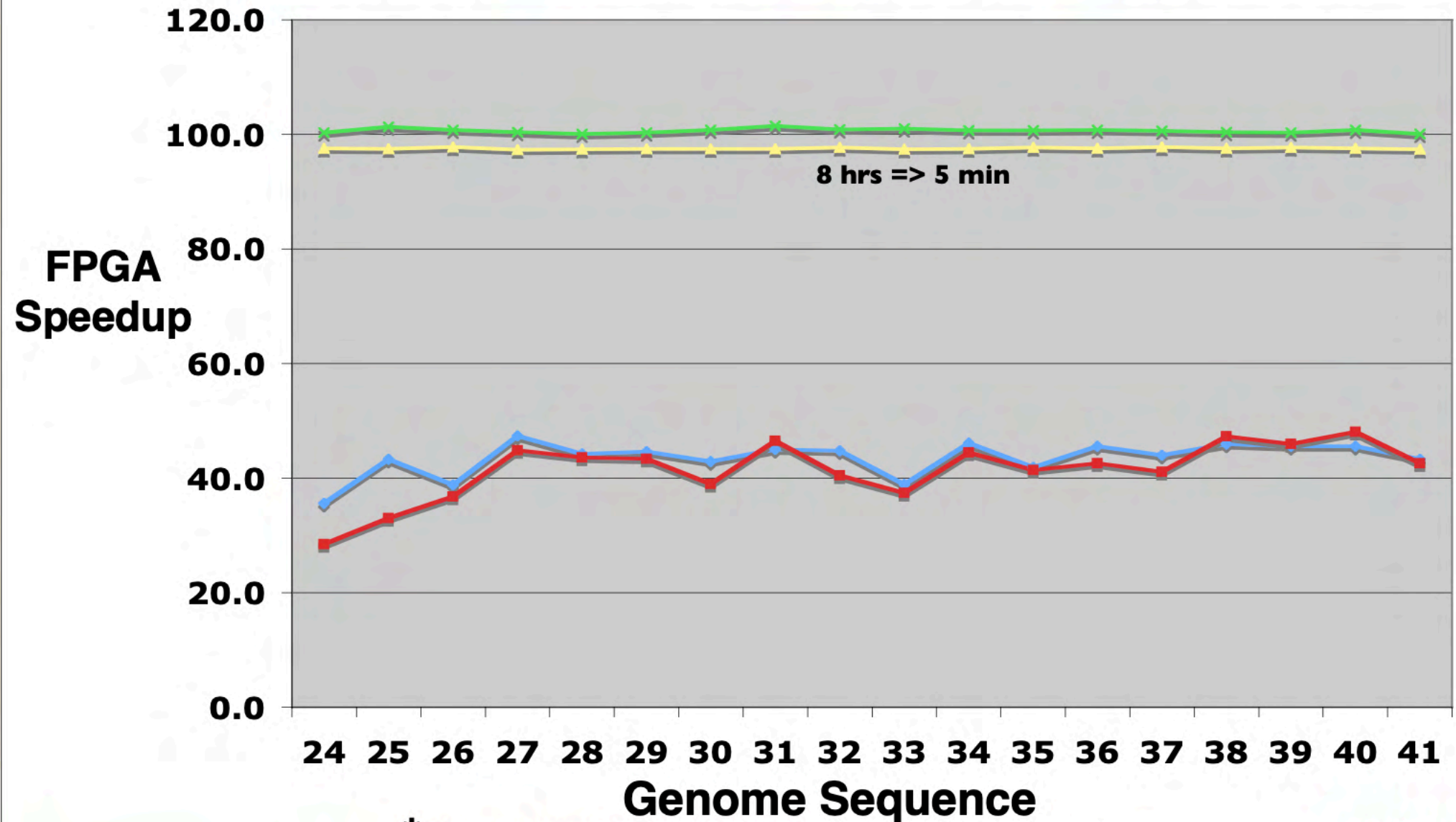


100x* DNA Sequence Speedup

Bacillus anthracis Human DNA comparison



8k w/align 16k w/align 8k w/o align 16k w/o align



*Virtex-4 FPGA vs 2.2 GHz Opteron on Cray XD1

ORNL Fast DNA sequencing

12.5 years on one 2.2 GHz Opteron

6 weeks on 150 Opterons

1 day on 150 FPGAs*



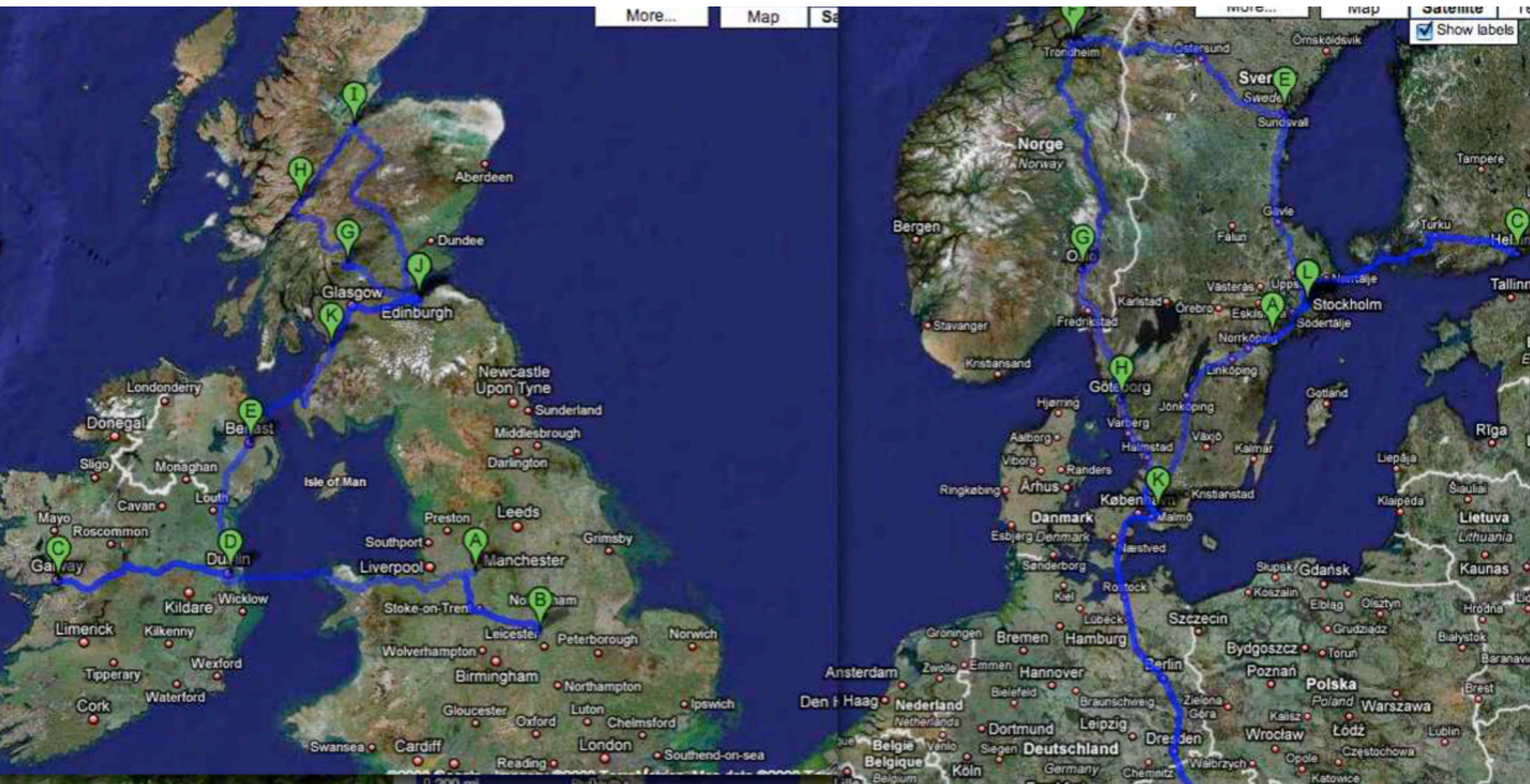
7,350X Speedup over one Opteron

also tested *64 FPGA Maxwell*
@Edinburgh University

*Thanks to NRL for use of 150 FPGA Cray XD1

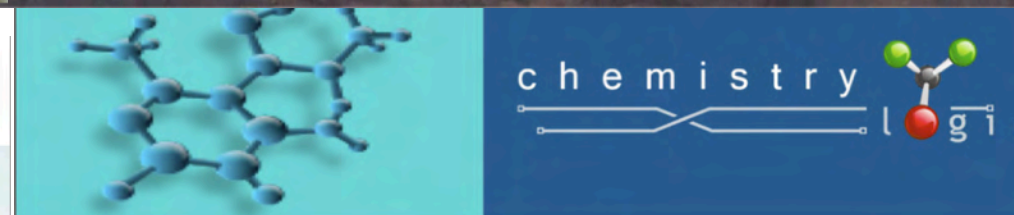


'08 Invited Talks: Mar-Jun, Apr U PostDoc*
Queens U (Belfast), Edinburgh*, Helsinki,
Trondheim, Oslo, Göteborg, Lund, Budapest
'05-08:UK, '05 Brazil, '13 NO SE FI ES, '15: NL Paris
'16 BE NO SE ES GEx2 FI Russia '17 UK: Queens+Imperial





Cray Users Group (Helsinki)



Meghívó

**Nagyságrendekkel hatékonyabb számítási módszerek
a gyógyszerkutatásban című konferenciára**

Programterv

9:00 – 9:30 Regisztráció

9:30 – 9:40 Köszöntő (Mészáros Csaba, evopro Kft. ügyvezetője)

9:40 – 10:00 A projekt története (Bérces Attila, Chemistry Logic Kft. ügyveze

10:00 – 10:10 Újrakonfigurálható számítástechnika

felhasználóknak (Fehér Béla, BME MIT)

10:10 – 10:50 Accelerating Genome Sequencing 100-1000X with FPGA

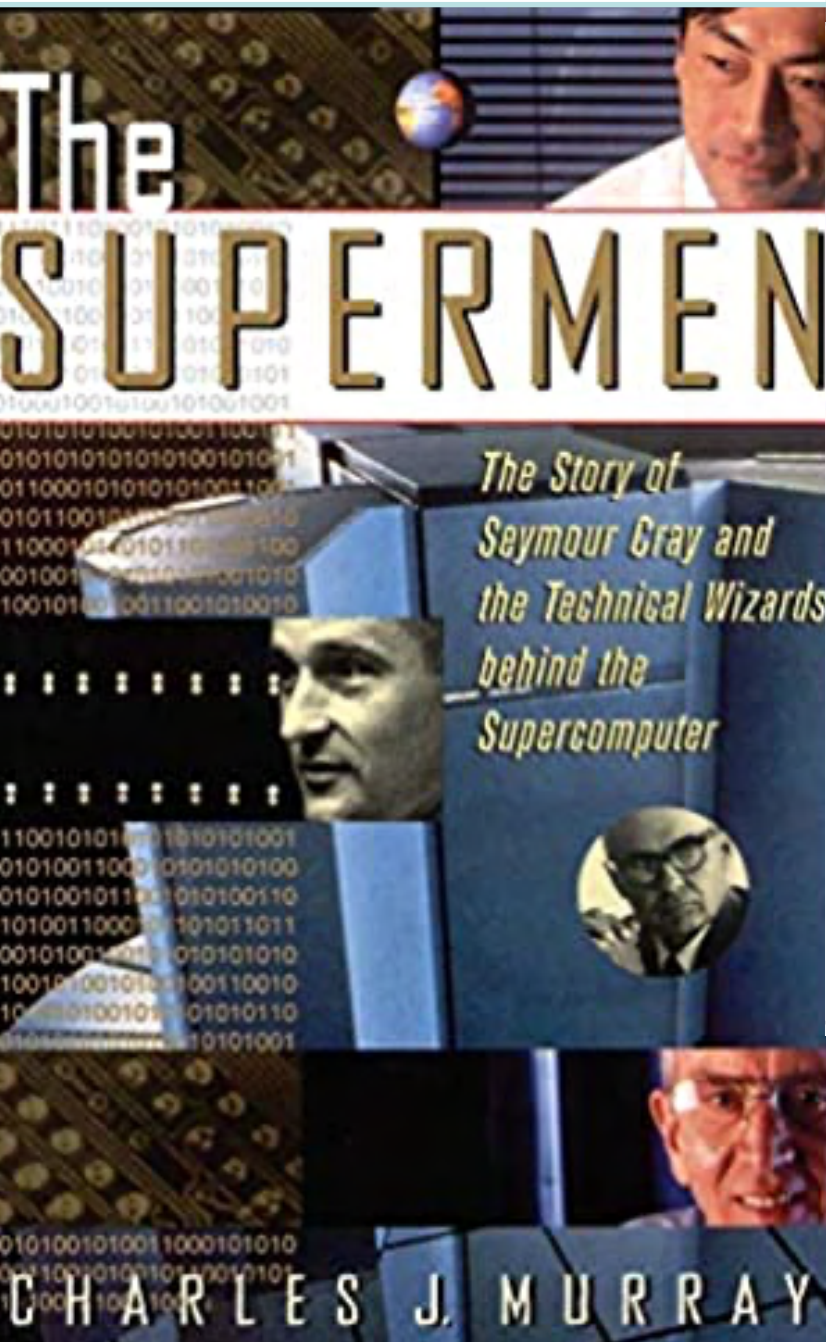
(Prof. Olaf Storaasli, Oak Ridge National National Laboratory kutatója)

“To Hell (Norway) & Back”



Motivation

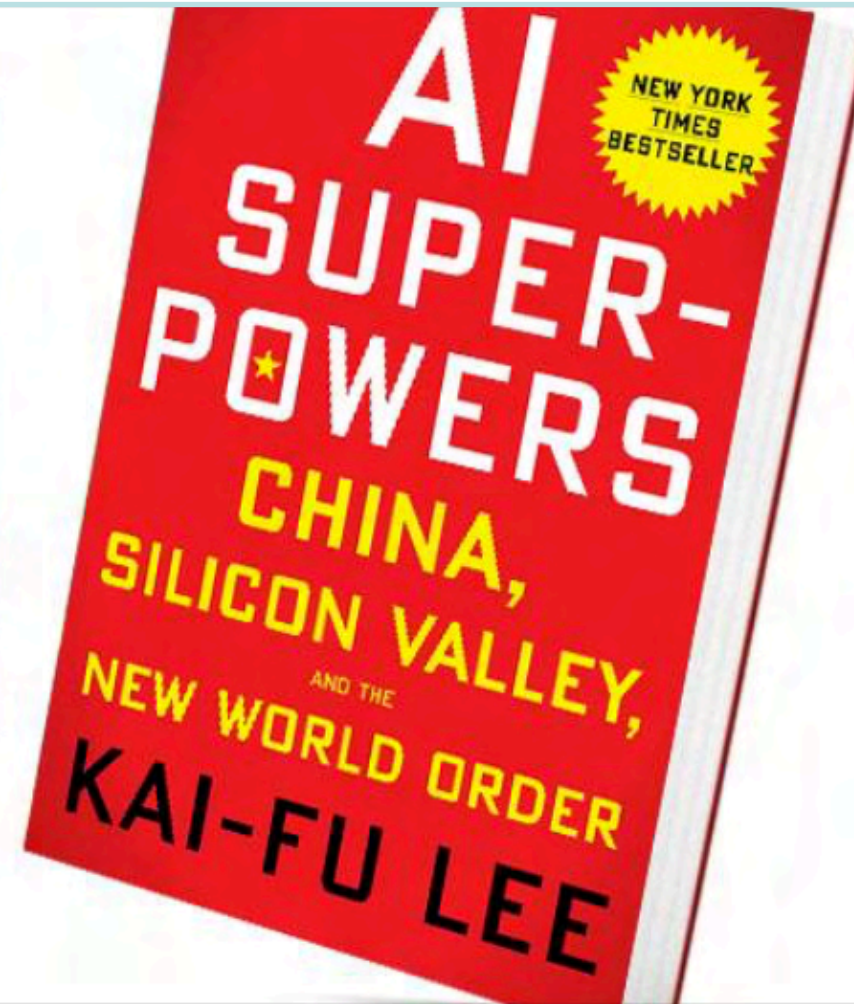
Past



Future



Google



This is the most important tech contest since the space race, and America is losing

Technical Computer Market

\$10B ('13) => \$15B ('18)

SC: \$4B => \$5.7B



Morgan
Stanley



TOYOTA



DREAMWORKS
ANIMATION SKG



BOEING®

bp



MERCK



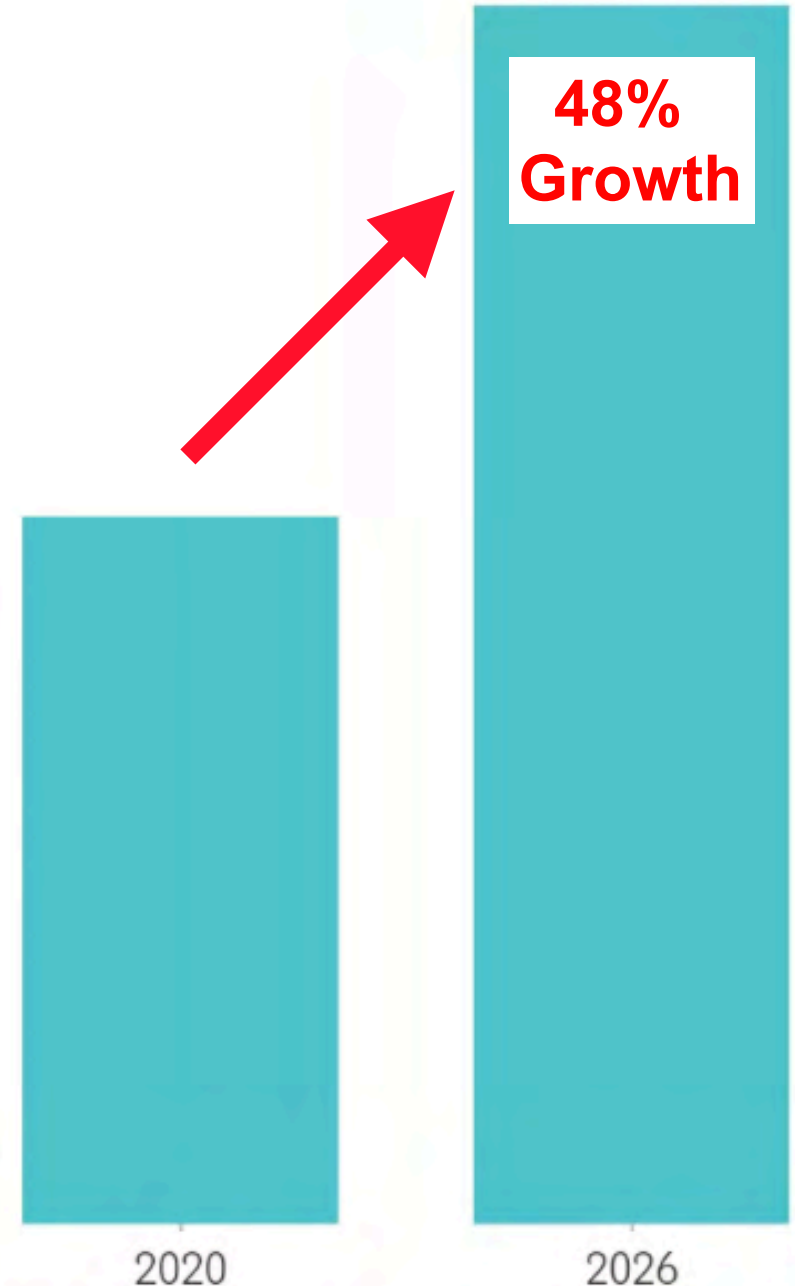
AIRBUS



Panasonic



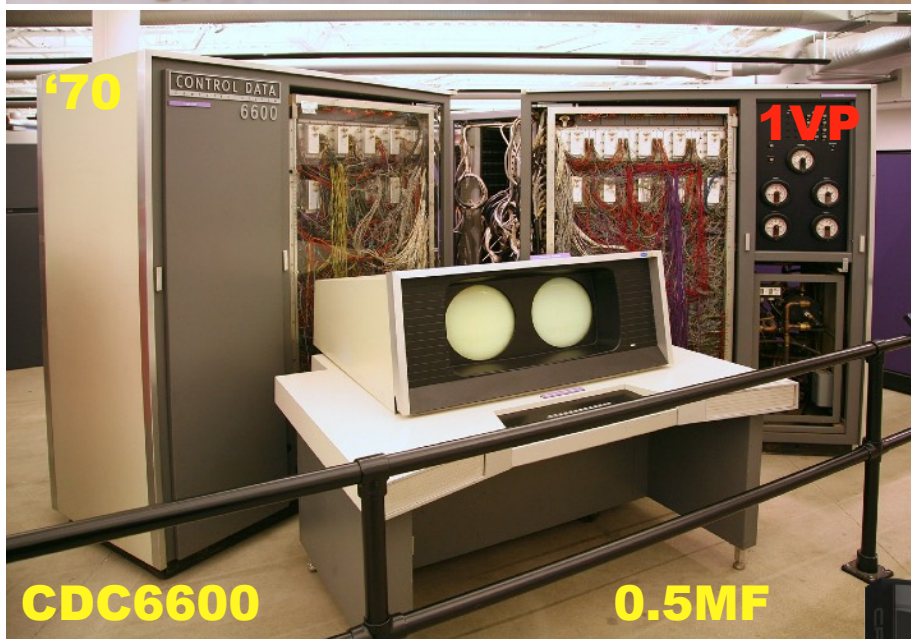
1960s



Source : Mordor Intelligence



Past 57-yr Speedup



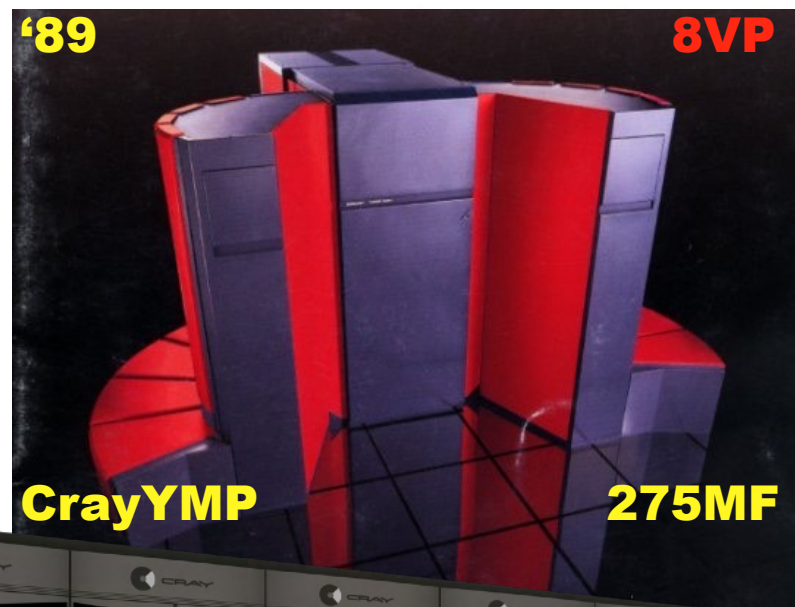
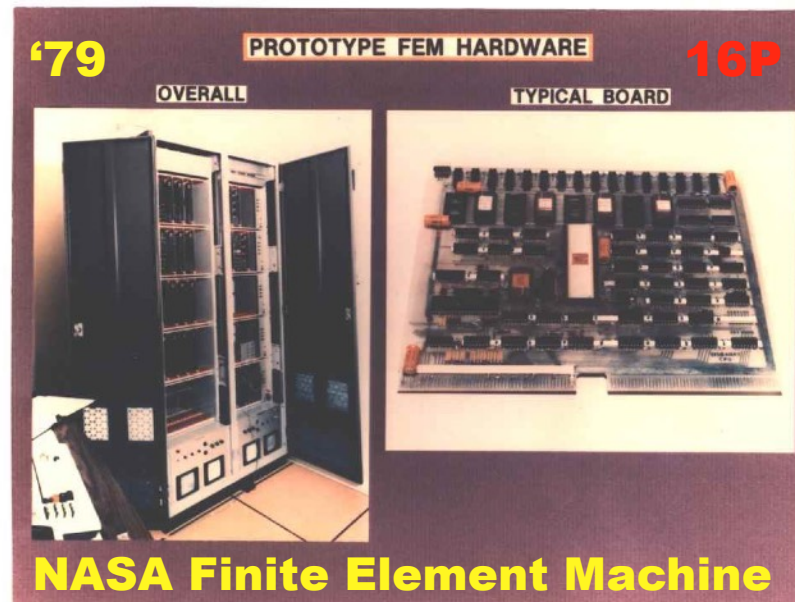
Now

Frontier: '21/'64 = 1.5EF/1.5KF

EF = 10^{18} / KF = 10^3

1,000,000,000,000,000 X faster

We hit
"Power
Wall"



World's 500 Fastest Computers

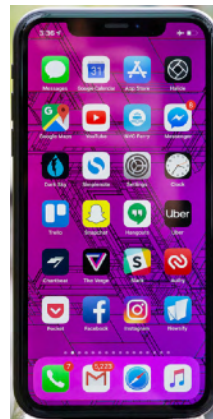


top500.org June/ISC, Nov/SC

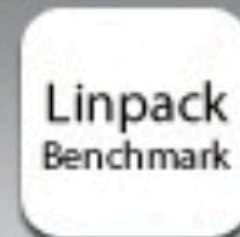
Linpack Benchmark: $Ax=b$ Jack Dongarra

Try! My iPhoneXr ~ **21GF**

*Craig Hunter MacPro28 ~ **1.5TF***



	SC18 Dallas, TX November 11-16, 2018		SC17 Denver, CO November 12-17, 2017 Conference Proceedings
	SC16 Salt Lake City, UT November 13-18, 2016 Conference Proceedings		SC15 Austin, TX November 15-20, 2015 Conference Proceedings
	SC14 New Orleans, LA November 16-21, 2014 Conference Proceedings		SC13 Denver, CO November 18-21, 2013 Conference Proceedings
	SC12 Salt Lake City, UT November 10-16, 2012 Conference Proceedings		SC11 Seattle, WA November 12-18, 2011 Conference Proceedings
	SC10 New Orleans, LA November 13-19, 2010 Conference Proceedings		SC09 Portland, OR November 14-20, 2009 Conference Proceedings
	SC08 Austin, TX November 2008 Conference Proceedings		SC07 Reno, NV November 10-16, 2007 Conference Proceedings



Linpack

5 Ratings

FREE

Linpack Benchmark

The LINPACK Benchmarks are a measure of a system's floating point computing power. They measure how fast a computer solves a dense N by

HPC Speedup: 1000X per Decade

Evolution of the fastest sustained performance
in real simulations



~1 Exaflop/s

~ 10^7 processing units
(ORNL?)

1.35 Petaflop/s

Cray XT5

$1.5 \cdot 10^5$ processor cores
(Shultness - ORNL)

1.02 Teraflop/s

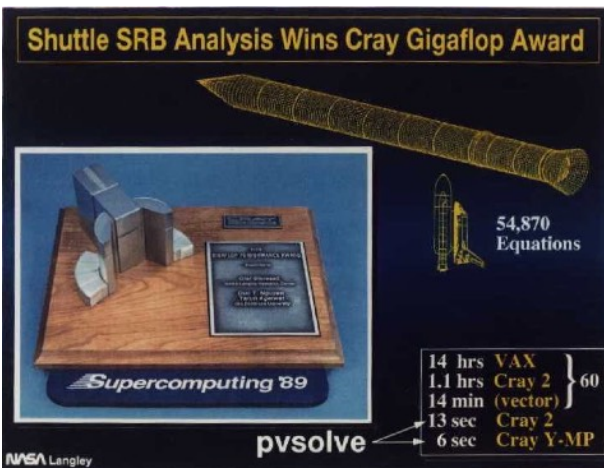
Cray T_{3D}

$1.5 \cdot 10^3$ processors
(ORNL)

1.5 Gigaflow/s

Cray YMP

$0.8 \cdot 10^1$ processors
(Storaasli - NASA)



1989

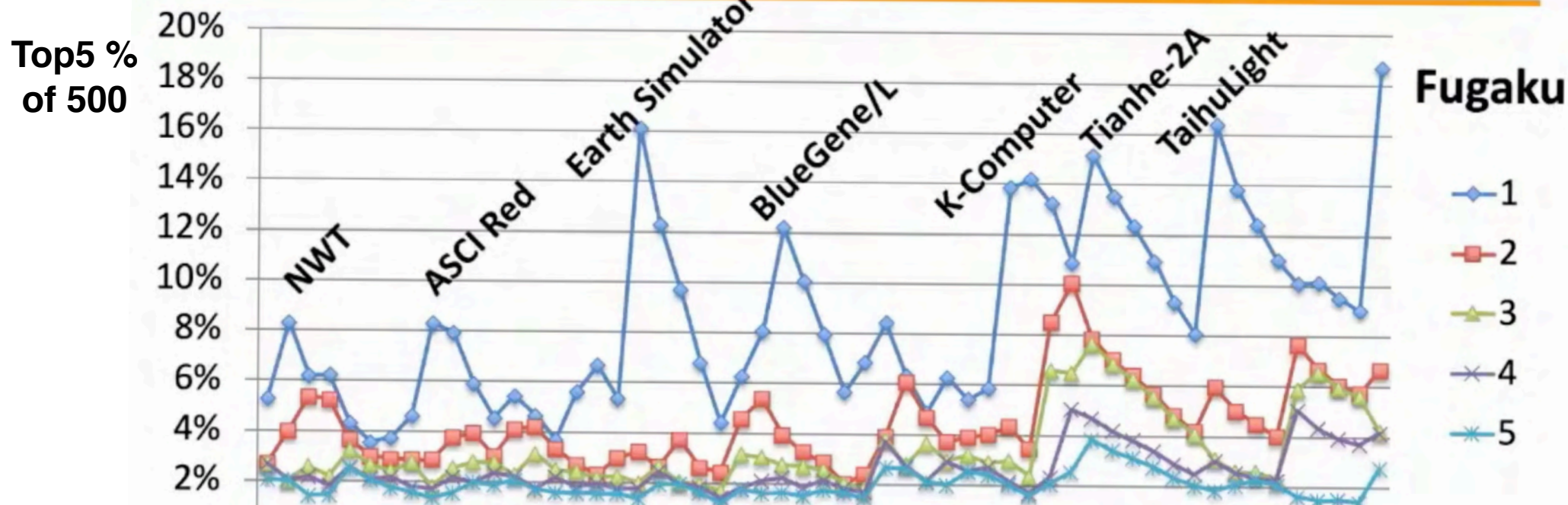
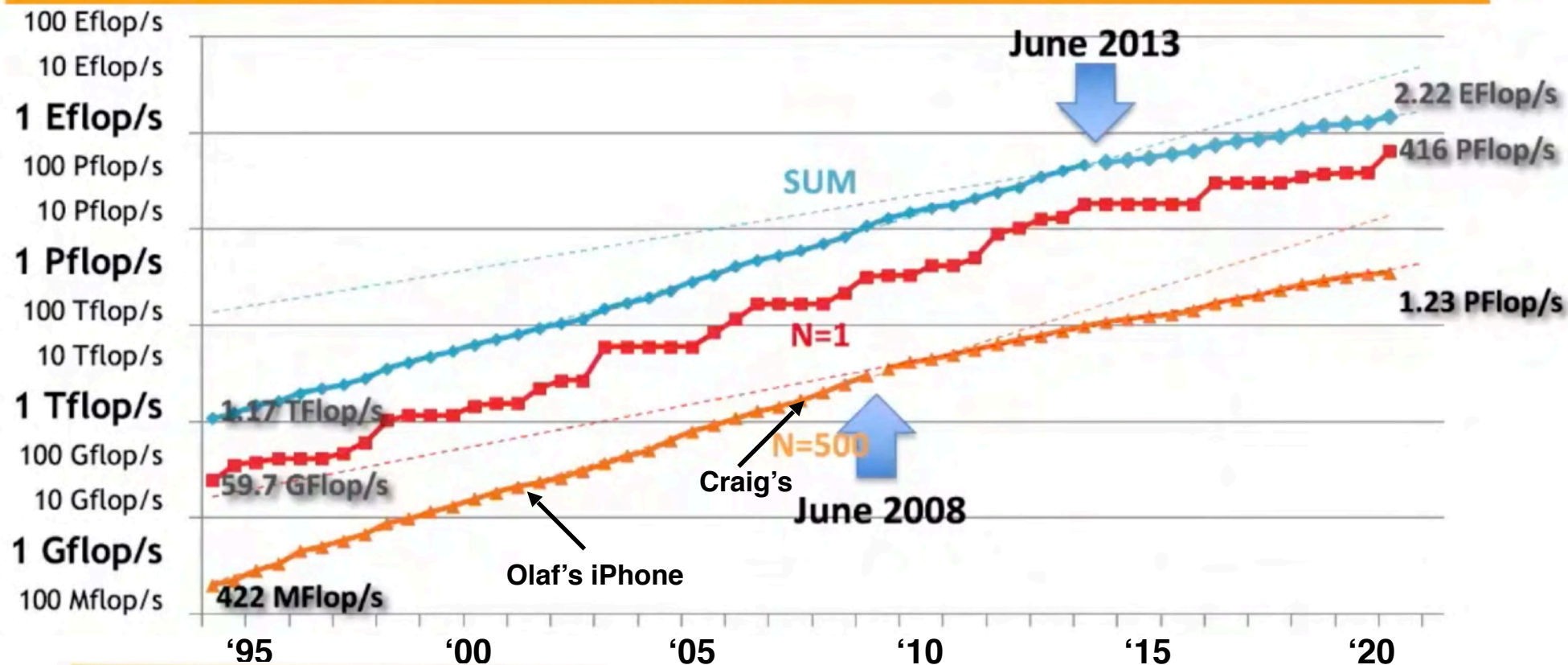
1998

2008

2021

10^{12} Mflops = 10^9 Gigaflops = 10^6 Teraflops = 1,000 Petaflops = 1 Exaflop

Supercomputer Speedup

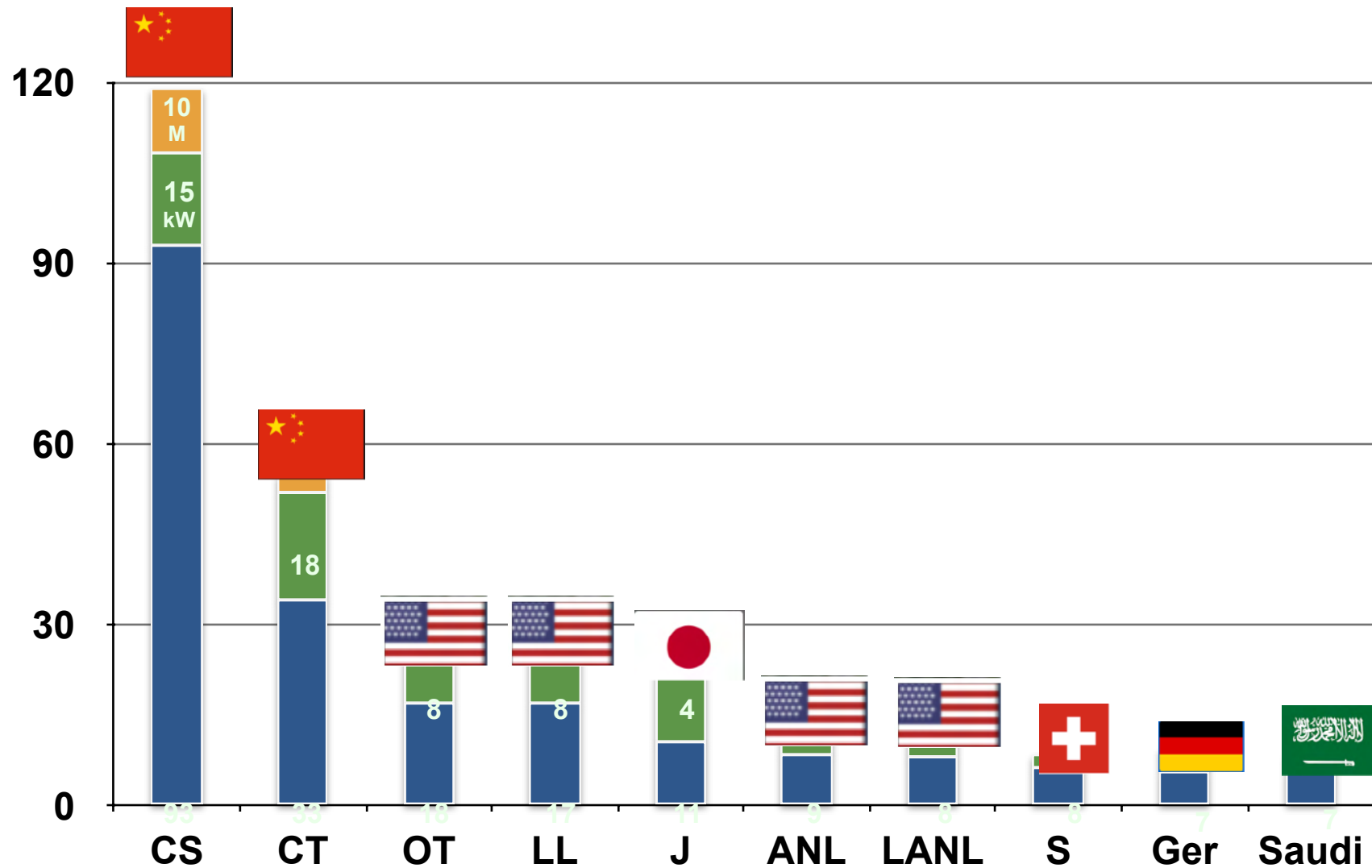


November 2012: The TOP10

Rank	Site	Computer	Country	Cores	Rmax [Pflops]	% of Peak	Power [MW]	MFlops /Watt
1	DOE / OS Oak Ridge Nat Lab	Titan, Cray XK7 (16C) + Nvidia Kepler GPU (14c) + custom	USA	560,640	17.6	66	8.3	2120
2	DOE / NNSA L Livermore Nat Lab	Sequoia, BlueGene/Q (16c) + custom	USA	1,572,864	16.3	81	7.9	2063
3	RIKEN Advanced Inst for Comp Sci	K computer Fujitsu SPARC64 VIIIfx (8c) + custom	Japan	705,024	10.5	93	12.7	827
4	DOE / OS Argonne Nat Lab	Mira, BlueGene/Q (16c) + custom	USA	786,432	8.16	81	3.95	2066
5	Forschungszentrum Juelich	JuQUEEN, BlueGene/Q (16c) + custom	Germany	393,216	4.14	82	1.97	2102
6	Leibniz Rechenzentrum	SuperMUC, Intel (8c) + IB	Germany	147,456	2.90	90*	3.42	848
7	Texas Advanced Computing Center	Stampede, Dell Intel (8) + Intel Xeon Phi (61) + IB	USA	204,900	2.66	67	3.3	806
8	Nat. SuperComputer Center in Tianjin	Tianhe-1A, NUDT Intel (6c) + Nvidia Fermi GPU (14c) + custom	China	186,368	2.57	55	4.04	636
9	CINECA	Fermi, BlueGene/Q (16c) + custom	Italy	163,840	1.73	82	.822	2105
10	IBM	DARPA Trial System, Power7 (8C) + custom	USA	63,360	1.51	78	.358	422

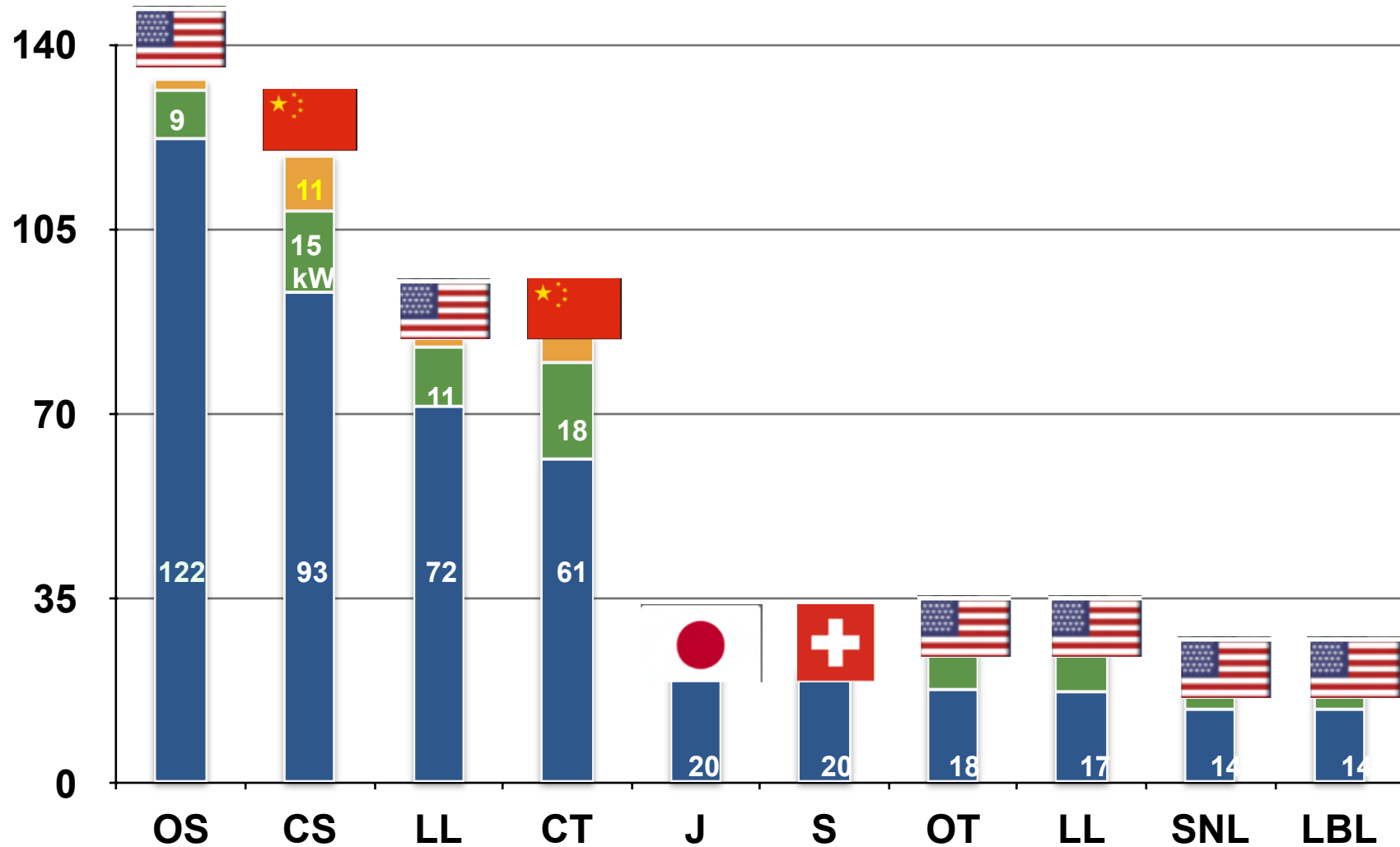
Top10 Supercomputers June 2016

Speed-TF, Power-kW, Cores-M

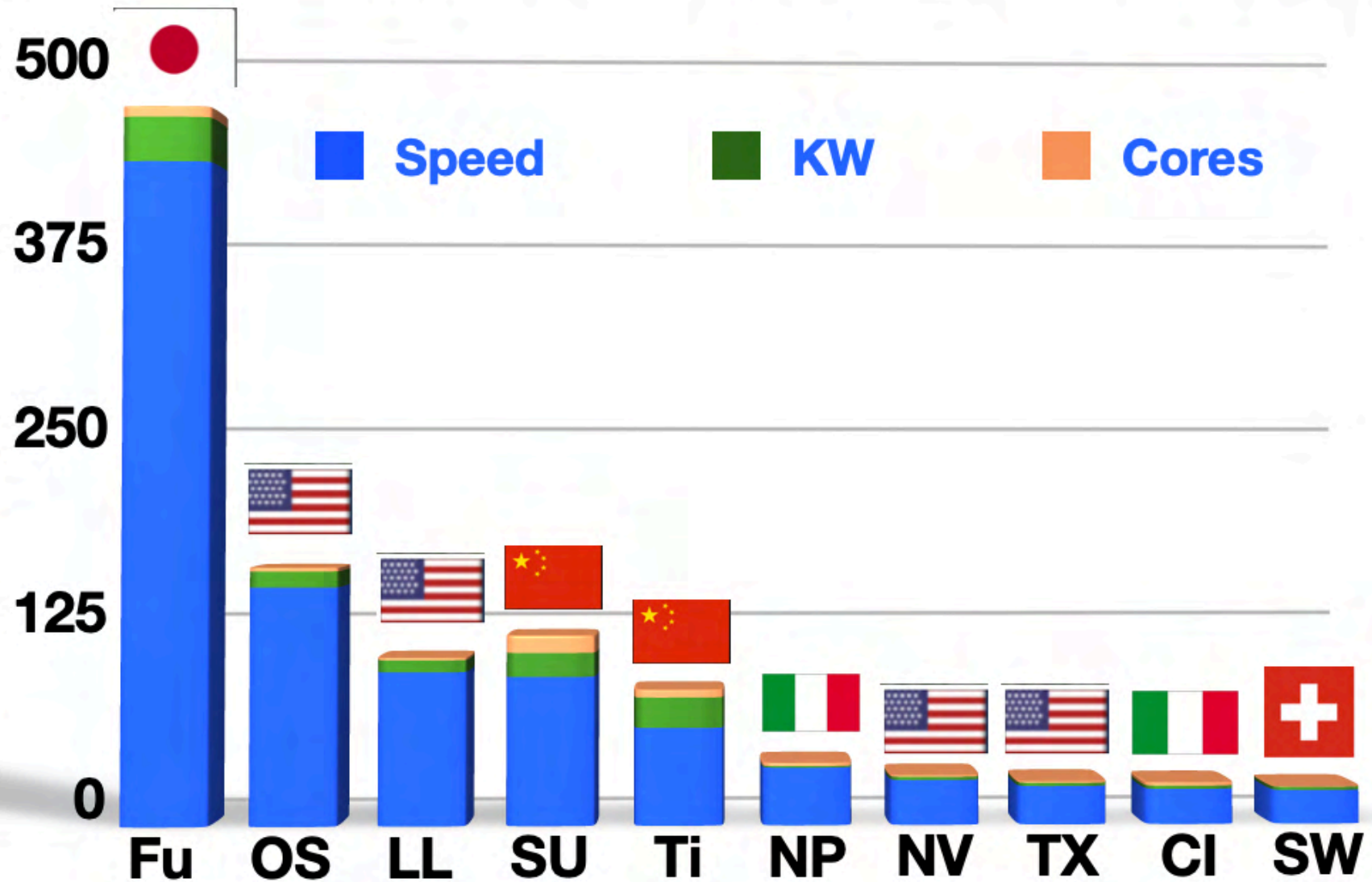


Top10 Supercomputers June 2018

Speed-TF, Power-kW, Cores-M



Top10 Supercomputers June 2020



Top10 Supercomputers June 2020

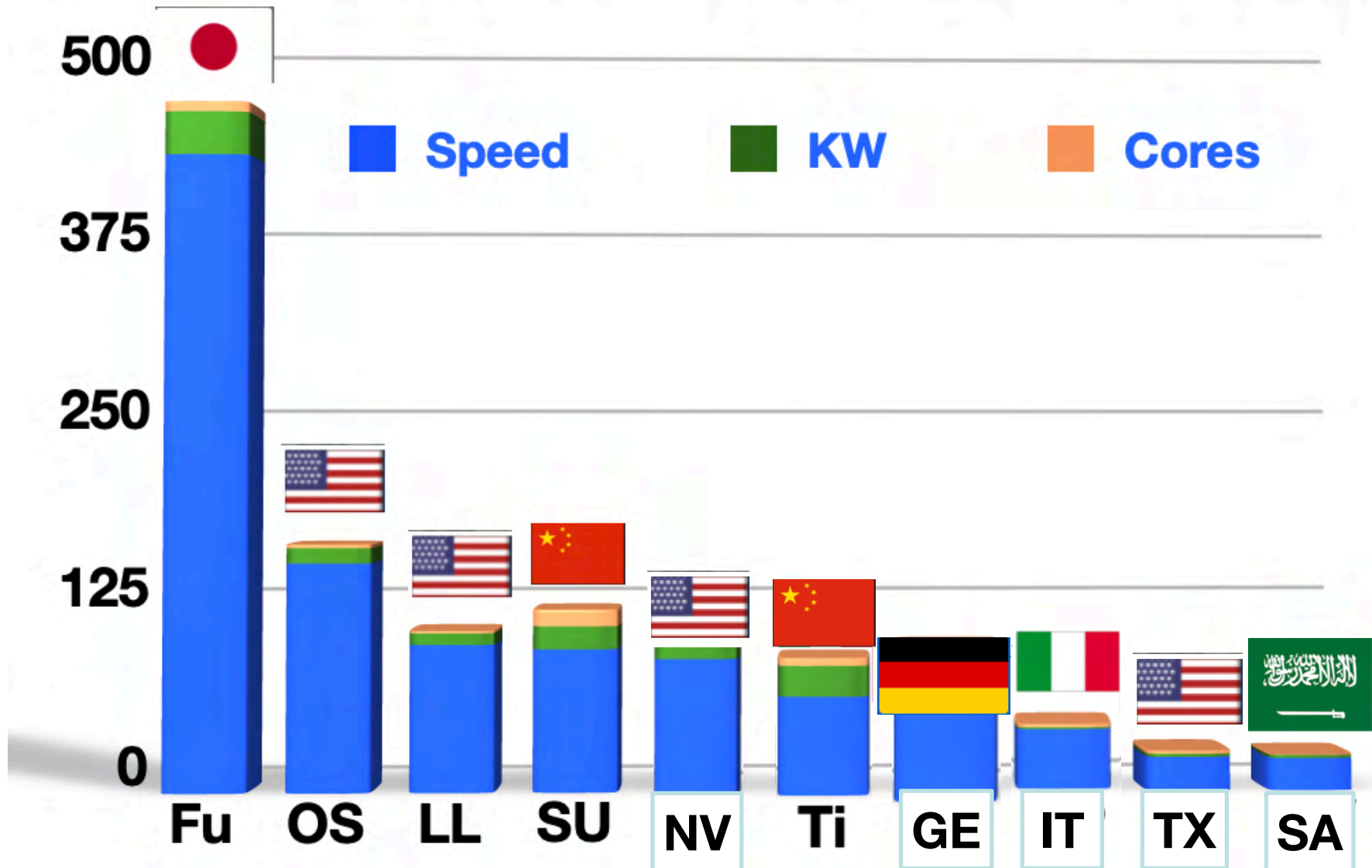
#	Site	Manufacturer	Computer	Country	Cores	Rmax [Pflops]	Power [MW]
1	RIKEN Center for Computational Science	Fujitsu	Fugaku Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D	Japan	7,299,072	415.5	28.3
2	Oak Ridge National Laboratory	IBM	Summit IBM Power System, P9 22C 3.07GHz, Mellanox EDR, NVIDIA GV100	USA	2,414,592	148.6	10.1
3	Lawrence Livermore National Laboratory	IBM	Sierra IBM Power System, P9 22C 3.1GHz, Mellanox EDR, NVIDIA GV100	USA	1,572,480	94.6	7.4
4	National Supercomputing Center in Wuxi	NRCP	Sunway TaihuLight NRCP Sunway SW26010, 260C 1.45GHz	China	10,649,600	93.0	15.4
5	National University of Defense Technology	NUDT	Tianhe-2A ANUDT TH-IVB-FEP, Xeon 12C 2.2GHz, Matrix-2000	China	4,981,760	61.4	18.5
6	Eni S.p.A	Dell EMC	HPC5 PowerEdge C4140, Xeon 24C 2.1GHz, NVIDIA T. V100, Mellanox HDR	Italy	669,760	35.5	2.25
7	NVIDIA Corporation	NVIDIA	Selene DGX A100 SuperPOD, AMD 64C 2.25GHz, NVIDIA A100, Mellanox HDR	USA	277,760	27.6	1.34
8	Texas Advanced Computing Center / Univ. of Texas	Dell	Frontera Dell C6420, Xeon Platinum 8280 28C 2.7GHz, Mellanox HDR	USA	448,448	23.5	
9	CINECA	IBM	Marconi-100 IBM Power System AC922, P9 16C 3GHz, Nvidia Volta V100, Mellanox EDR	Italy	347,776	21.6	1.98
10	Swiss National Supercomputing Centre (CSCS)	Cray	Piz Daint Cray XC50, Xeon E5 12C 2.6GHz, NVIDIA Tesla P100, Aries	Switzerland	387,872	21.2	2.38

 new to Top10

#1 EF for HPL-AI (less precision)

15GF/W 1-3
6-3GF/W 4-5

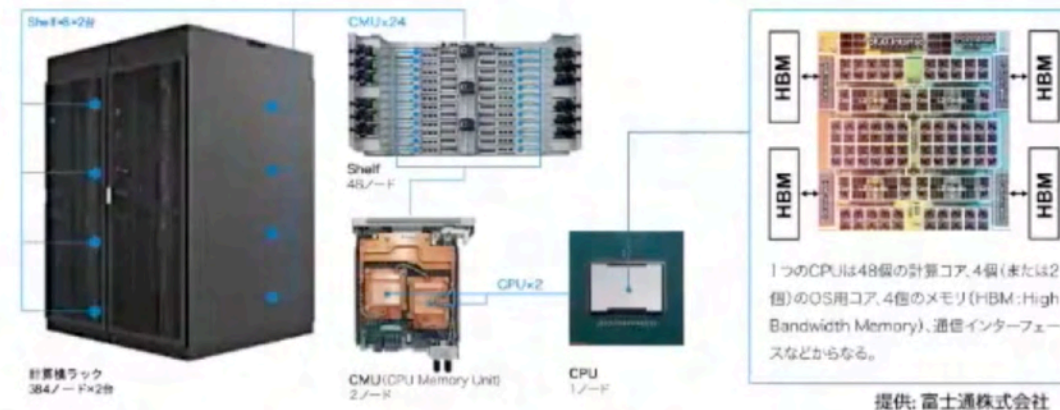
Top10 Supercomputers Nov 2020



#1 Supercomputer Fugaku = 537 PF

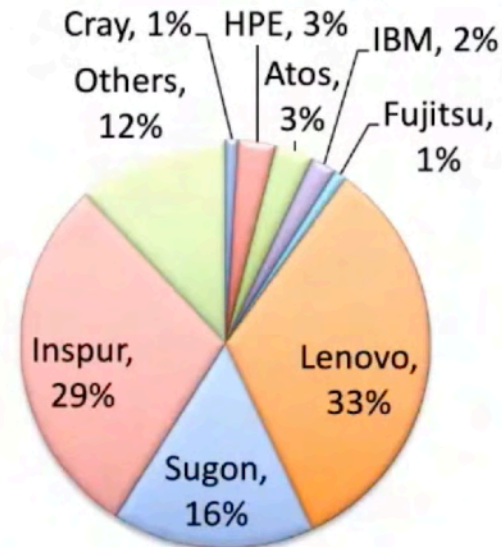
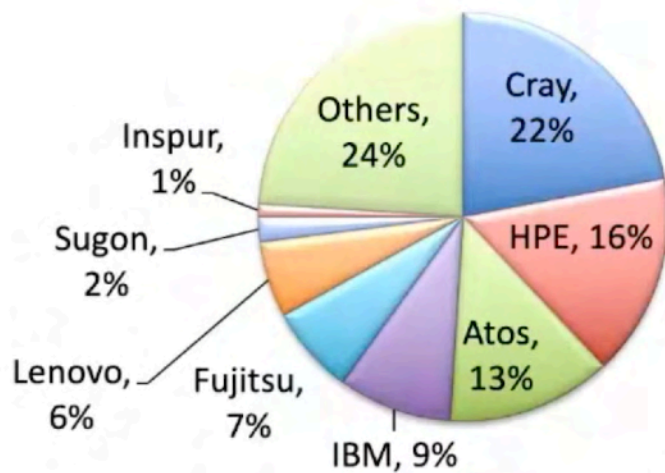
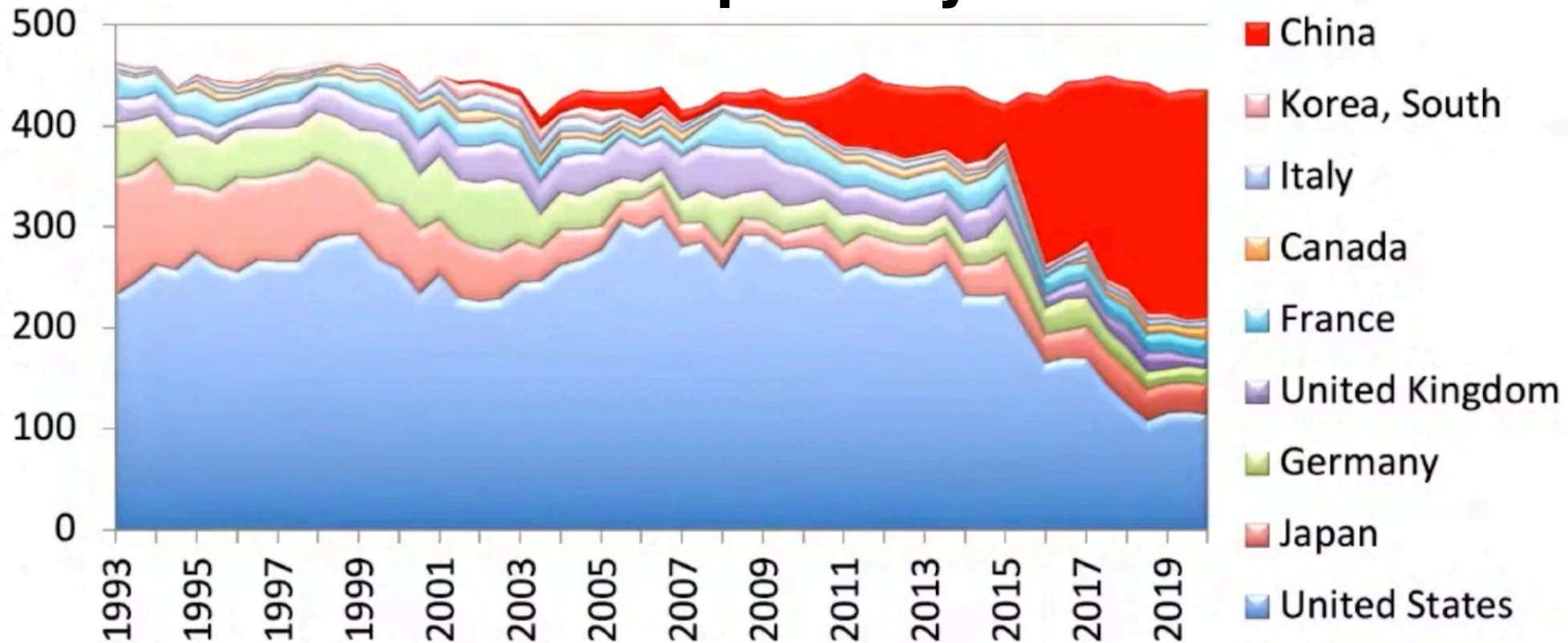


- **Total # Nodes: 158,976 nodes**
 - 384 nodes/rack x 396 (full) racks = 152,064 nodes
 - 192 nodes/rack x 36 (half) racks = 6,912 nodes
- **Theoretical Peak Compute Performances**
 - Boost Mode (CPU Frequency 2.2GHz)
 - 64 bit Double Precision FP: 537 Petaflops
 - 32 bit Single Precision FP: 1.07 Exaflops
 - 16 bit Half Precision FP (AI training): 2.15 Exaflops
 - 8 bit Integer (AI Inference): 4.30 Exaops
- **Theoretical Peak Memory Bandwidth: 163 Petabytes/s**



For detail see Jack Dongarra's report at: <http://bit.ly/fugaku-report>

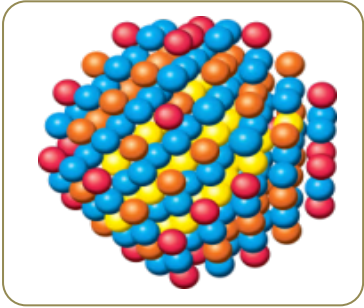
China leads #Top500 Systems



Research

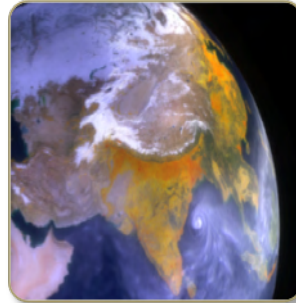
Commercial

Science Applications



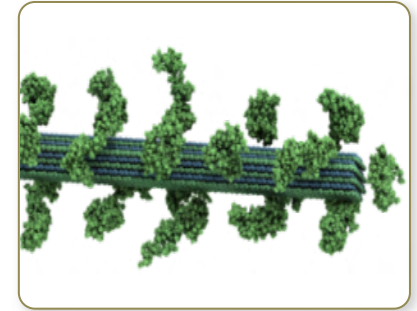
Material Science (WL-LSMS)

Role of material disorder, statistics & fluctuations in nanoscale materials & systems.



Climate Change (CAM-SE)

Realistic climate change adaptation & mitigation scenarios: precipitation & tropical storm patterns/statistics.

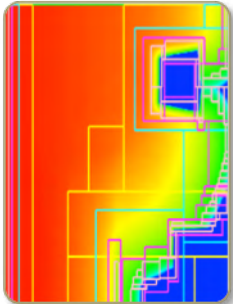


Biofuels (LAMMPS)

Multiple function molecular dynamics

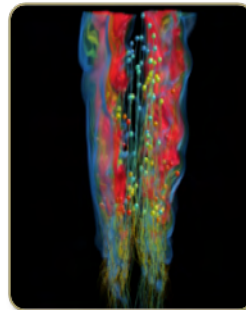
Astrophysics (NRDF)

Radiation transport for astrophysics, laser fusion, combustion, atmospheric dynamics & medical imaging.



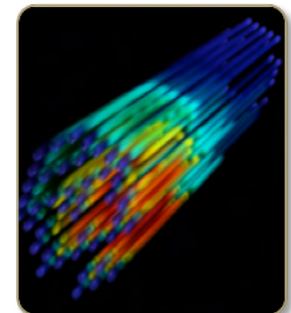
Combustion (S3D)

Combustion simulations to enable next generation diesel/bio-fuels to burn more efficiently.



Nuclear Energy (Denovo)

Calculate Radiation transport for nuclear energy & technology apps.

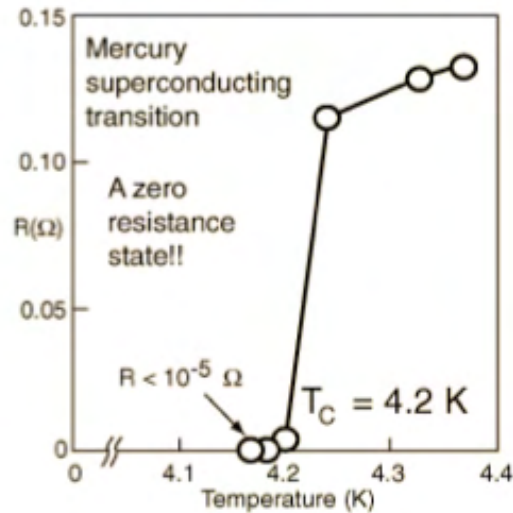


Superconductivity: a state of matter with zero electrical resistivity

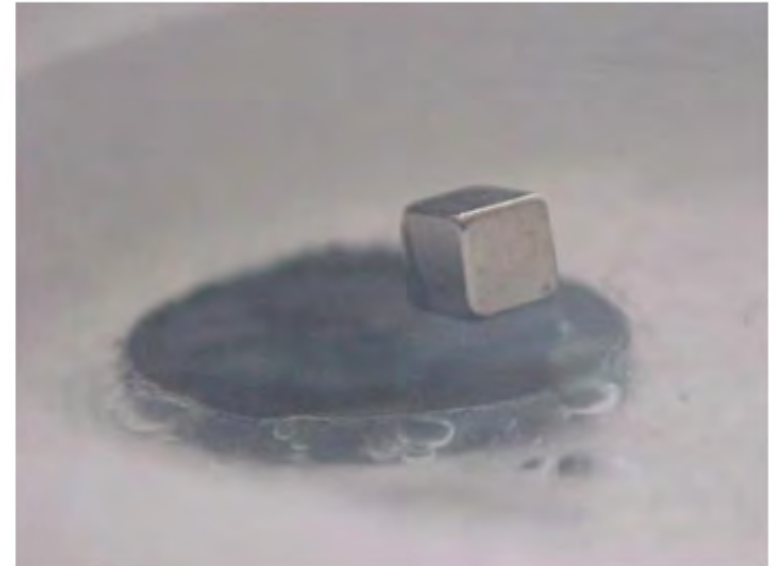
Discovery 1911



Heike Kamerlingh Onnes (1853-1926)



Superconductor repels magnetic field
Meissner and Ochsenfeld, **Berlin 1933**



Microscopic Theory for Superconductivity 1957

PHYSICAL REVIEW

VOLUME 106, NUMBER 5

DECEMBER 1, 1957

Theory of Superconductivity*

J. BARDEEN, L. N. COOPER,† and J. R. SCHRIEFFER‡
Department of Physics, University of Illinois, Urbana, Illinois
(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electron states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by an amount proportional to an average $(\hbar\omega)^2$, consistent with the isotope effect. A mutually orthogonal set of excited states in

one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about 3.5kT_c at T=0°K to zero at T_c. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.



BCS Theory generally accepted in the early 1970s

Courtesy of Thomas Schulth

Who?

New algorithm to enable
1+ PFlop/s sustained performance
in simulations of disorder effects
in high- T_c superconductors

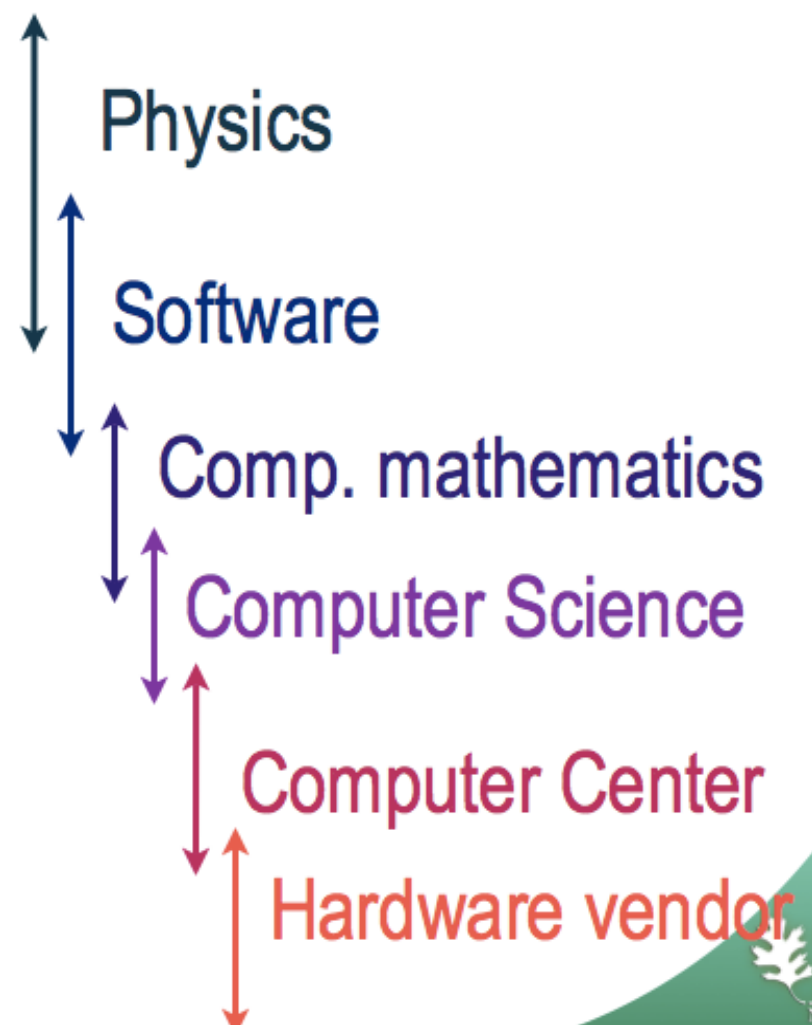
Models,
Methods,
& Implementation

Map to Hardware

Operations

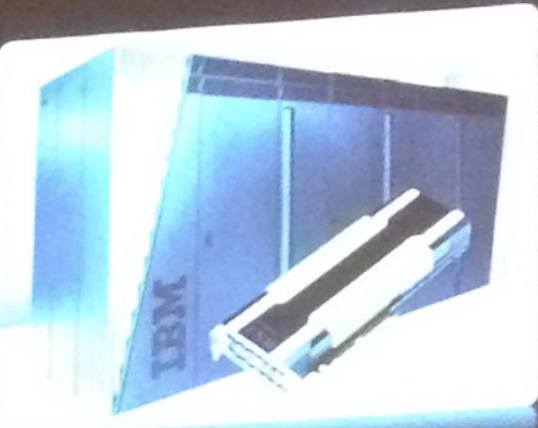
System design

- T. A. Maier**
- P. R. C. Kent**
- T. C. Schulthess**
- G. Alvarez**
- M. S. Summers**
- E. F. D'Azevedo**
- J. S. Meredith**
- M. Eisenbach**
- D. E. Maxwell**
- J. M. Larkin**
- J. Levesque**



Bill Dally NVIDIA Chief Scientist, Stanford Prof HiPEAC'15 Keynote Amsterdam Jan 19, 2015

US to Build Two Flagship Supercomputers



OAK
RIDGE
National Laboratory
SUMMIT

Lawrence Livermore
National Laboratory
SIERRA

150-300 PFLOPS Peak Performance
IBM POWER9 CPU + NVIDIA Volta GPU
NVLink High Speed Interconnect
40 TFLOPS per Node, >3,400 Nodes
2017

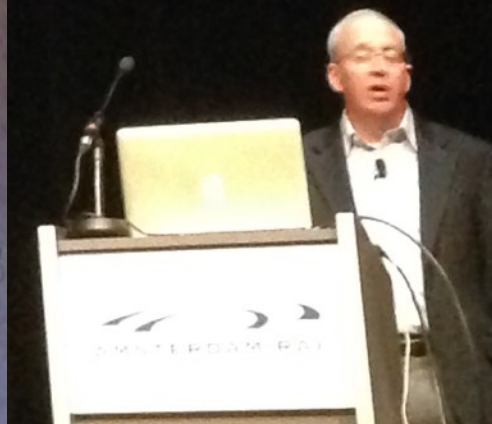
CPUs use 12x power of GPUs

CPU
1690 pJ/flop

Optimized for Latency
Caches

GPU
140 pJ/flop

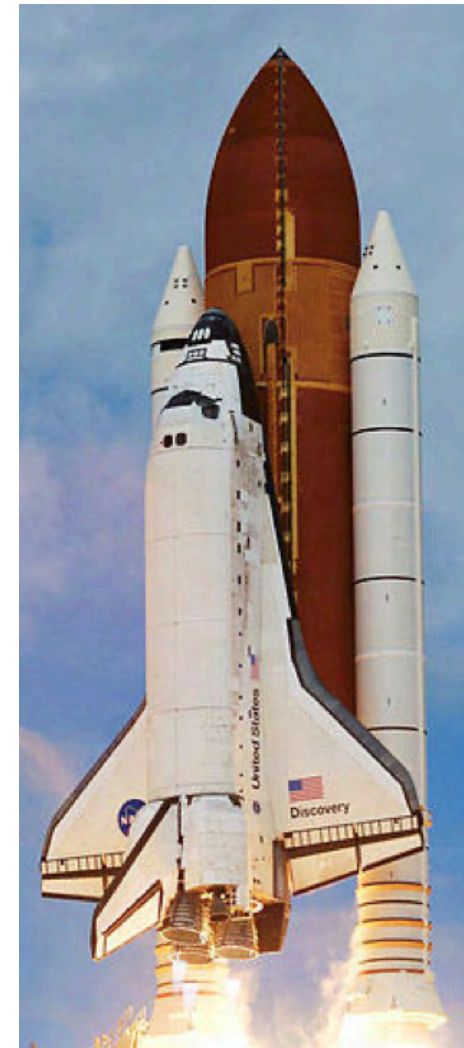
Optimized for Throughput
Explicit Management
of On-chip Memory



Summit



Summary



GREAT Life after Langley! Opportunities, travel ...
Exciting Supercomputer research: **10^{15}** speedup
Efficient GF/W: 2 ('15) $\Rightarrow$ 15 ('21)
Exaflop Future: Frontier(GPUs), Fugatu(ARM) + ?
Change is Good! *Who moved the cheese?*

Thanks for listening!

Question



Answer

Contact

Google

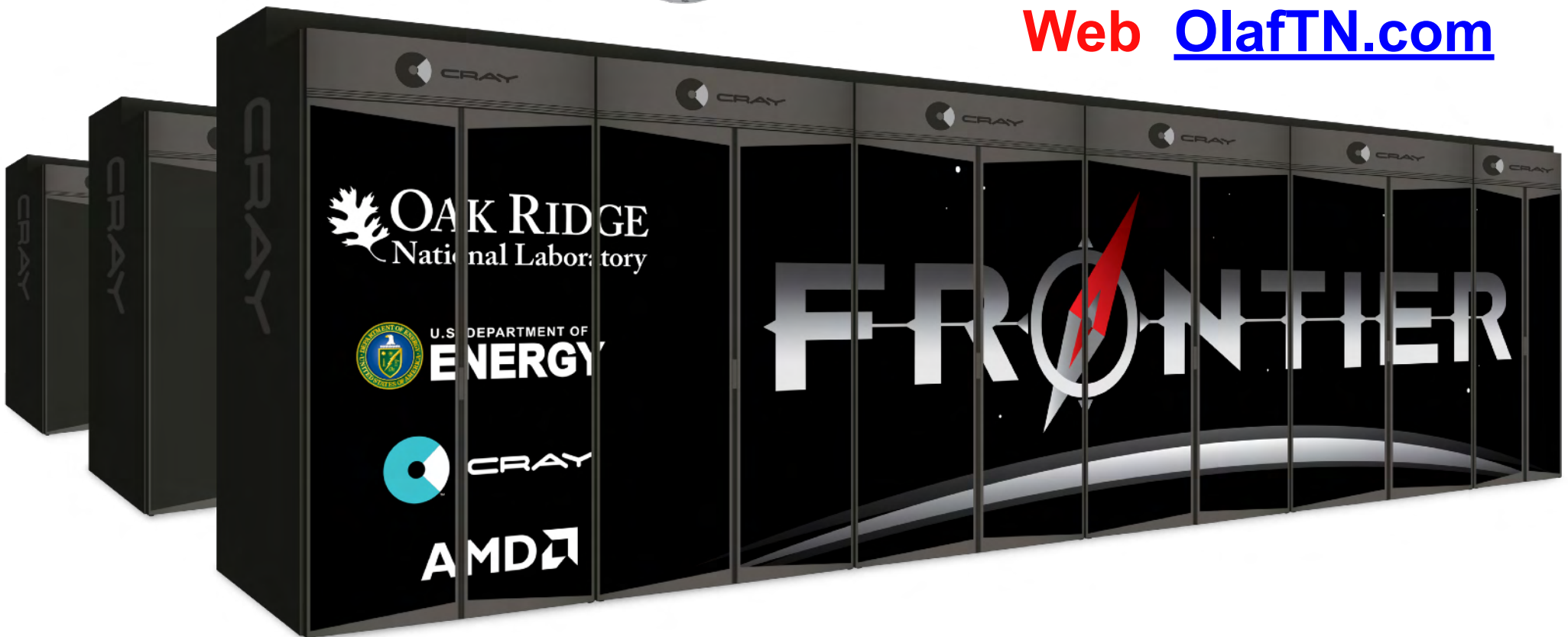


Storaasli



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**Additional Slides
(not used)**

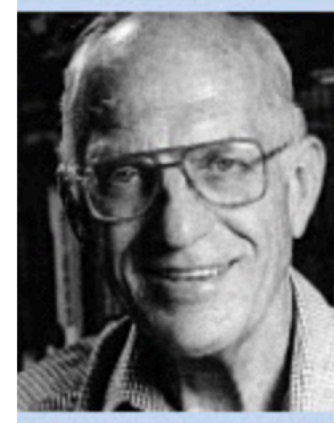
Developer of Finite Element Analysis Method Ray Clough Dies

BY Staff

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[Distinguished Members](#) [earthquake engineering](#) [finite element method](#) [Ray Clough](#) [structural analysis](#)

Ray William Clough, Ph.D., P.E., NAE, Dist.M.ASCE, renowned as a developer of the finite element method for structural analysis of buildings, has died. He was 96.



Clough

Clough was professor emeritus of civil and environmental engineering at the University of California, Berkeley. He was a faculty member at Berkeley's Department of Civil and Environmental Engineering from 1949 to 1987, and served as Earthquake Engineering Research Center director from 1973 to 1977.

It was on a sabbatical leave in Trondheim, Norway, in 1956-57, that Clough developed the theories that would become the finite element method. He coauthored a paper in 1956 outlining the method, forever changing the field of structural analysis and the design of buildings and other structures.

In the 1960s, Clough had the vision to see how powerful computers could be in conducting structural analyses on giant structures. He published a series of papers that became the basis for commercial computer programs, now industry standards. His paper, "Dynamics of

Top10 Supercomputers Nov 2020

Rank (previous)	Rmax Rpeak (PFLOPS)	Name	Model	CPU cores	Accelerator (e.g. GPU) cores	Interconnect	Manufacturer	Site country	Year	Operat syste
1	442.010 537.212	<u>Fugaku</u>	<u>Supercomputer Fugaku</u>	158,976 × 48 <u>A64FX @2.2 GHz</u>	0	Tofu interconnect D	<u>Fujitsu</u>	<u>RIKEN Center for Computational Science</u> Japan	2020	Linux (<u>RHEL</u>)
2 ▼ (1)	148.600 200.795	<u>Summit</u>	<u>IBM Power System AC922</u>	9,216 × 22 <u>POWER9 @3.07 GHz</u>	27,648 × 80 <u>Tesla V100</u>	<u>InfiniBand EDR</u>	<u>IBM</u>	<u>Oak Ridge National Laboratory</u> United States	2018	Linux (<u>RHEL</u>)
3 ▼ (2)	94.640 125.712	<u>Sierra</u>	<u>IBM Power System S922LC</u>	8,640 × 22 <u>POWER9 @3.1 GHz</u>	17,280 × 80 <u>Tesla V100</u>	<u>InfiniBand EDR</u>	<u>IBM</u>	<u>Lawrence Livermore National Laboratory</u> United States	2018	Linux (<u>RHEL</u>)
4 ▼ (3)	93.015 125.436	<u>Sunway TaihuLight</u>	<u>Sunway MPP</u>	40,960 × 260 <u>SW26010 @1.45 GHz</u>	0	<u>Sunway</u> ^[26]	<u>NRCPC</u>	<u>National Supercomputing Center in Wuxi</u> China ^[26]	2016	Linux (<u>Raise</u>)
5 ▲ (7)	63.460 79.215	<u>Selene</u>	<u>Nvidia</u>	1,120 × 64 Epyc <u>7742 @2.25 GHz</u>	4,480 × 108 <u>Ampere A100</u>	<u>Mellanox HDR Infiniband</u>	<u>Nvidia</u>	<u>Nvidia</u> United States	2020	Linux (<u>Ubuntu</u>)
6 ▼ (5)	61.445 100.679	<u>Tianhe-2A</u>	<u>TH-IVB-FEP</u>	35,584 × 12 Xeon <u>E5-2692 v2 @2.2 GHz</u>	35,584 × 128 <u>Matrix- 2000</u> ^[27]	<u>TH Express-2</u>	<u>NUDT</u>	<u>National Supercomputer Center in Guangzhou</u> China	2013	Linux (I
7 ▲ (new)	44.120 70.980	<u>JUWELS (booster module)</u> ^[28]	<u>BullSequana XH2000</u>	1,872 × 24 AMD <u>EPYC 7402 @2.8 GHz</u>	3,744 × 108 <u>Ampere A100</u>	<u>Mellanox HDR Infiniband</u>	<u>ATOS</u>	<u>Forschungszentrum Jülich</u> Germany	2020	Linux (<u>CentO</u>)
8 ▼ (6)	35.450 51.721	<u>HPC5</u>	<u>Dell</u>	3,640 × 24 Xeon <u>Gold 6252 @2.1 GHz</u>	7,280 × 80 <u>Tesla V100</u>	<u>Mellanox HDR Infiniband</u>	<u>Dell EMC</u>	<u>Eni</u> Italy	2020	Linux (<u>CentO</u>)
9 ▼ (8)	23.516 38.746	<u>Frontera</u>	<u>Dell C6420</u>	16,016 × 28 Xeon <u>Platinum 8280 @2.7 GHz</u>	0	<u>InfiniBand HDR</u>	<u>Dell EMC</u>	<u>Texas Advanced Computing Center</u> United States	2019	Linux (<u>CentO</u>)
10 ▲ (new)	22.400 55.424	<u>DAMMAM- 7</u>	<u>CRAY CS-Storm</u>	1,978 × Xeon <u>Gold 6248 @2.5 GHz</u>	7,912 × 80 <u>Tesla V100</u>	<u>InfiniBand HDR 100</u>	<u>Cray</u>	<u>Saudi Aramco</u> Saudi Arabia	2020	Linux (<u>RHEL</u>)

Next: June Top10

#1 EF for HPL-AI (less precision)

15GF/W 1-3,5
6,3GF/W 4,6