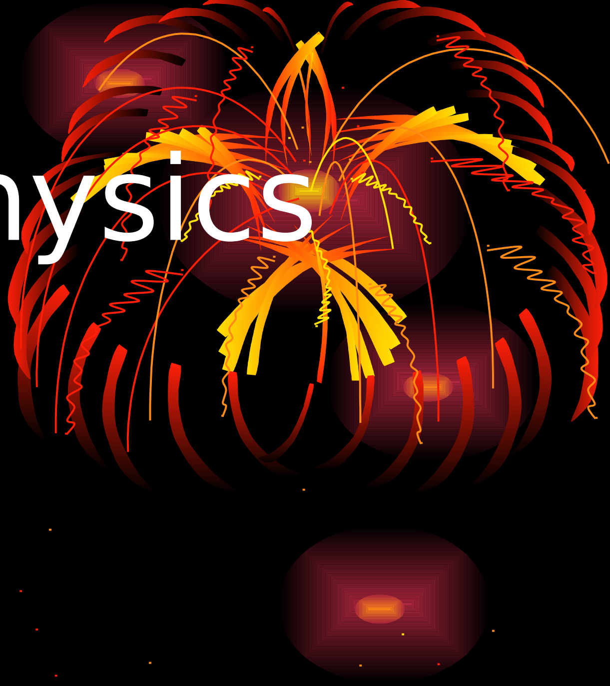
Computational Physics

Computerphysik



Rainer Spurzem, Astronomisches Rechen-Institut Zentrum für Astronomie, Universität Heidelberg
Ralf Klessen, Institut f. Theoretische Astrophysik, Zentrum für Astronomie, Universität Heidelberg

spurzem@ari.uni-heidelberg.de, spurzem@nao.cas.cn
klessen@uni-heidelberg.de

the SILK ROAD PROJECT at NAOC/KIAA
丝绸之路 计划

Chinese President Xi Jinping welcomes “Foreign Experts”

千人計劃
RECRUITMENT
PROGRAM OF GLOBAL EXPERTS

Pictures from:
http://www.chinatourselect.com/

http://silkroad.bao.ac.cn

National Astronomical Observatory of Chinese Academy of Sciences, Beijing China
Kavli Institute for Astronomy and Astrophysics, Peking University, Beijing, China
Fesenkov Astrophysical Institute, Space Institute, Almaty, Kazakhstan
Main Astronomical Observatory of Ukrainian Academy of Sciences, Kiev, Ukraine
Astronomisches Rechen-Institut,Zentrum f. Astronomie (ZAH) and
Computer Engineering and Architecture (ZITI), Univ. Of Heidelberg, Germany
Max-Planck Institute for Astrophysics (MPA), Garching/Munich, Germany

Observations (Experiment)

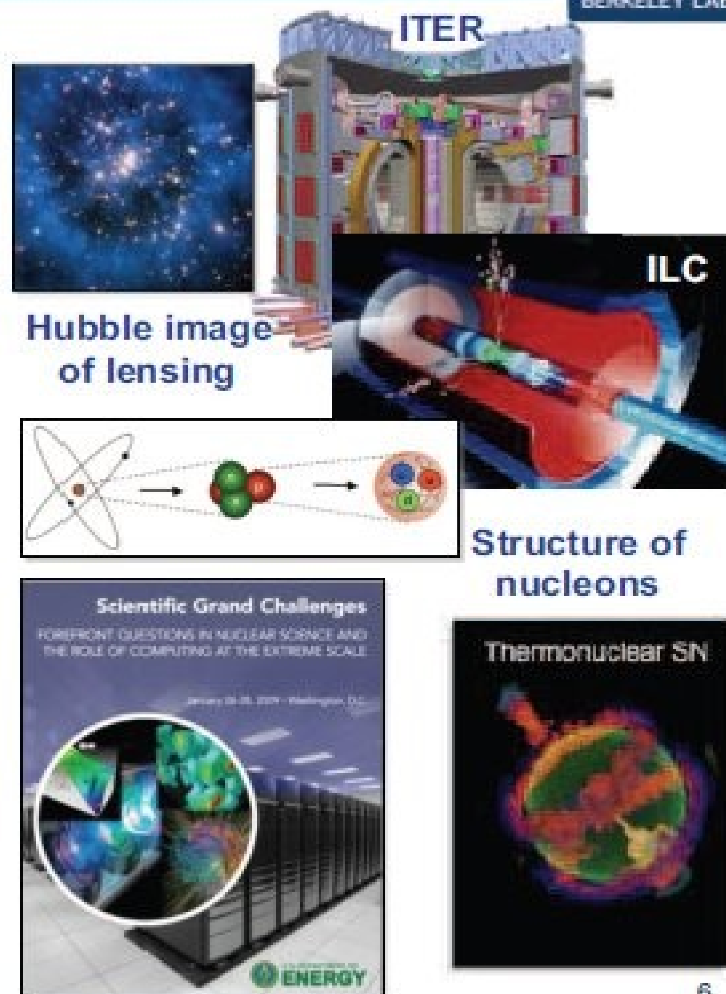
Theory

Computational Physics

Exascale simulation will enable fundamental advances in basic science

- High Energy & Nuclear Physics
  - Dark-energy and dark matter
  - Fundamentals of fission fusion reactions
- Facility and experimental design
  - Effective design of accelerators
  - Probes of dark energy and dark matter
  - ITER shot planning and device control
- Materials / Chemistry
  - Predictive multi-scale materials modeling: observation to control
  - Effective, commercial technologies in renewable energy, catalysts, batteries and combustion
- Life Sciences
  - Better biofuels
  - Sequence to structure to function

These breakthrough scientific discoveries and facilities require exascale applications and resources



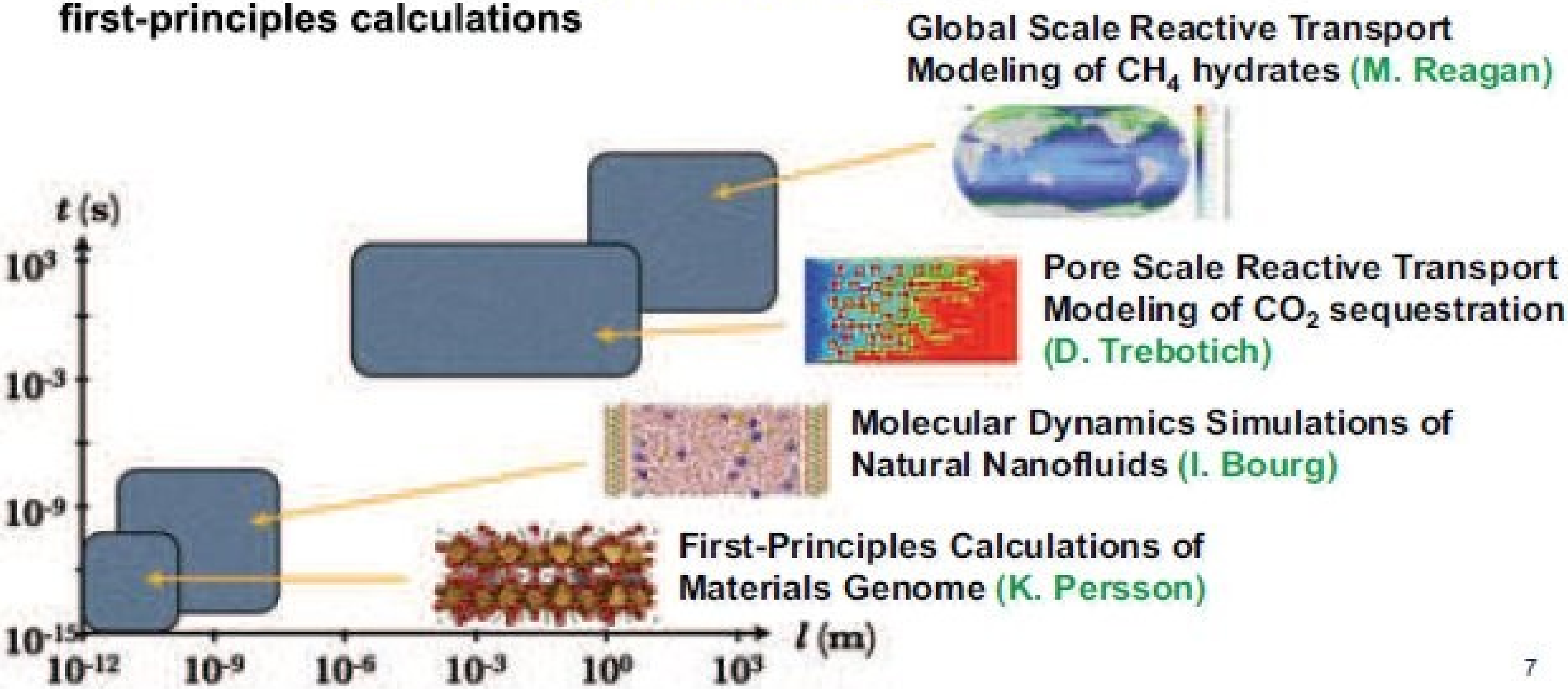
Slide: Horst Simon, Exascale Computing

Advanced Computation in Energy Science at LBNL

Probe natural systems under constraints that are difficult or impossible to impose in the field or laboratory

Reveal the manner in which large-scale phenomena arise from smaller-scale properties

Discover new materials for green technology applications through first-principles calculations

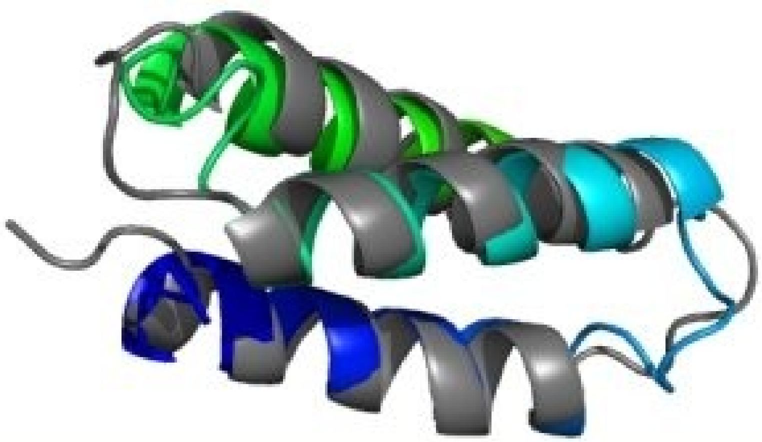


Slide: Horst Simon, Exascale Computing

Research

http://www.fz-juelich.de/ias/jsc/EN/Research/research_node.html

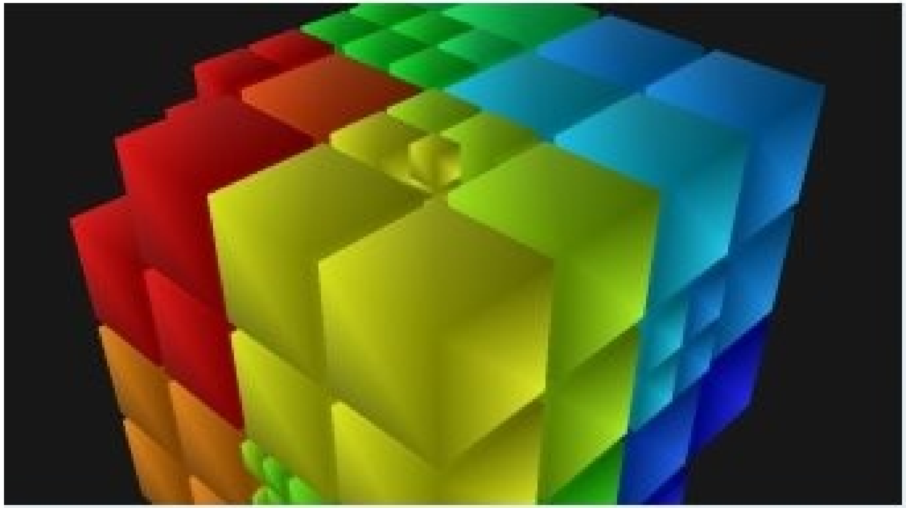
JSC's research and development concentrates on mathematical modelling and numerical, especially parallel algorithms for quantum chemistry, molecular dynamics and Monte-Carlo simulations. The focus in the computer sciences is on cluster computing, performance analysis of parallel programs, visualization, computational steering and grid computing.



Modelling and Simulation

The simulation of complex systems in natural science or engineering depends on the development of adequate mathematical models. Thus the development of realistic and yet efficient models is a core activity at JSC. Examples of simulations are:

- Computational Plasma Physics
- Protein Folding
- Quantum Information Processing
- Civil Security and Traffic



Algorithms and Methods

Efficient simulations need powerful algorithms and methods. JSC focusses on the development of the following methods:

- Fast Coulomb Solvers
- Parallel-In-Time Integration
- Fast Multipole Method
- Parallel I/O

Why Computational Physics? Our view at this lecture...

- Differential Equations (ODE/PDE)– no analytical solution!

  Relation to nonlinear dynamcs, theory of chaos

- Ordinary differential equations (ODE) – initial value problems – particle simulations

  Plasma physics, molekular dynamics, stellar dynamics…

- Ordinary differential equations (ODE) – boundary values problems – *quantum mechanics (time-indep.), statistical mechanics, stationary states*

- Partial differential equations (PDE) – initial and boundary value problems – mesh based or finite elements

fluid dynamics, numerical relativity, quantum mechanics (time-dep.)

- Monte Carlo methods – use of (pseudo) random numbers

numerical integration, stellar dynamics, particle physics (many dims.)

- Computational mathematics – ``exact'' mathematical computations

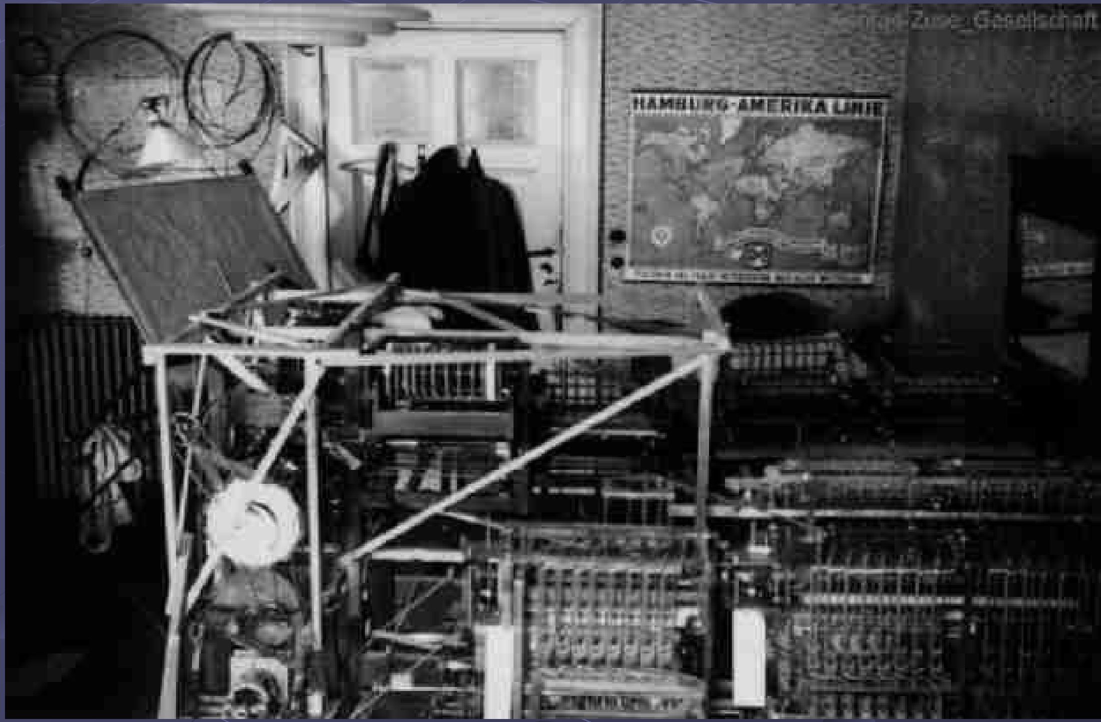
  Mathematica, Maple, MatLab, …

HARDWARE

...before von Neumann...

- Konrad Zuse (1910-1995) Berlin

Invented freely programmable Computer

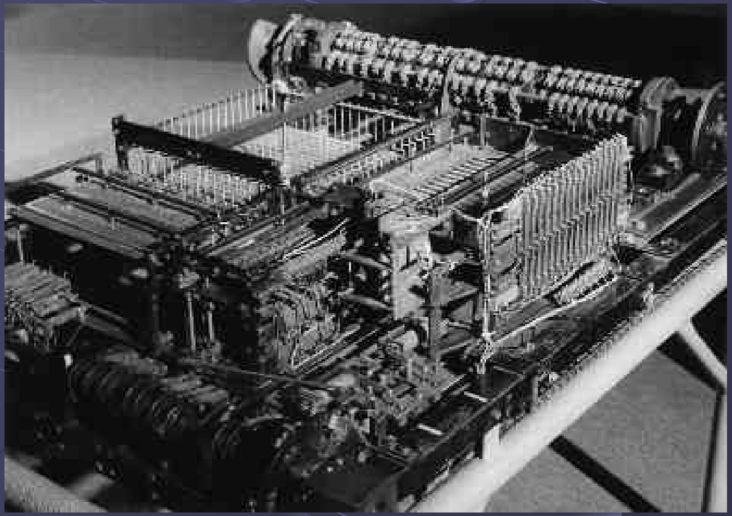


Z1 in parental flat 1936

HARDWARE

Zuse Z4: 1944 Berlin, 1950 Zürich, 1954 Frankreich

1959 Deutsches Museum München



Computing Speed 0.03 MHz

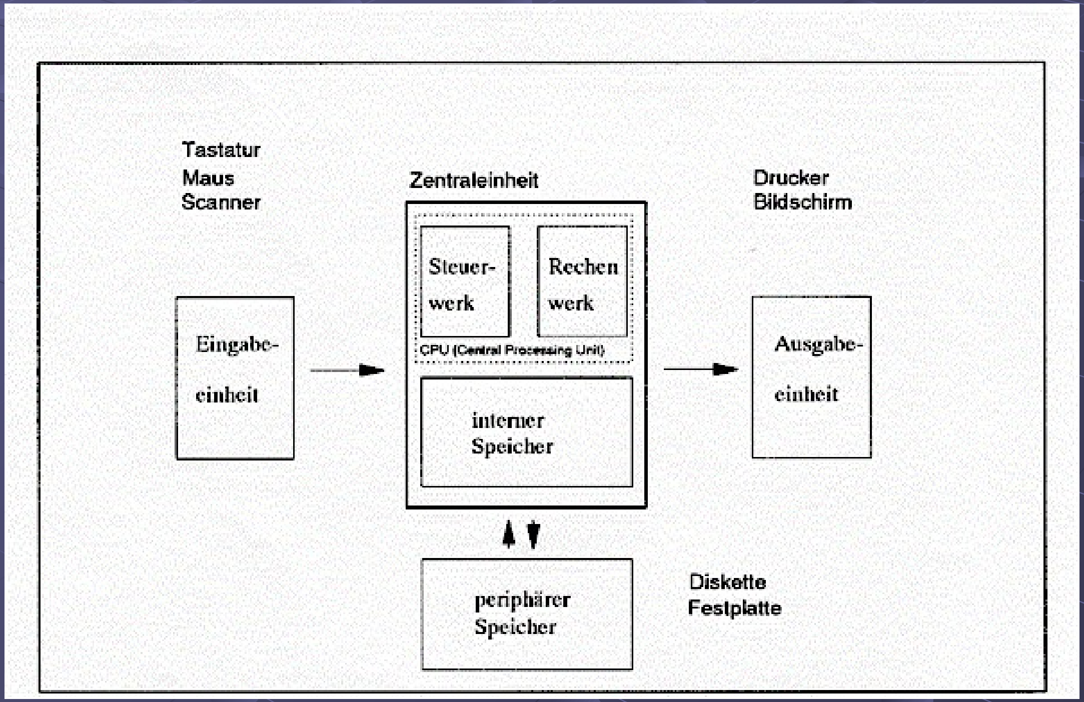
Memory 256 byte

HARDWARE

- John von Neumann (1903-1957)

Born Budapest, Lecturer Berlin, since 1930 Princeton Univ.

Requirements for the Construction of an electronic computing device(1946)



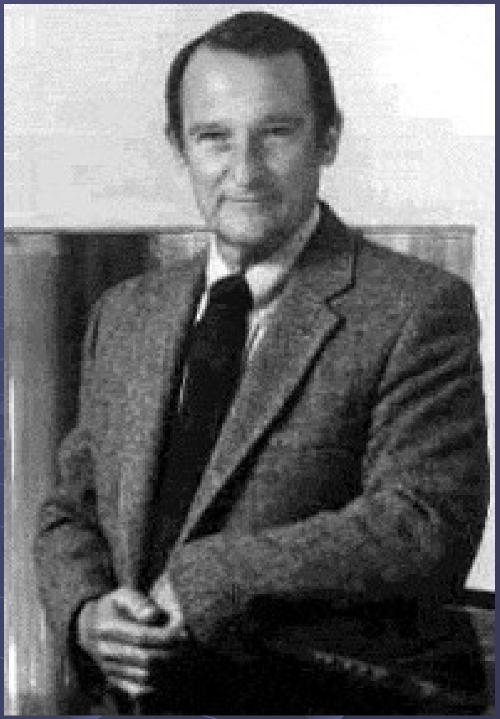
Astronomisches Rechen-Institut (ARI) at Univ. of Heidelberg, Germany

Siemens 2002
Computer in 1964
At ARI

HARDWARE

- ``The father of supercomputing´´

- Seymour Cray (1925-1996)



CRAY1: Vectorregisters (1976)

160 Mflop, 80 MHz, 8 MByte RAM

CRAY2: (1984)

1Gflop, 120MHz, 2GByte RAM

HARDWARE

Supercomputer

JUGENE

IBM Blue Gene

Jülich

Supercomputing

Centre (JSC)

223 Tflop/s

...Petaflop/s...

2019: Exaflop/s System

(...Trillion...)

Opening with J. Rüttgers June 2008

Computational Science...

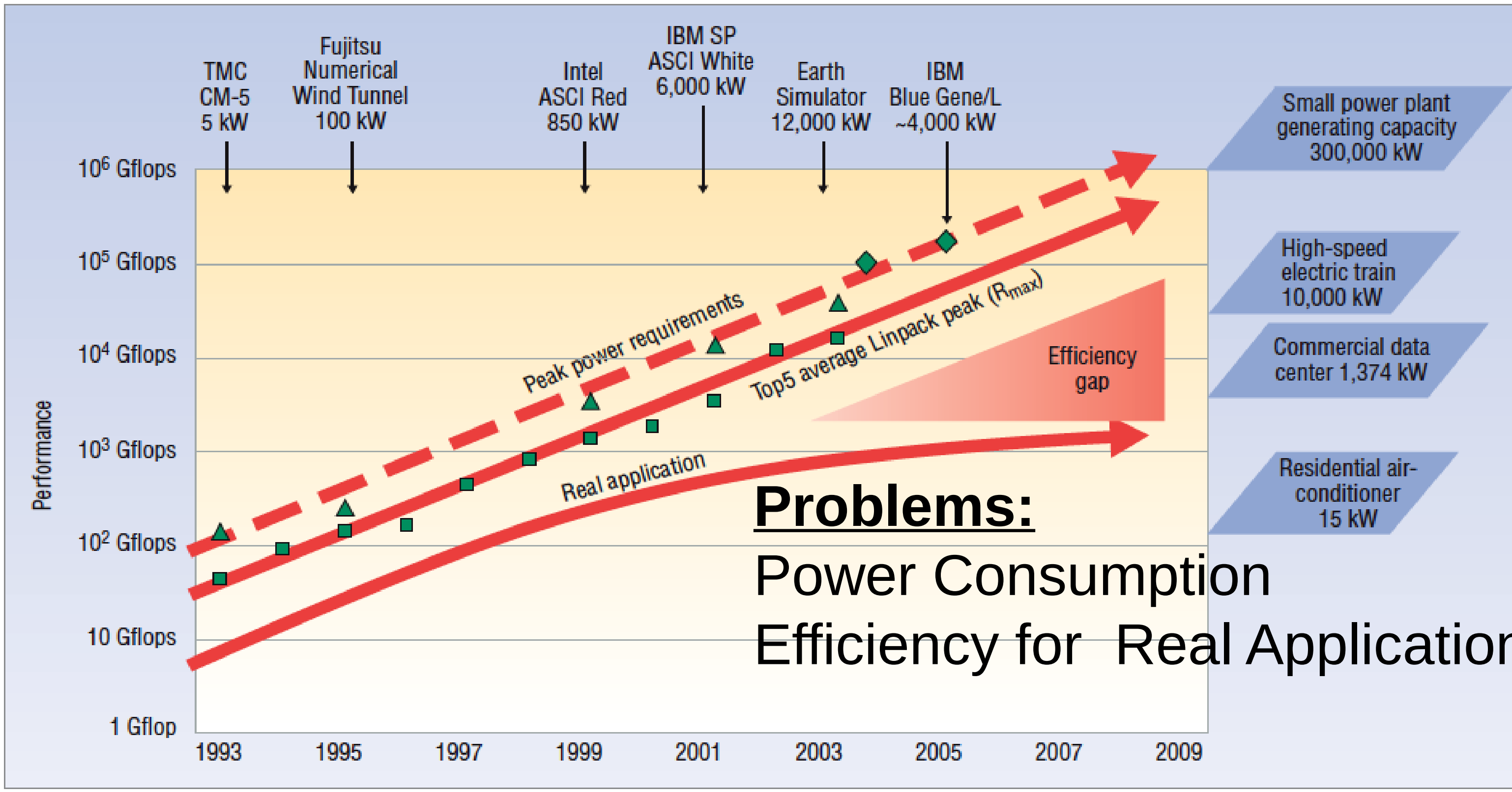
...after von Neumann...

Exaflop/s?

Petaflop/s

Teraflop/s

Gigaflop/s



Problems:

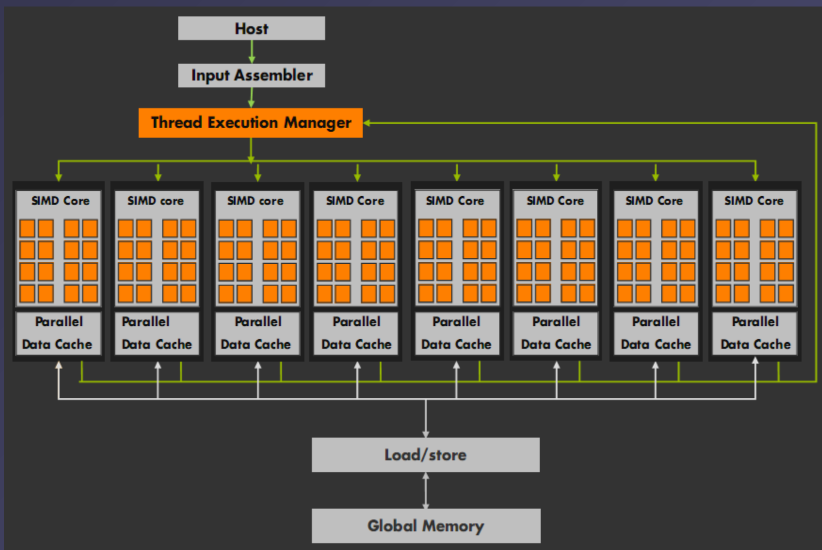
Power Consumption

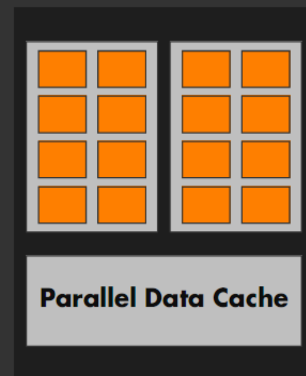
Efficiency for Real Applications

Thanks to Horst Simon, LBNL/NERSC for this diagram.

***Figure 1. Rising power requirements.** Peak power consumption of the top supercomputers has steadily increased over the past 15 years.*

Hardware





Each core

- 8 functional units
- SIMD 16/32 "warp"
- 8-10 stage pipeline
- Thread scheduler
- 128-512 threads/core
- 16 KB shared memory

Total #threads/chip

16 * 512 = 8K

NVIDIA Tesla C1060 :

1.3 GHz *240 processors * 3 flopclock = 930 Gflops

NAOC laohu cluster

Beijing, China

Heidelberg **Kepler GPU cluster.** VolkswagenStiftung

Kepler GPU cluster

12 nodes = 12 x 16 = 192 CPU cores (@ 2 GHz)

12 x 64 GB = 768 GB RAM CPU memory

12 GPUs K20m = 12 x 2496 ~ 30k GPU threads

12 x 4.8 GB ~ 57 GB GPU device memory

4 x Xilinx Virtex-6 FPGA (ML 605)

since beg. 2013 operated.

Nr. 1 Supercomputer from China: 33 Pflop/s Linpack

Tianhe-2 (MilkyWay-2) - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P

http://www.top500.org

32000 Intel Xeon 12 core, 48000 Intel Phi Accelerators 57 Core

Top 10 List November 2010

From www.top500.org - list of fastest supercomputers in the world... ... last year Nov. 2010:

1	National Supercomputing Center in Tianjin China	**Tianhe-1A** - NUDT TH MPP, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C NUDT
2	DOE/SC/Oak Ridge National Laboratory United States	**Jaguar** - Cray XT5-HE Opteron 6-core 2.6 GHz Cray Inc.
3	National Supercomputing Centre in Shenzhen (NSCS) China	**Nebulae** - Dawning TC3600 Blade, Intel X5650, NVidia Tesla C2050 GPU Dawning
4	GSIC Center, Tokyo Institute of Technology Japan	**TSUBAME 2.0** - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows NEC/HP
5	DOE/SC/LBNL/NERSC United States	**Hopper** - Cray XE6 12-core 2.1 GHz Cray Inc.
6	Commissariat a l'Energie Atomique (CEA) France	**Tera-100** - Bull bullx super-node S6010/S6030 Bull SA
7	DOE/NNSA/LANL United States	**Roadrunner** - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband IBM
8	National Institute for Computational Sciences/University of Tennessee United States	**Kraken XT5** - Cray XT5-HE Opteron 6-core 2.6 GHz Cray Inc.
9	Forschungszentrum Juelich (FZJ) Germany	**JUGENE** - Blue Gene/P Solution IBM
10	DOE/NNSA/LANL/SNL United States	**Cielo** - Cray XE6 8-core 2.4 GHz Cray Inc.

GPU (rows 1, 3, 4)

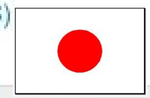
FR (row 6)

China Grabs Supercomputing Leadership Spot in Latest Ranking of World's Top 500 Supercomputers

Thu, 2010-11-11 22:42

MANNHEIM, Germany; BERKELEY, Calif.; and KNOXVILLE, Tenn.—The 36th edition of the closely watched TOP500 list of the world's most powerful supercomputers confirms the rumored takeover of the top spot by the Chinese Tianhe-1A system at the National Supercomputer Center in Tianjin, achieving a performance level of 2.57 petaflop/s (quadrillions of calculations per second).

Top 10 List June 2014

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National University of Defense Technology China 	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT ***Xeonϕ***	3120000	33862.7	54902.4	17808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc. ***GPU***	560640	17590.0	27112.5	8209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1572864	17173.2	20132.7	7890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan 	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705024	10510.0	11280.4	12660
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786432	8586.6	10066.3	3945
6	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell ***Xeonϕ***	462462	5168.1	8520.1	4510
7	Forschungszentrum Juelich (FZJ) Germany 	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458752	5008.9	5872.0	2301
8	DOE/NNSA/LLNL United States	**Vulcan** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	393216	4293.3	5033.2	1972
9	Leibniz Rechenzentrum Germany 	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR	147456	2897.0	3185.1	3423

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	**4,503.17**	GSIC Center, Tokyo Institute of Technology	TSUBAME-KFC - LX 1U-4GPU/104Re-1G Cluster, Intel Xeon E5-2620v2 6C 2.100GHz, Infiniband FDR, NVIDIA K20x	27.78
2	**3,631.86**	Cambridge University	Wilkes - Dell T620 Cluster, Intel Xeon E5-2630v2 6C 2.600GHz, Infiniband FDR, NVIDIA K20	52.62
3	**3,517.84**	Center for Computational Sciences, University of Tsukuba	HA-PACS TCA - Cray 3623G4-SM Cluster, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband QDR, NVIDIA K20x	78.77
4	**3,185.91**	Swiss National Supercomputing Centre (CSCS)	Piz Daint - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Level 3 measurement data available	1,753.66
5	**3,130.95**	ROMEO HPC Center - Champagne-Ardenne	romeo - Bull R421-E3 Cluster, Intel Xeon E5-2650v2 8C 2.600GHz, Infiniband FDR, NVIDIA K20x	81.41
6	**3,068.71**	GSIC Center, Tokyo Institute of Technology	TSUBAME 2.5 - Cluster Platform SL390s G7, Xeon X5670 6C 2.930GHz, Infiniband QDR, NVIDIA K20x	922.54
7	**2,702.16**	University of Arizona	iDataPlex DX360M4, Intel Xeon E5-2650v2 8C 2.600GHz, Infiniband FDR14, NVIDIA K20x	53.62
8	**2,629.10**	Max-Planck-Gesellschaft MPI/IPP	iDataPlex DX360M4, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband, NVIDIA K20x	269.94
9	**2,629.10**	Financial Institution	iDataPlex DX360M4, Intel Xeon E5-2680v2 10C 2.800GHz, Infiniband, NVIDIA K20x	55.62
10	**2,358.69**	CSIRO	CSIRO GPU Cluster - Nitro G16 3GPU, Xeon E5-2650 8C 2.000GHz, Infiniband FDR, Nvidia K20m	71.01

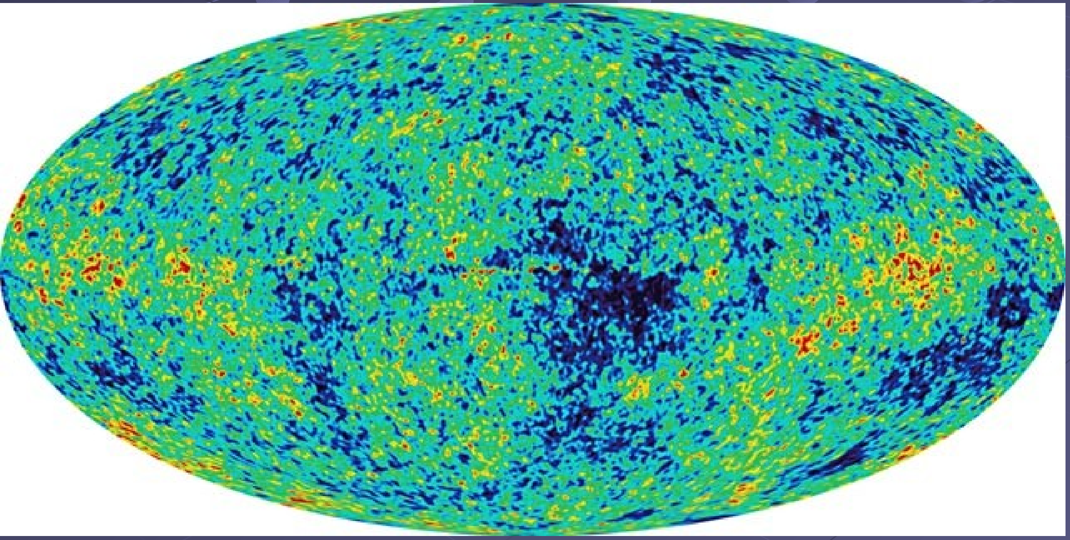
Computer Physics - Astrophysics

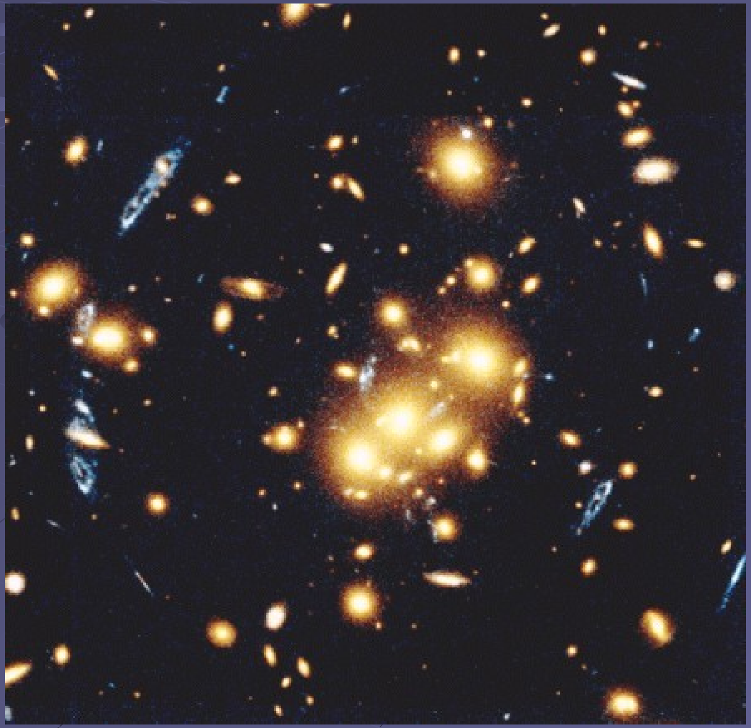
Cosmology

Computer Physics – Astrophysics

- Structure Formation in the Universe

In the year 100.000....

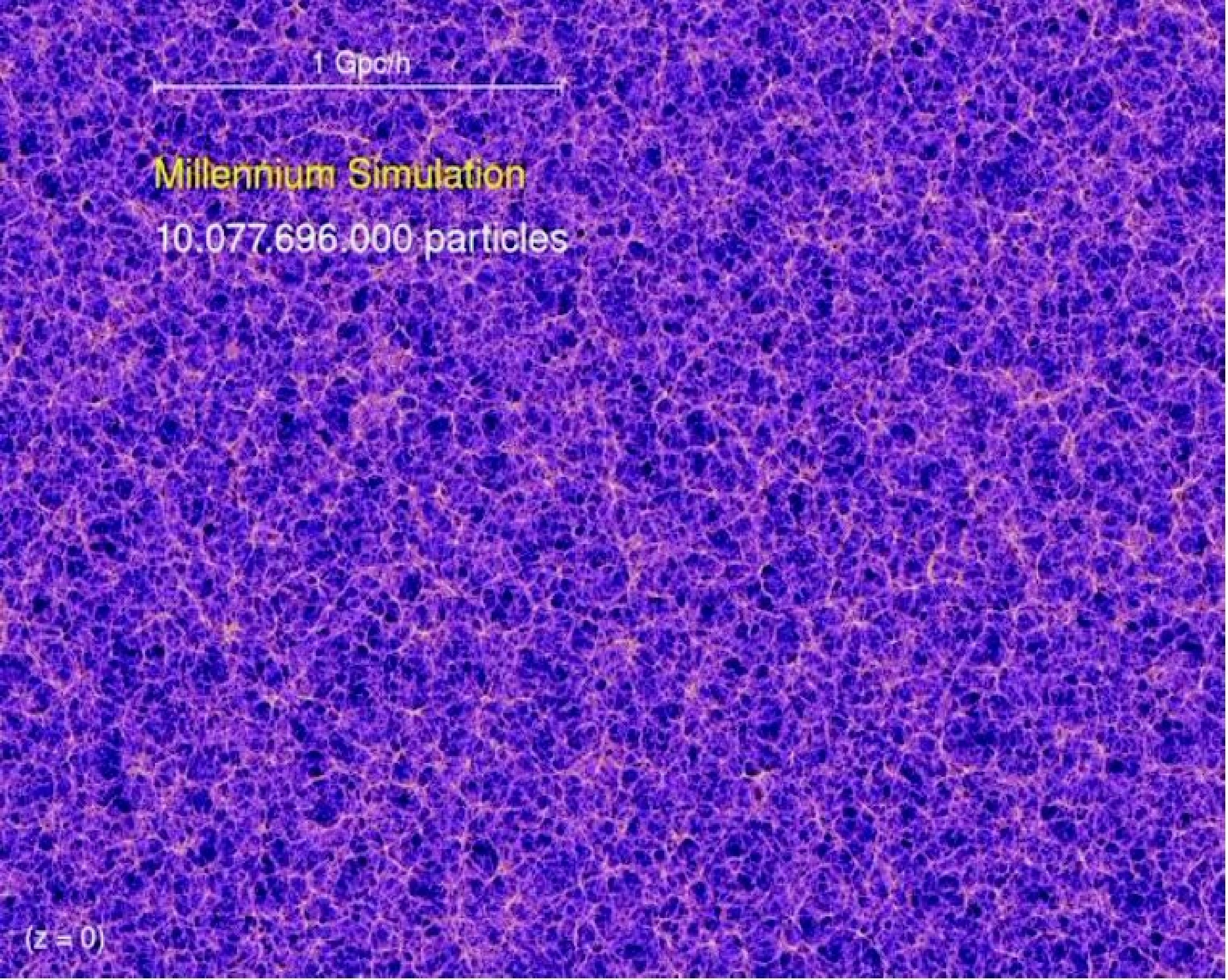




- Wilkinson Microwave Anisotropy Probe (WMAP)

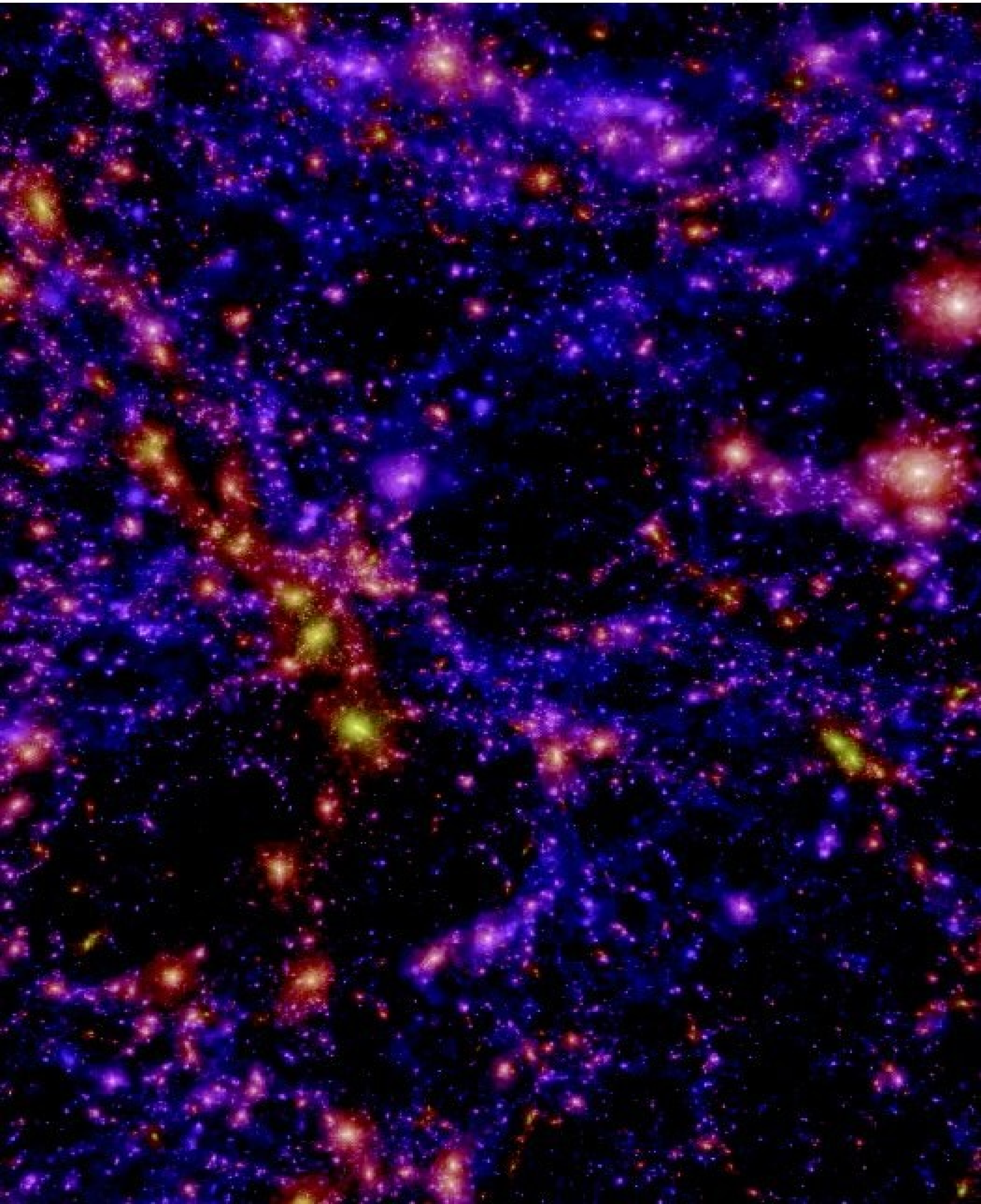
(Cosmic Microwave Background)

...and ``today´´



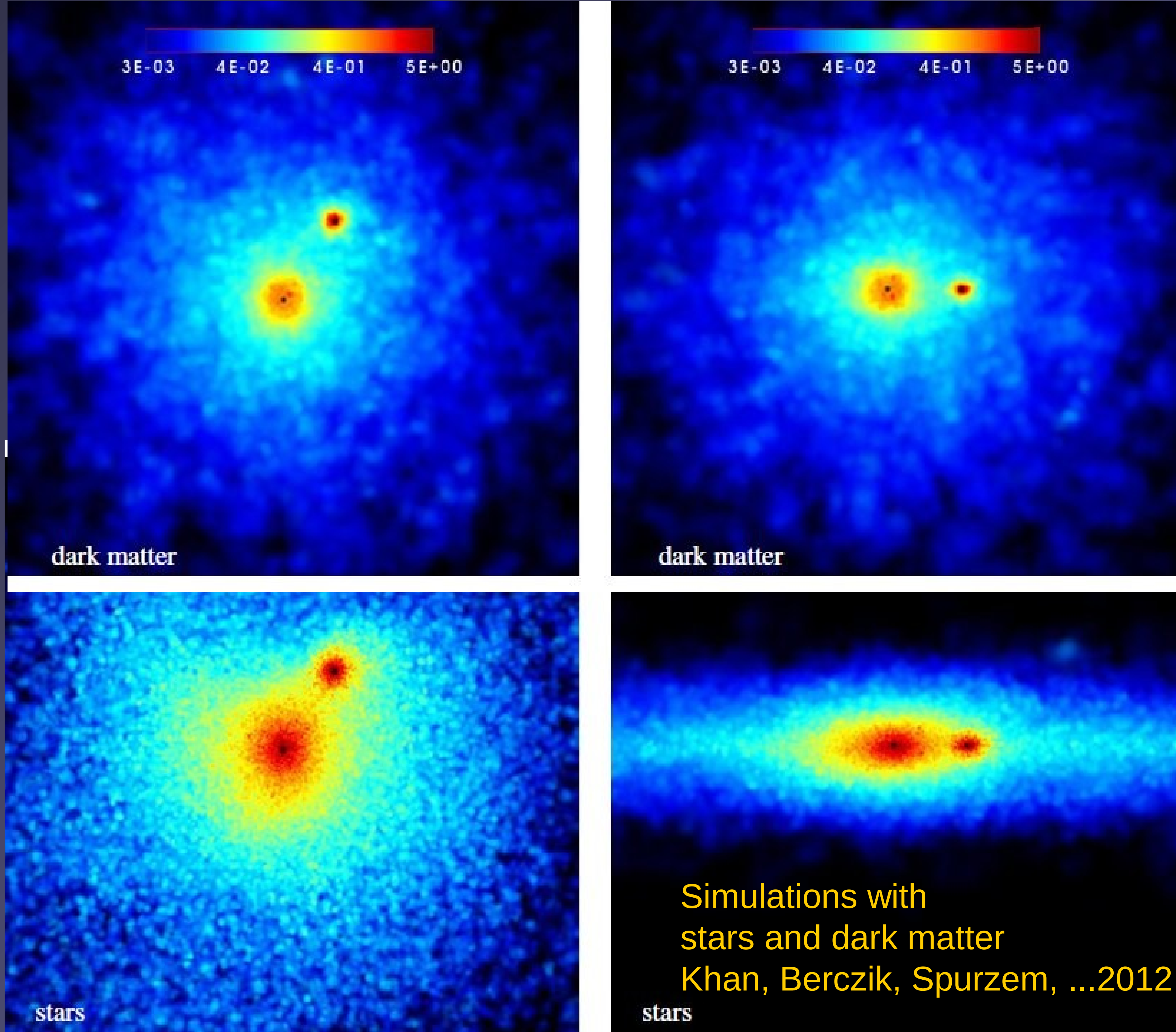
Millenium Simulaiton (Springel et al.)

Millenium Simulaiton (Springel et al.)



Computer Physics - Astrophysics

Black Holes in Galaxies



Simulations with
stars and dark matter
Khan, Berczik, Spurzem, ...2012

Post-Newtonian Dynamics Gravitational Wave Templates

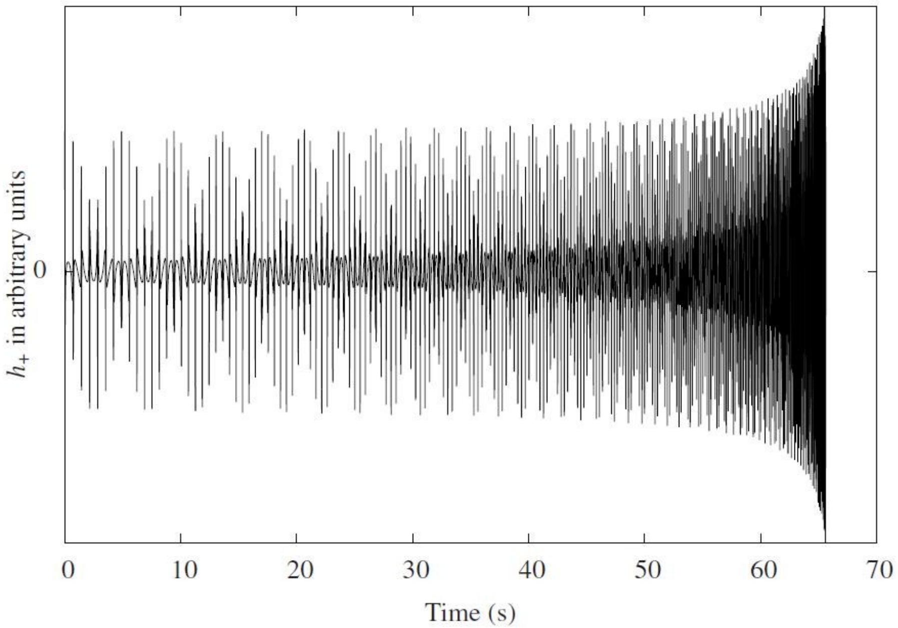


Figure 3.11: Waveform for two equal mass objects on a an orbit with $e = 0.5$.

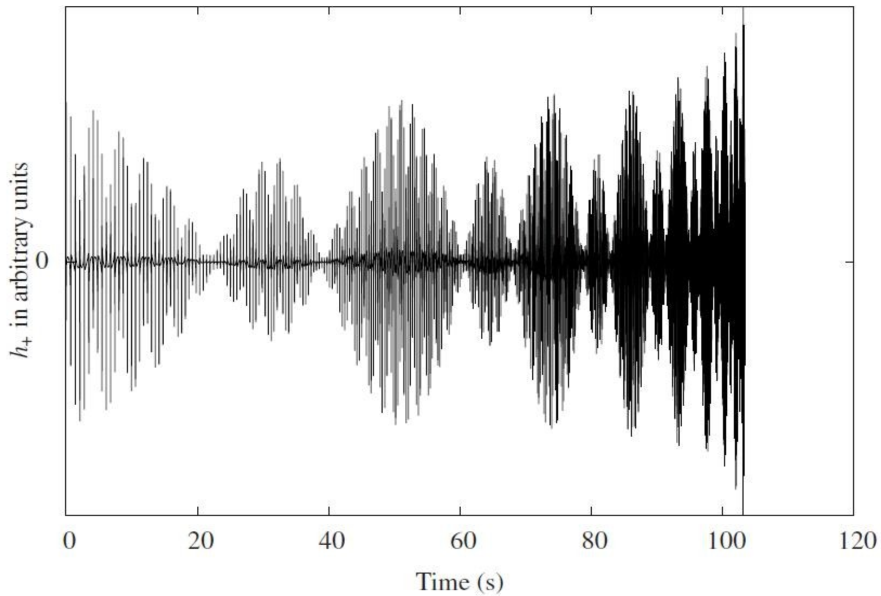


Figure 3.12: Waveform for two objects with a mass ratio of $q = 1/10$ on an orbit with $e = 0.5$ and spins $a_{1,x} = 1.0$, $a_{2,y} = 1.0$.

Handle spin-orbit and spin-spin coupling
(P.Brem, R. Spurzem, Univ. Heidelberg)

Example: VIRGO Detector in Cascina near Pisa, Italy

VIRGO – Pisa 3km
LIGO – Livingston, LA
Hanford, WA
1km
GEO600 – Hannover
600m
AIGO – Australien
(planned, 5 km)

http://www.ligo-la.caltech.edu/
http://www.ego-gw.it
http://www.geo600.uni-hannover.de

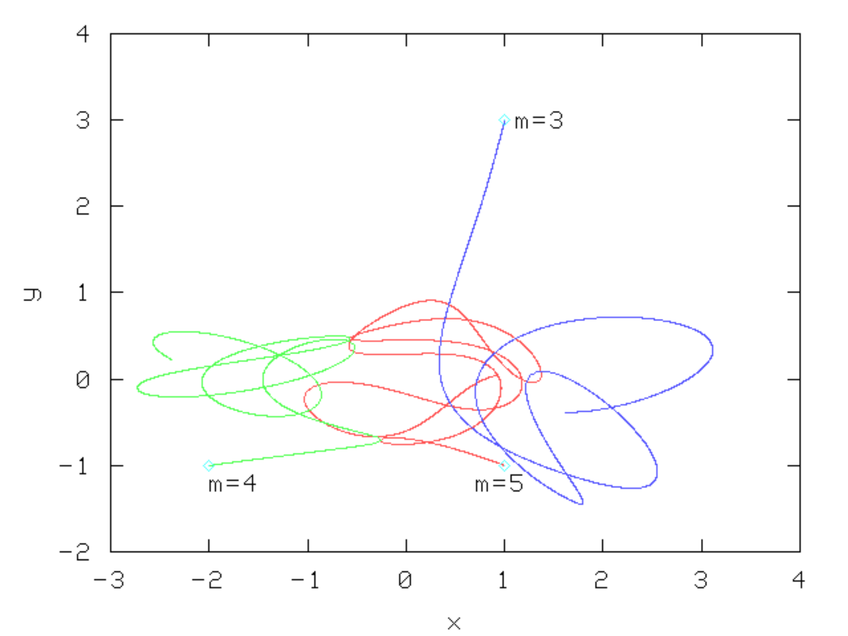
Outreach to 50 Millionen light years (Neutron Stars)

Computer Physics - Astrophysics

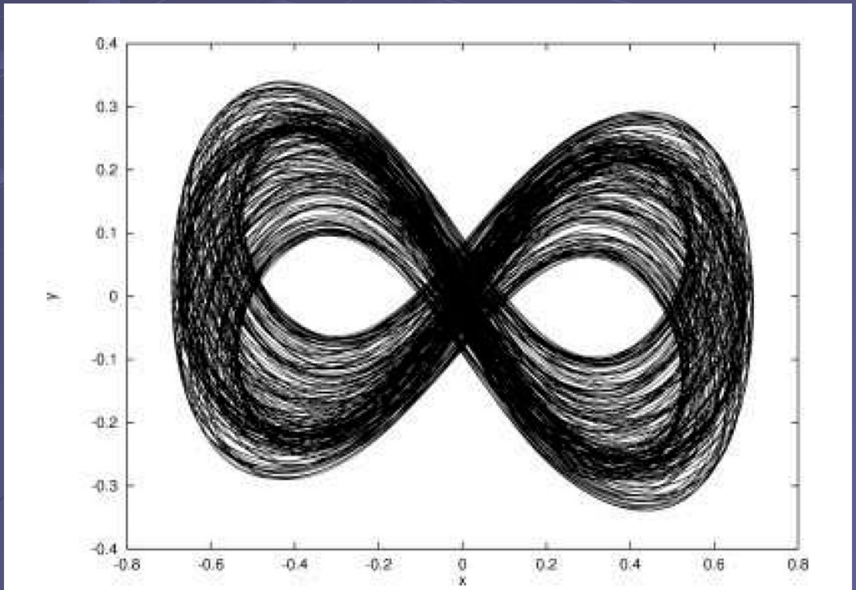
Nonlinear Dynamics and Chaos

3-Body Problems

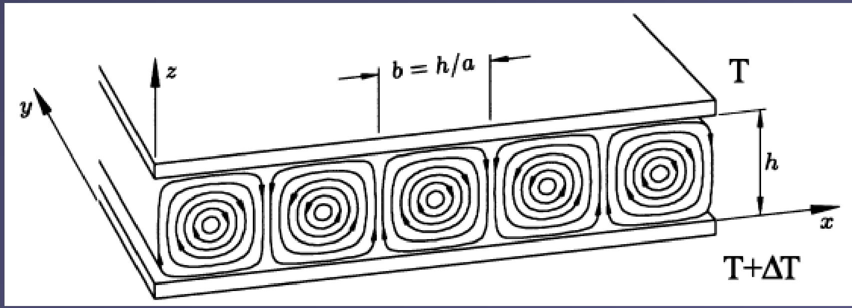
Burrau's Problem

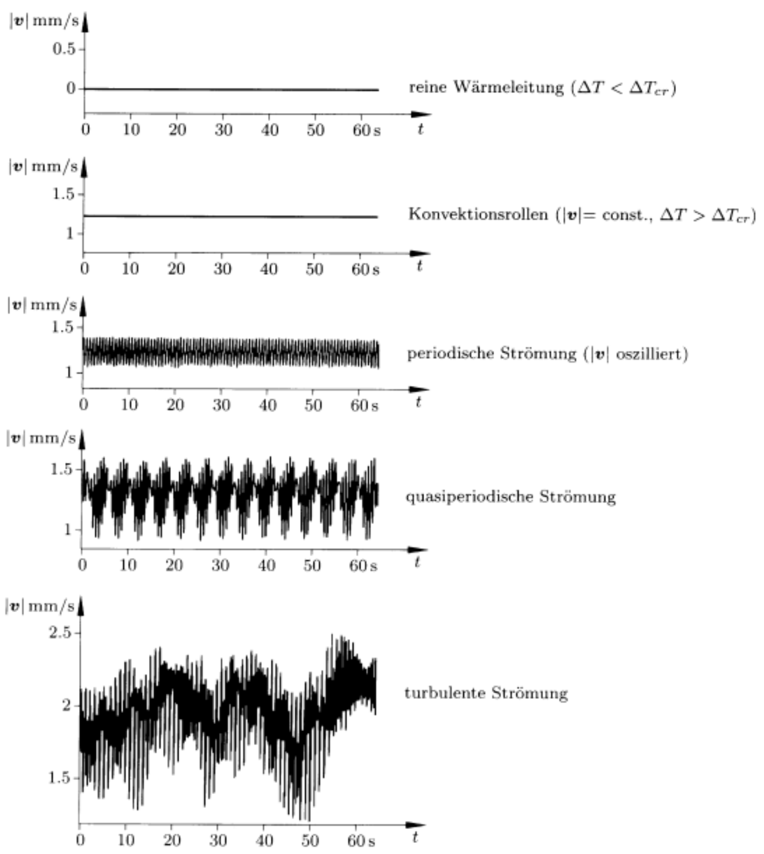


„The Eight“

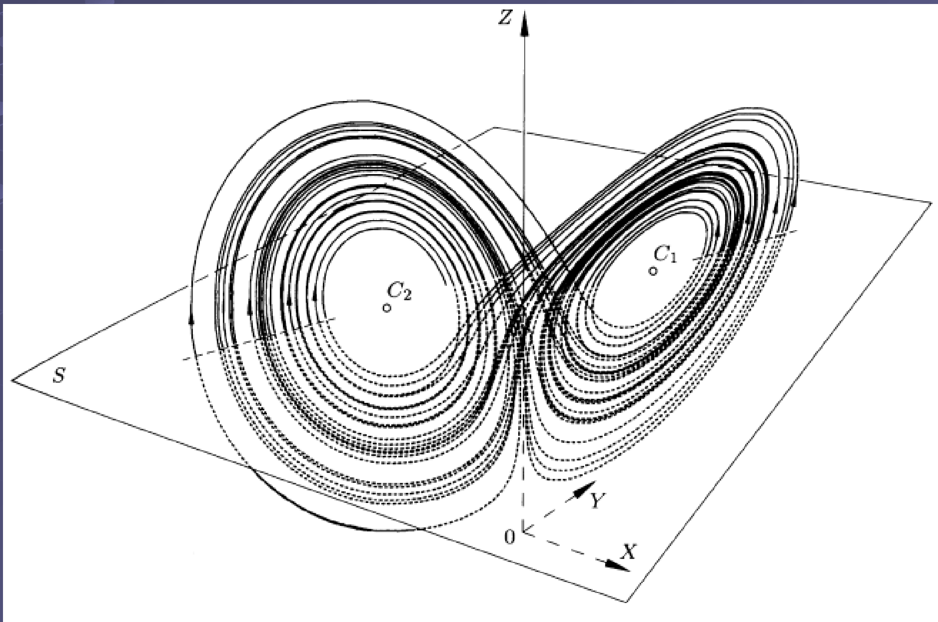


Lorenz-Attraktor





Fünf unterschiedliche Strömungszustände des Bénard-Experiments bei steigender Temperaturdifferenz ΔT (nach Graham, 1982)



Lorenz-Attraktor für $r = 28, \sigma = 10$ und $b = 8/3$.
Der Trajektorienbereich, den die Ebene $Z = r - 1 = 27$ verdeckt, ist punktiert (Lanford, 1977)

Logistische Abbildung