High Performance Computing and Modern Science
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Abstract

High Performance Computing (HPC) became an instrument for many modern sciences. In particular numerical simulations are based on parallel computing in HPC systems. Beside experiment and theory they are considered as the third pillar of knowledge gaining. However, HPC became very expensive over the last ten years. In particular, modern systems ask for huge amounts of electrical power such that the possible research starts to be limited by the research institution’s budget for power. Moreover, programming these systems that exhibit massiv parallelism in their components requires scientists knowledgeable in software engineering. Finally, there is now a new challenge for our researchers: the aggregation of measured and generated digital data leads to new epistemological concepts. It is usually called data intensive science or the Fourth Paradigm. Available data becomes the primary product for new and unique insights. The talk will discuss current challenges in HPC and data intensive science and will highlight the potential development in the field until the end of the decade. Beyond 2020 the development in computer technology is difficult to predict - modern science and modern life ask however for a sustained progress.
Computational Performance

0.123456 x 0.654321
this is ONE floating point operation (FLOP)

if you need 100 seconds to calculate this
your computational performance is 1/100 Flops
Computers and Performance

The first computer in 1941 (Zuse’s Z3) made
0.3 Flops

The No. 1 computer in Nov 2013 (Tianhe-2) makes
33,862,700,000,000,000 Flops
33x10^{15} Flops
33 quadrillion Flops
33 PetaFlops
Computers and Science & Engineering

Zuse’s Z3
- Fluid dynamics and wing profile optimizations

ENIAC (1946, 385 Flops!)
- Artillery firing tables
- Simulate hydrogen bomb (John von Neuman)
- First numerical weather forecast (John von Neuman, 1950)

Tianhe-2
- Fluid dynamics
- Cosmology
- Business Opinion Analysis
- Security e-Government Cloud
factor of 1,000 in 12 years

notebook 2014 😊

7 years
Zuse's Z3 - 0.3 Flops (1941)
1MFlops
1TFlops
1GFlops
1MFlops
1KFlops
1Flops
0.001Flops


Zuse’s Z3 – 0.3 Flops (1941)
Zuse’s Z3 – 0.3 Flops (1941)

Bruk’s M-1 – 20 Flops (1950)
Zuse's Z3 – 0.3 Flops (1941)
Glushkov’s KIEV – 3 KFlops (1958)
Bruk’s M-1 – 20 Flops (1950)
Zuse’s Z3 – 0.3 Flops (1941)

Glushkov’s KIEV – 3 KFlops (1958)

Bruk’s M-1 – 20 Flops (1950)
1953: Zuse’s Z3 – 0.3 Flops (1941)
1950: Bruk’s M-1 – 20 Flops (1950)
1958: Glushkov’s KIEV – 3 KFlops (1958)
1972: EC 1020 – 20 KFlops (1972)
Zuse’s Z3 – 0.3 Flops (1941)

Glushkov’s KIEV – 3 KFlops (1958)

Bruk’s M-1 – 20 Flops (1950)

EC 1020 – 20 KFlops (1972)
Zuse’s Z3 – 0.3 Flops (1941)

Glushkov’s KIEV – 3 KFlops (1958)

Bruk’s M-1 – 20 Flops (1950)

EC 1020 – 20 KFlops (1972)
- **Zuse’s Z3** – 0.3 Flops (1941)
- **Bruk’s M-I** – 20 Flops (1950)
- **Glushkov’s KIEV** – 3 KFlops (1958)
- **EC 1020** – 20 KFlops (1972)

The graph shows the evolution of computing power from 1943 to 2032 with notable points including:

1953: Glushkov’s KIEV - 3 KFlops
1963: Bruk’s M-I - 20 Flops
1973: EC 1020 - 20 KFlops
1983: Zuse’s Z3 - 0.3 Flops

The graph projects a trend line indicating the potential for computing performance in 2032 (represented as 2032 (?)).
Increase in Computational Performance

from 0.3 Flops in 1941
to 33x10^{15} Flops in 2013
as constant exponential growth

means factor 1.000 every 12.5 years
for already more than 70 years
Exponential Acceleration
A 1941 Ford
Geneva - Bourg-en-Bresse

100 km in 1 hour
A Ford as Fast as Light

1,079,252,849 km/h will be reached in 1970
by the way: „Tianhe“ means Milky Way (5 min for our Ford)
The Universe and the 2020 Ford (Exascale)

- Afterglow Light Pattern 380,000 yrs.
- Dark Ages
- Development of Galaxies, Planets, etc.
- Dark Energy Accelerated Expansion
- Inflation
- Quantum Fluctuations
- 1st Stars about 400 million yrs.
- Big Bang Expansion 13.7 billion years

- 90 billion lightyears
- 2 months
The Universe and the 2032 Ford (Zetascale)

- Afterglow Light Pattern 380,000 yrs.
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- Development of Galaxies, Planets, etc.
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  - 13.7 billion years

- 90 billion lightyears
- 2.5 h
Energy Consumption

A killer argument against high performance computing today and tomorrow

- Tianhe-2 uses 17 MW
- May cost 17 million Euro per year for power
- Same problem with most compute HPC centers

But…
Time will tell...

Currently energy efficiency increases by a factor of 10 every 7 years

1987

25 years of DKRZ

2012
What Type of Science?

Basically we do numerical simulations

- Climate and weather simulation
  - Cloud simulation
- Cosmology
  - The origin of the universe
- Particle physics
- Proteine folding
  - Individualized medical treatment
- Brain simulation
Orders of Magnitude

Human brain
- 100x10^9 neurons

Tianhe-2 in 2013
- 33x10^{15} Flops
  - 330,000 Flops/neuron

Exaflops in 2020
- 1x10^{18} Flops
  - 10 million Flops/neuron

Zetaflops in 2032
- 1x10^{21} Flops
  - 10 billion Flops/neuron
datadeluge
The Fourth Paradigm

Refer to Jim Gray et al.:
“The Fourth Paradigm –
Data-Intensive Scientific Discovery”

„Data are not consumed by the ideas and innovations they spark but are an endless fuel for creativity“

„Harnessing the Power of Digital Data for Science and Society“
by the Interagency Working Group on Digital Data
January 2009
Climate research was and is dependent on data

- Keep data for long term in order to validate models in the future
- Keep all model variables because we do not know what will be necessary in future analyses
- Use a fine global grid in order to select later local regions
- ...

DKRZ archived around 8 PB on tape in 2013

- This is all output data of simulation runs
Data Generation

DKRZ (115 TFlop/s, 26 TByte main memory) produces an estimated data transfer mem<->disk

- 5-10 GB/s (430-860 TB/day)
- ca. 100 TB/day are saved for further inspection
- ca. 20 TB/day are archived to tape
The 5th Coupled Model Intercomparison Project

- Provides key input for the next IPCC report (5th AR)
  - Intergovernmental Panel on Climate Change
- ~20 modeling centers around the world (DKRZ being one of the biggest)
- Produces 10s of PBytes of output data from ~60 experiments (“digital born data”)

Data are produced without knowing all applications beforehand and these data are stored and archived for interdisciplinary utilization by yet unknown researchers.
Example Workflow CMI P5

Data creation
- German contribution produced at DKRZ
- Used ½ year of its compute capacity

Data archival
- 600 TB raw + 60 TB with quality control

Data dissemination
- Will be heavily used during the next 5 years

Expected CMI P6 data volume: factor 20-50 higher
The Next 10 Years
Future Computer and Storage

Next generation climate computer
- 2-3 PFlop/s
- 45 PByte on disk
- An estimated $\frac{1}{2}$ EByte as tape library capacity

- Storage: 30-50% of investment and energy costs
- Currently it is more like 10%

- Storage 50% of the overall complexity?
Where will this lead us to?
Where will this lead us to?

- Unprecedented science
  - E.g. life sciences: genetic design, artificial DNA

- Unprecedented products
  - E.g. medical science: prosthesis, medical treatments

- Unprecedented problems
  - Ethical question will be undiscussed
  - Societal considerations will be undiscussed
  - Legal aspects will be undiscussed
The technological singularity, or simply the singularity, is a hypothetical moment in time when artificial intelligence will have progressed to the point of a greater-than-human intelligence, radically changing civilization, and perhaps human nature. Because the capabilities of such an intelligence may be difficult for a human to comprehend, the technological singularity is often seen as an occurrence beyond which the future course of human history is unpredictable or even unfathomable. (Wikipedia)

“Singularity” – mentioned first in 1958 by John von Neumann
See also his book The Computer and the Brain

See Ray Kurzweil’s non-fiction book: “The Singularity is Near”