Computational Physics

Computerphysik

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Computer Physics

- Traditional:

Theory **Experiment/Observation**

- Modern:

Theory

Experiment

Observation

Computer-Experiment

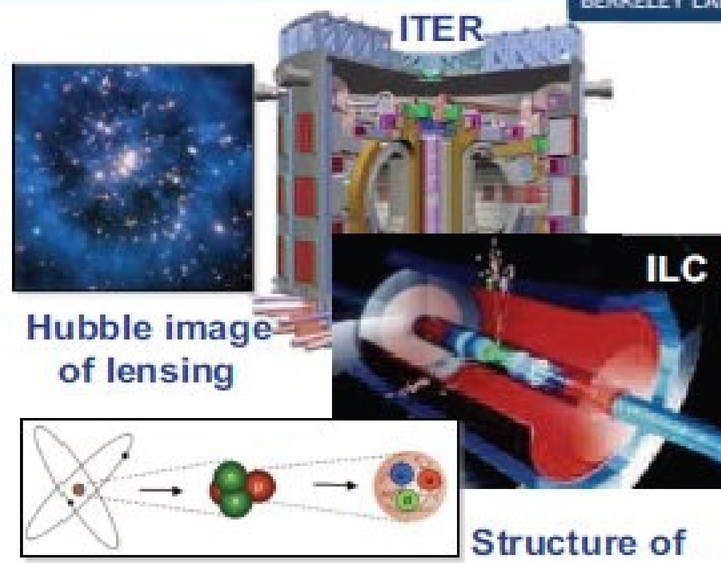
Checking Theories!

Predict Experiments/Observations!

Exascale simulation will enable fundamental advances in basic science

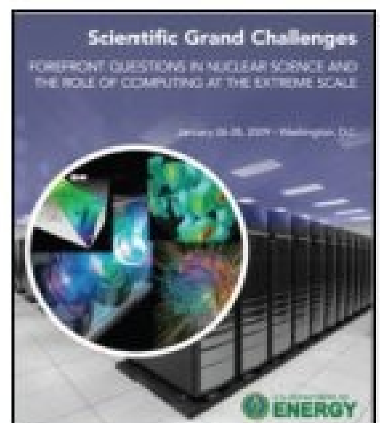
- High Energy & Nuclear Physics
  - Dark-energy and dark matter
  - Fundamentals of fission fusion reactions
- Facility and experimental design
  - Effective design of accelerators
  - Probes of dark energy and dark matter
  - ITER shot planning and device control
- Materials / Chemistry
  - Predictive 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

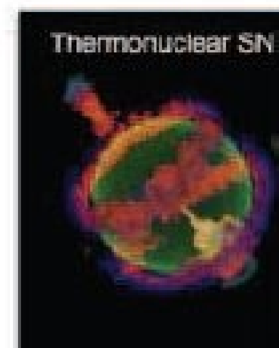
These breakthrough scientific discoveries and facilities require exascale applications and resources



Hubble image of lensing

Structure of nucleons





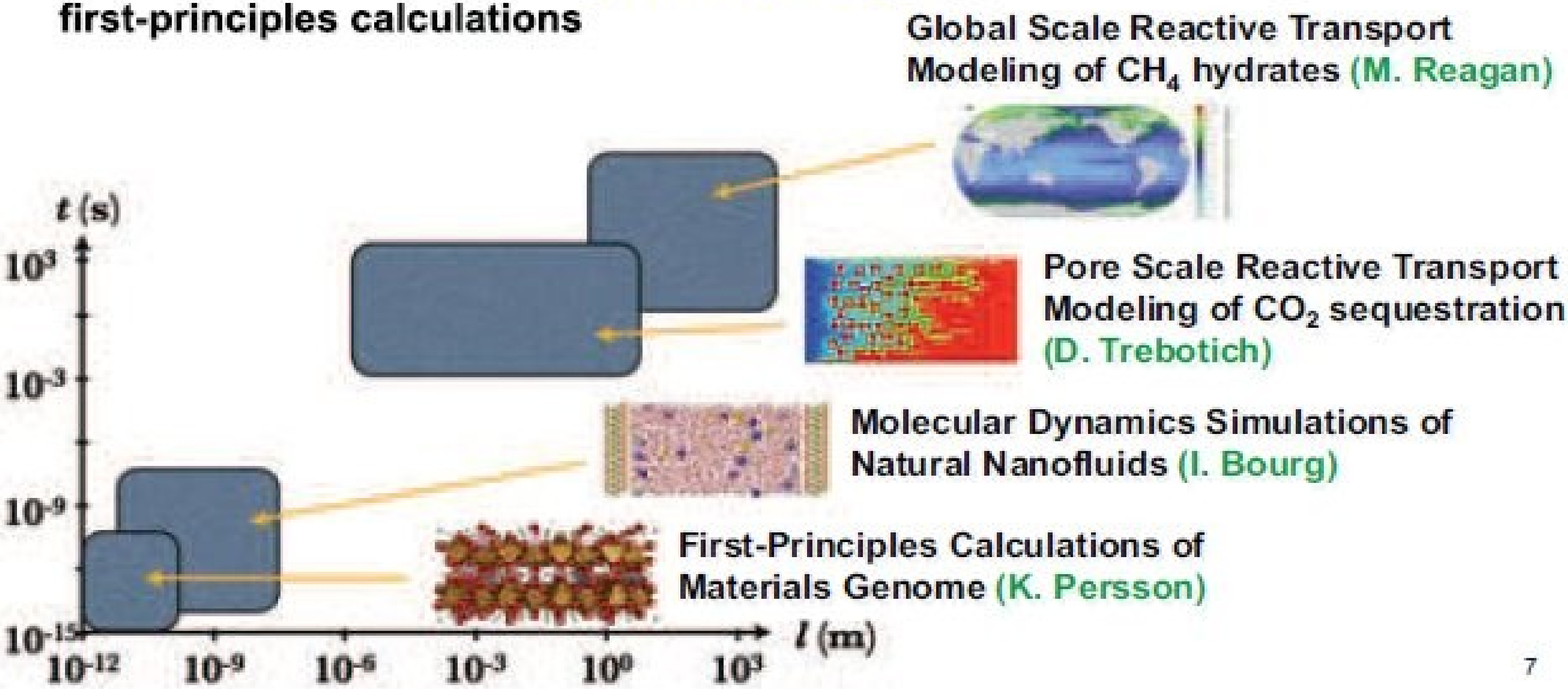
Slide: Horst Simon, Exascale Computing

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

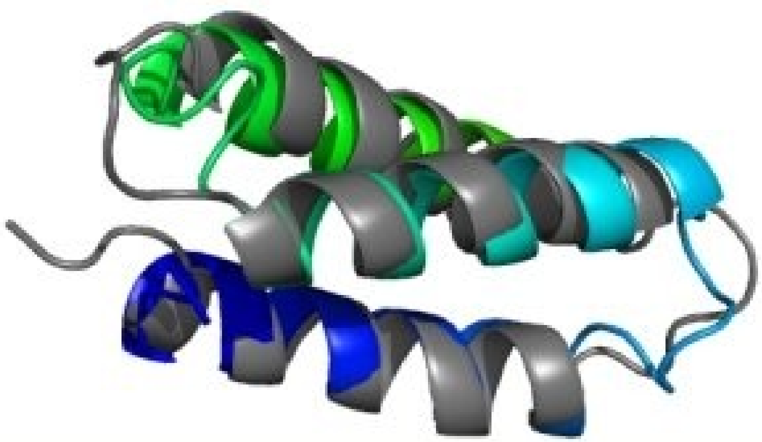
Discover new materials for green technology applications through first-principles calculations



Slide: Horst Simon, Exascale Computing

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

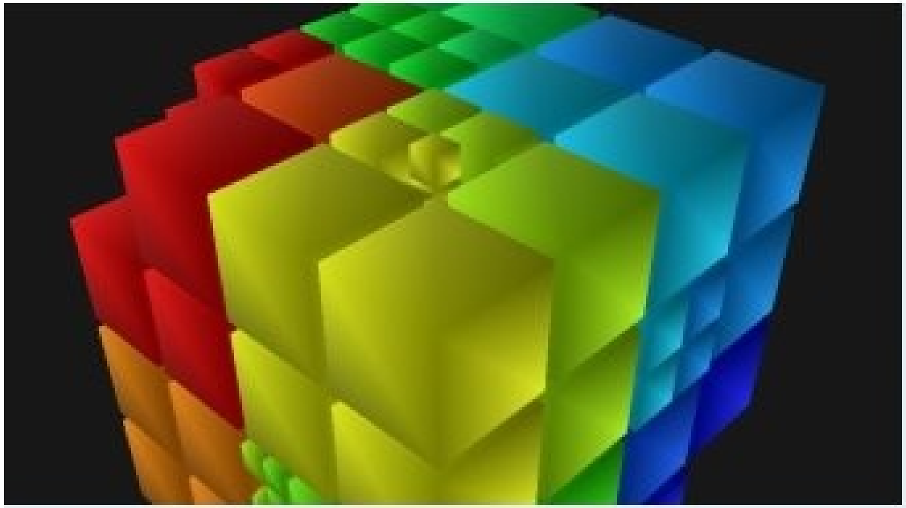
JSC's research and development concentrates on mathematical modelling and numerical, especially parallel algorithms for quantum chemistry, molecular dynamics and Monte-Carlo simulations. The focus in the computer sciences is on cluster computing, performance analysis of parallel programs, visualization,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

History

- Erik Holmberg (1908-2000)

Dissertation Univ. Lund (Sweden) (1937):
``A study of double and multiple galaxies´´
Galaxies distributed in groups and pairs –
Satellite galaxies have uneven distribution
(Holmberg-Effect)

- **Father of numerical Astrophysics....**
  - **...with 200 light bulbs**

History

- The Astrophysical Journal, Nov. 1941

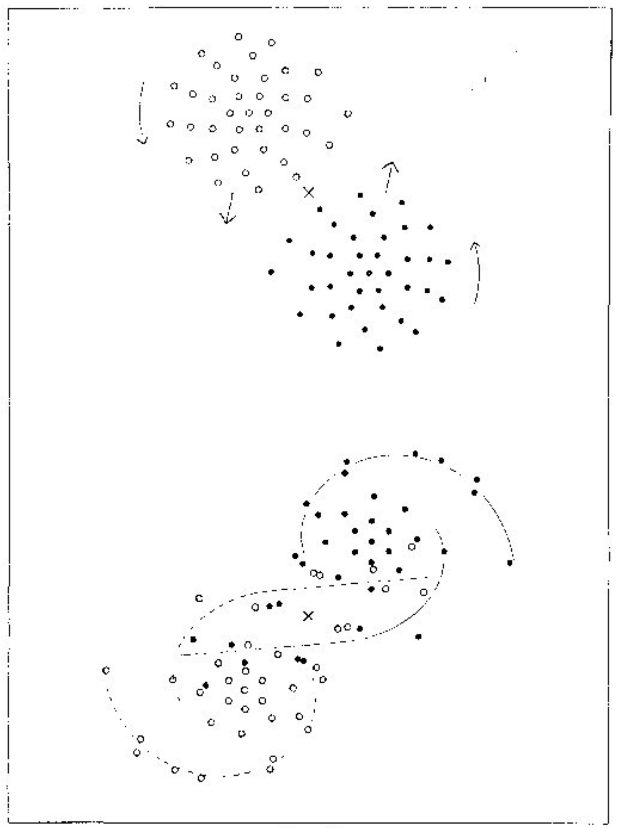


FIG. 4b

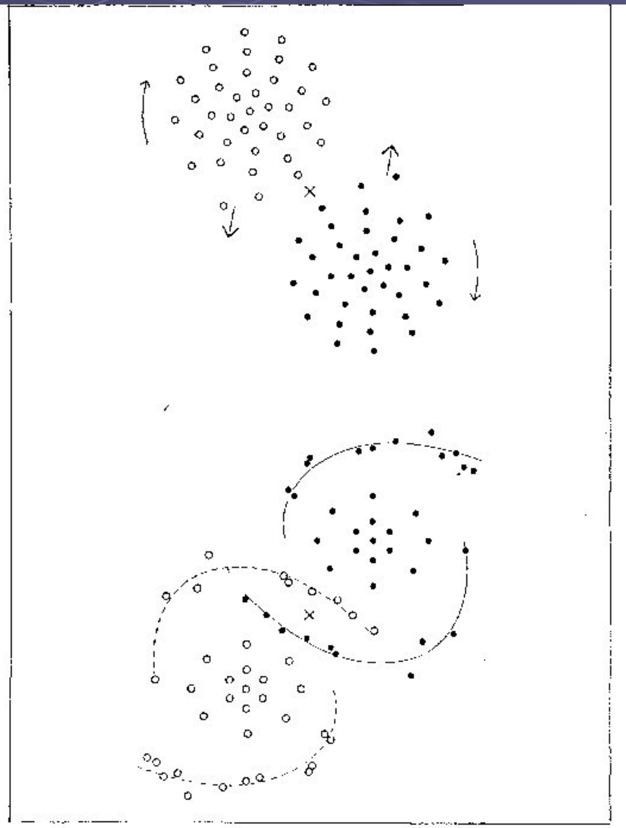


FIG. 4a

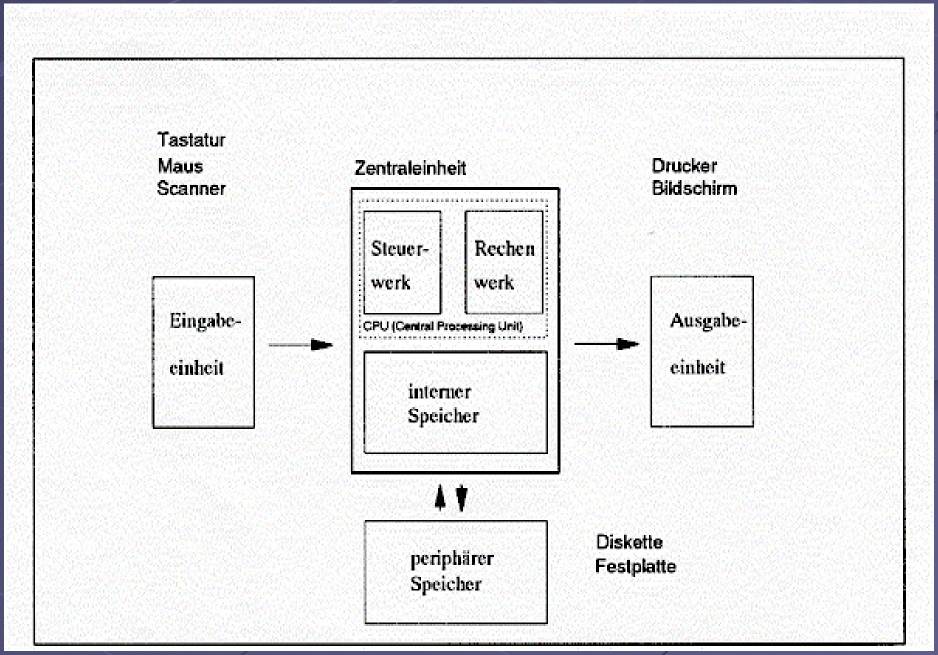
Geschichte

- John von Neumann (1903-1957)

Geb. Budapest, Dozent Berlin,

ab 1930 Princeton Univ. NJ USA Princeton

„Requirements for an electronic computing machine“ (1946)



Introduction – Supercomputers

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...

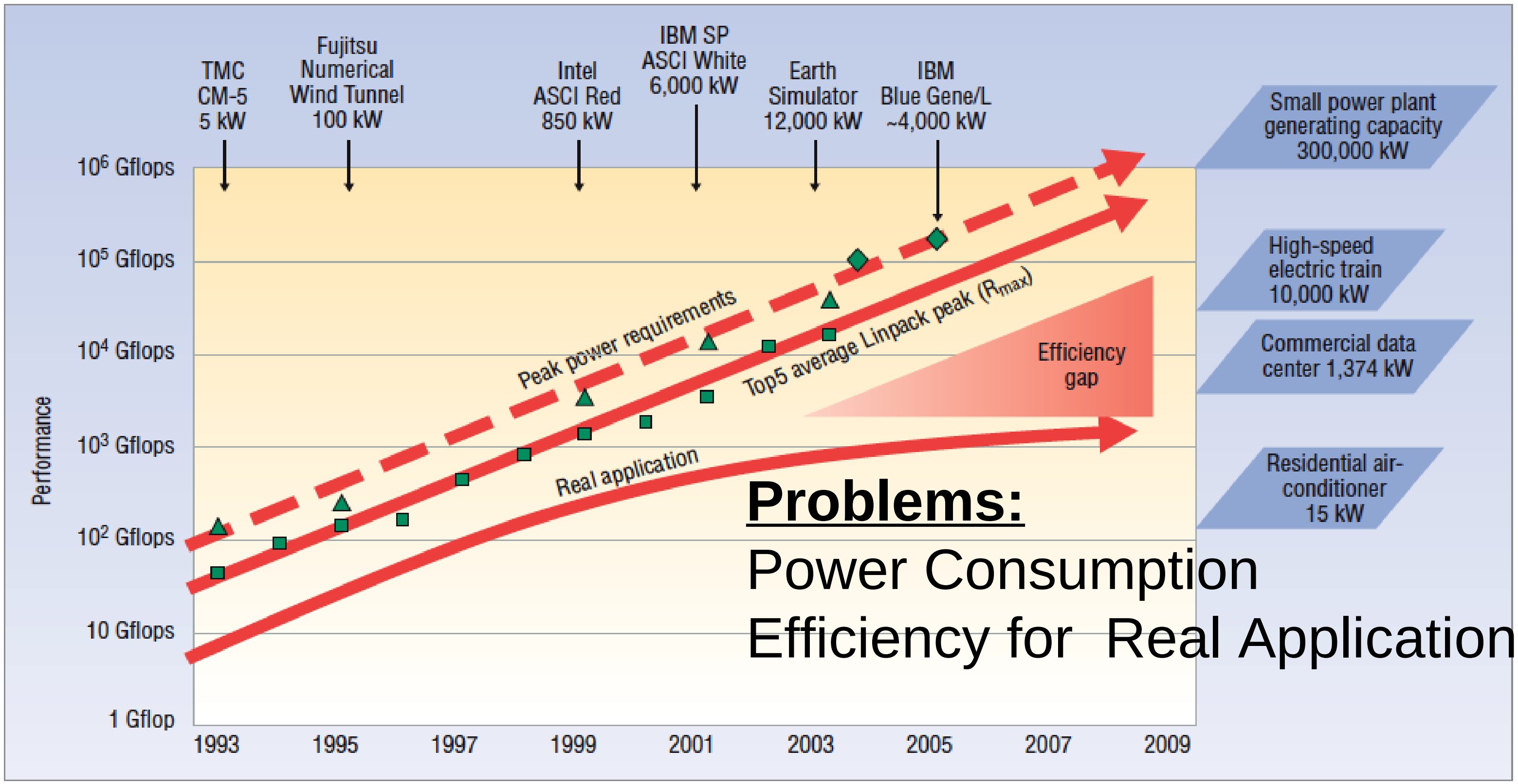
...after von Neumann...

Exaflop/s?

Petaflop/s

Teraflop/s

Gigaflop/s



Problems:

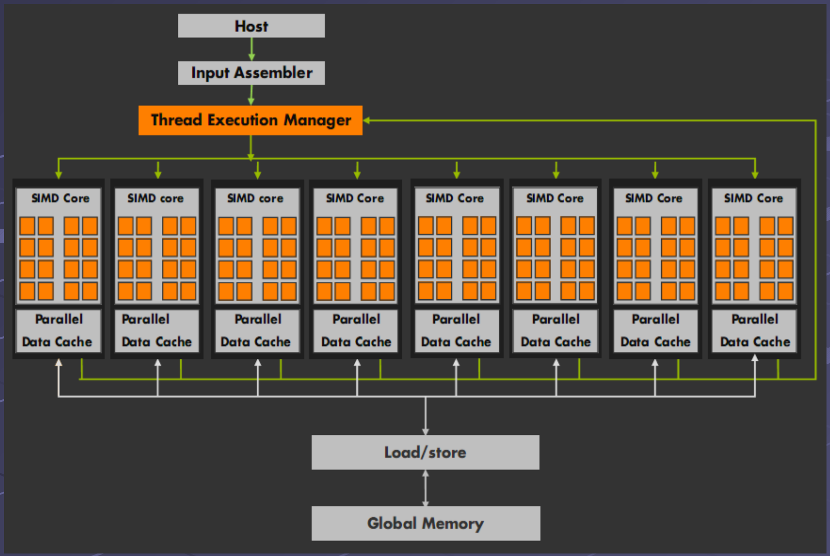
Power Consumption

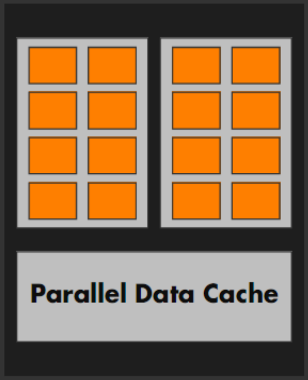
Efficiency for Real Applications

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:

Rank	Site	Country	System	Vendor	
1	National Supercomputing Center in Tianjin	China	**Tianhe-1A** - NUDT TH MPP, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C	NUDT	***GPU***
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	***GPU***
4	GSIC Center, Tokyo Institute of Technology	Japan	**TSUBAME 2.0** - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows	NEC/HP	***GPU***
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	FR
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.	

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

Thu, 2010-11-11 22:42

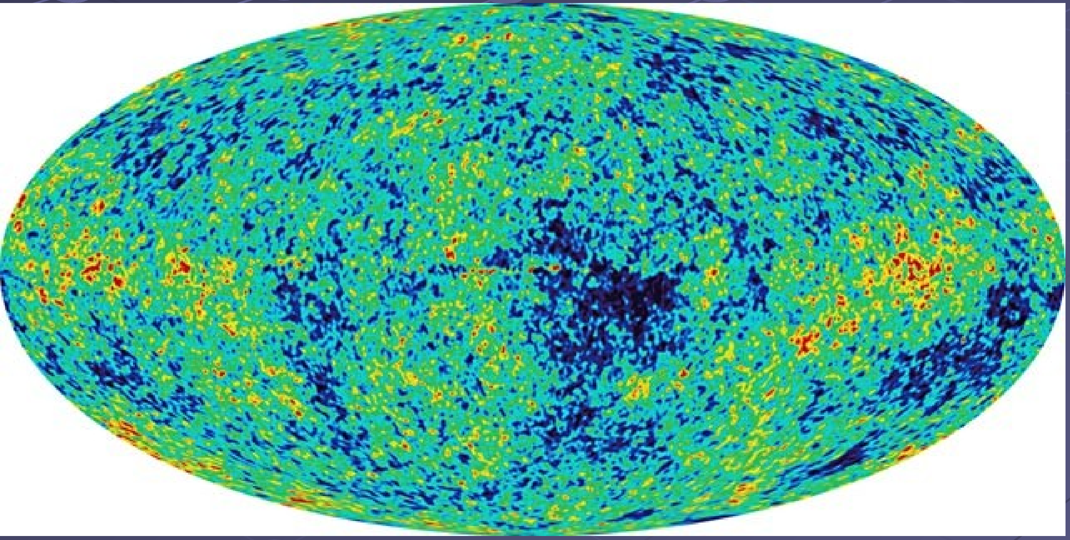
MANNHEIM, Germany; BERKELEY, Calif.; and KNOXVILLE, Tenn.—The 36th edition of the closely watched TOP500 list of the world's most powerful supercomputers confirms the rumored takeover of the top spot by the Chinese Tianhe-1A system at the National Supercomputer Center in Tianjin, achieving a performance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

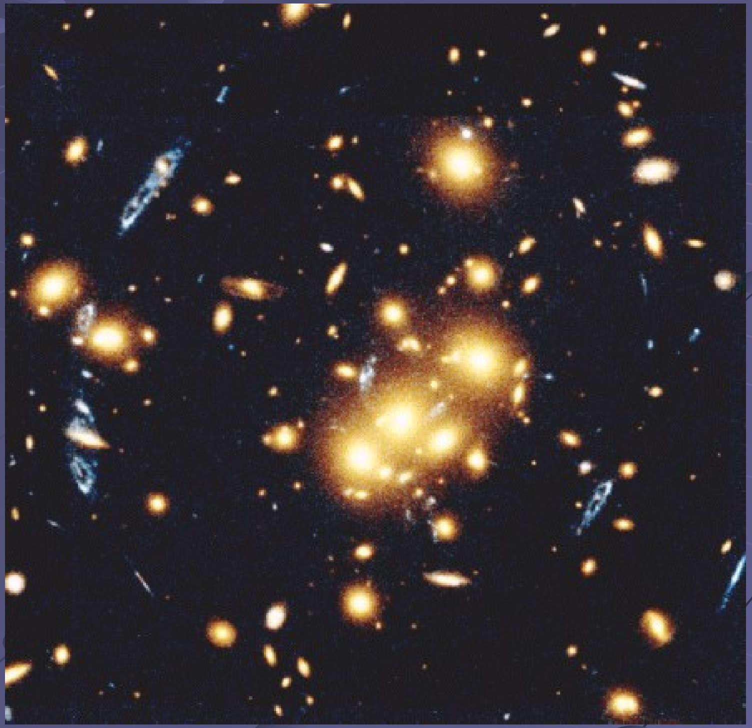
Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	4,503.17	GSIC Center, Tokyo Institute of Technology	TSUBAME-KFC - LX 1U-4GPU/104Re-1G Cluster, Intel Xeon E5-2620v2 6C 2.100GHz, Infiniband FDR, NVIDIA K20x	27.78
2	3,631.86	Cambridge University	Wilkes - Dell T620 Cluster, Intel Xeon E5-2630v2 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

Cosmology

- Structurr Formation in the Universe

In the year 100.000....

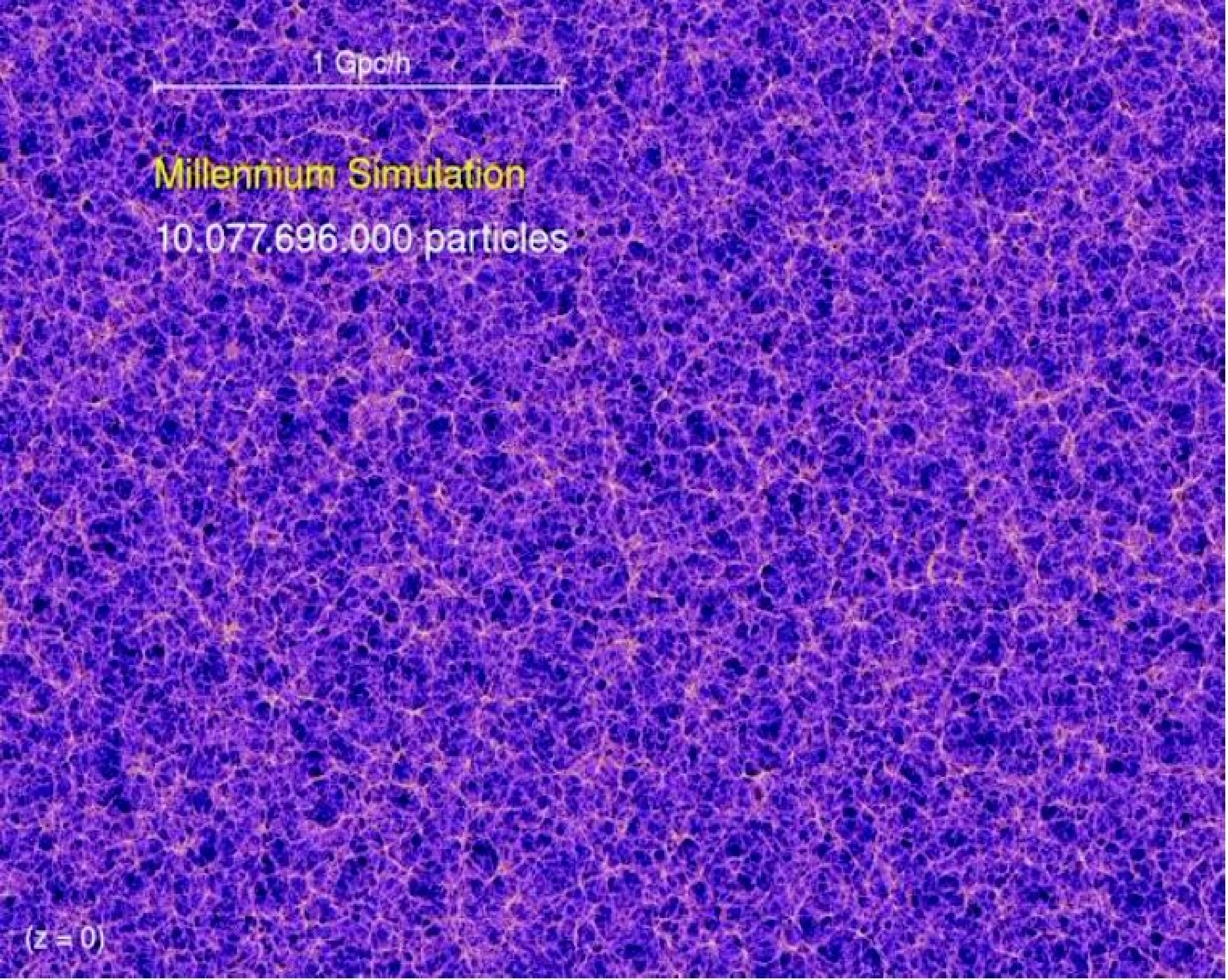




- Wilkinson Microwave Anisotropy Probe (WMAP)

(Cosmic Microwave Background)

...and ``today´´



Millenium Simulaiton (Springel et al.)

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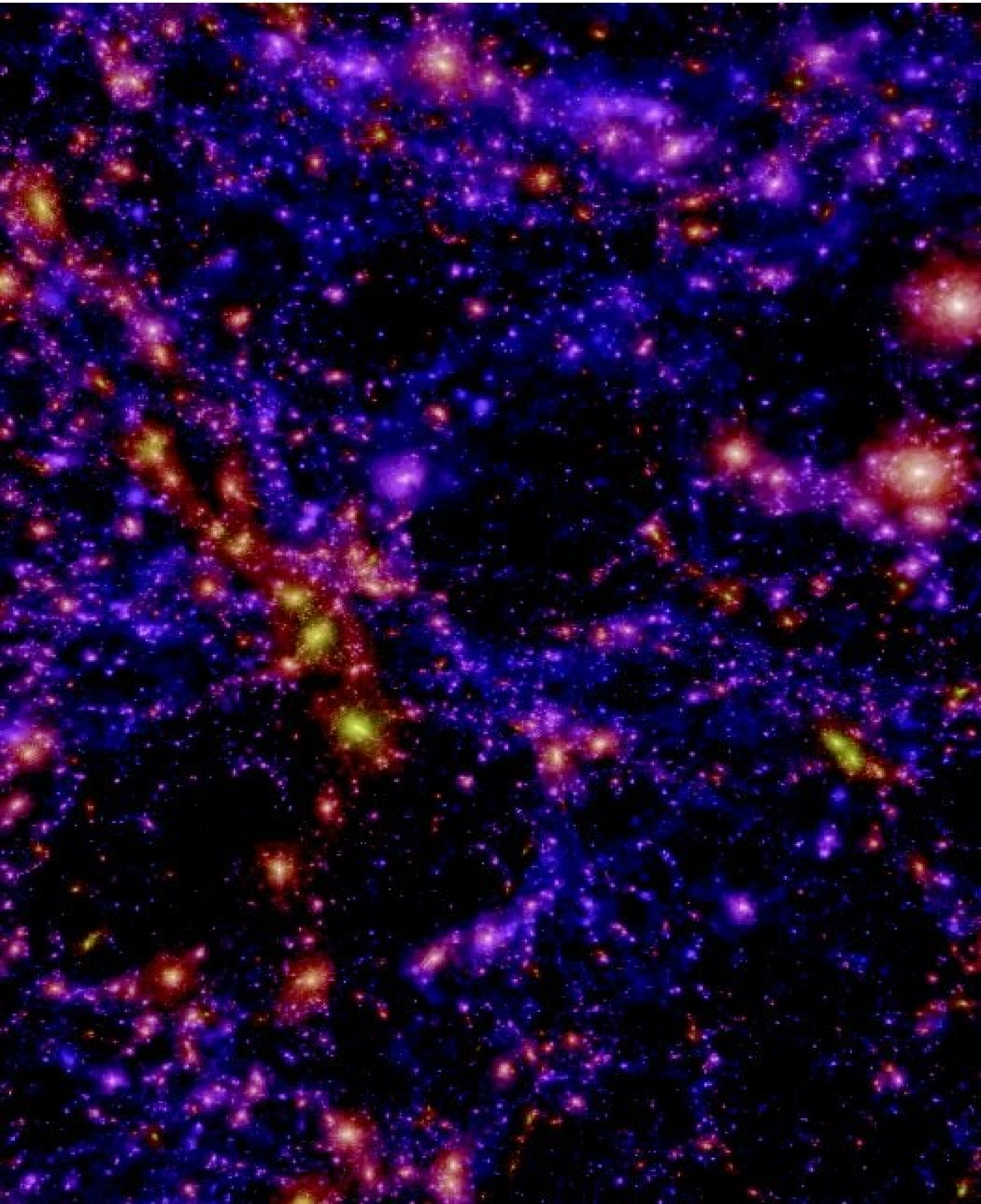
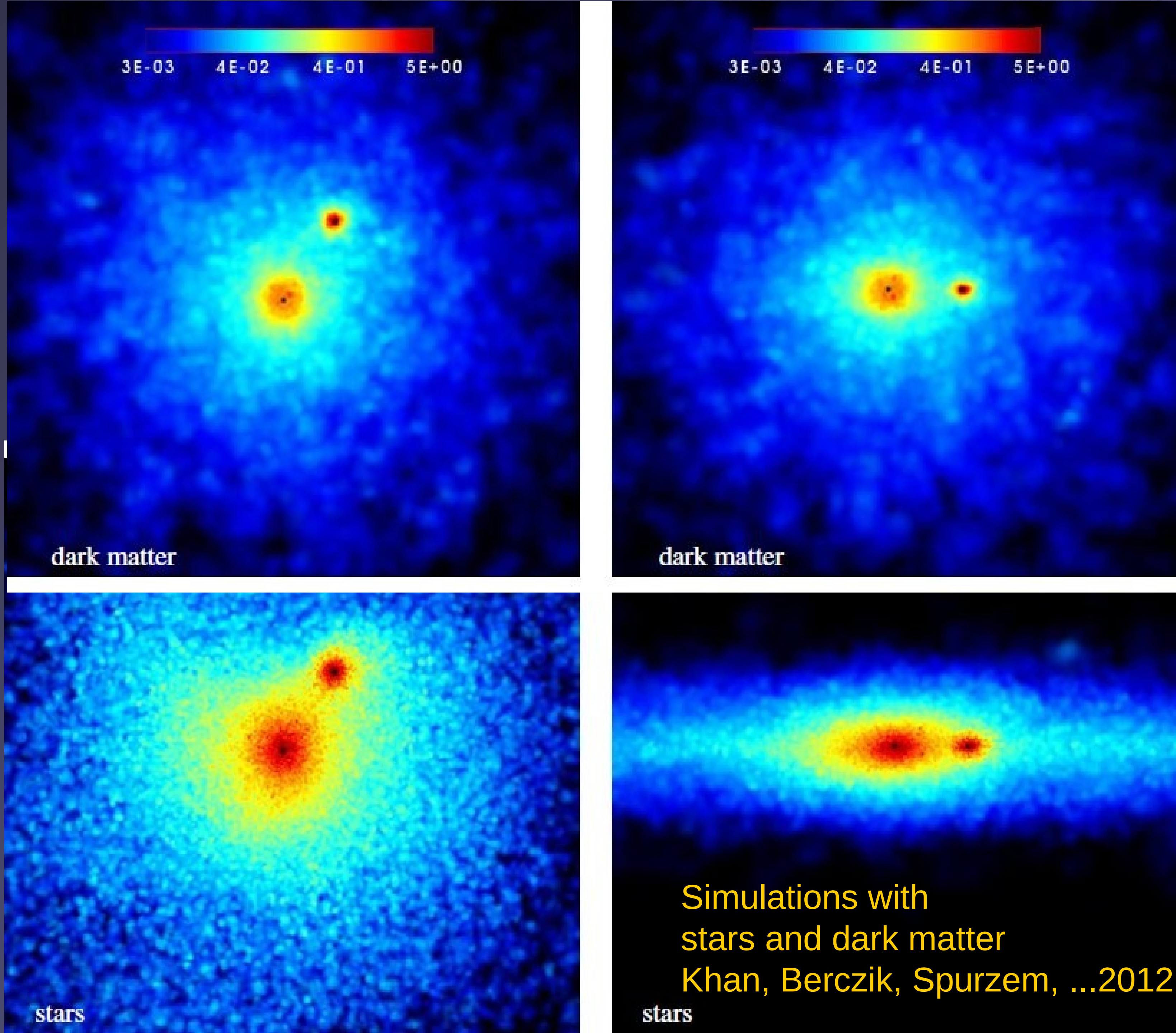


Black Holes in Galaxies


3E-03
4E-02
4E-01
5E+00
dark matter
3E-03
4E-02
4E-01
5E+00
dark matter
stars
stars
Simulations with
stars and dark matter
Khan, Berczik, Spurzem, ...2012

Post-Newtonian Dynamics Gravitational Wave Templates

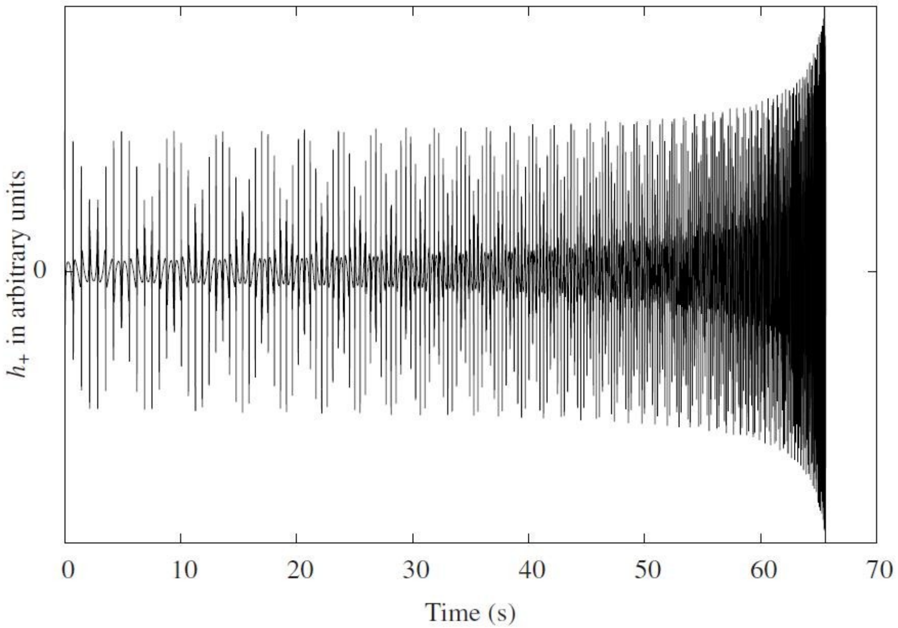


Figure 3.11: Waveform for two equal mass objects on a an orbit with $e = 0.5$.

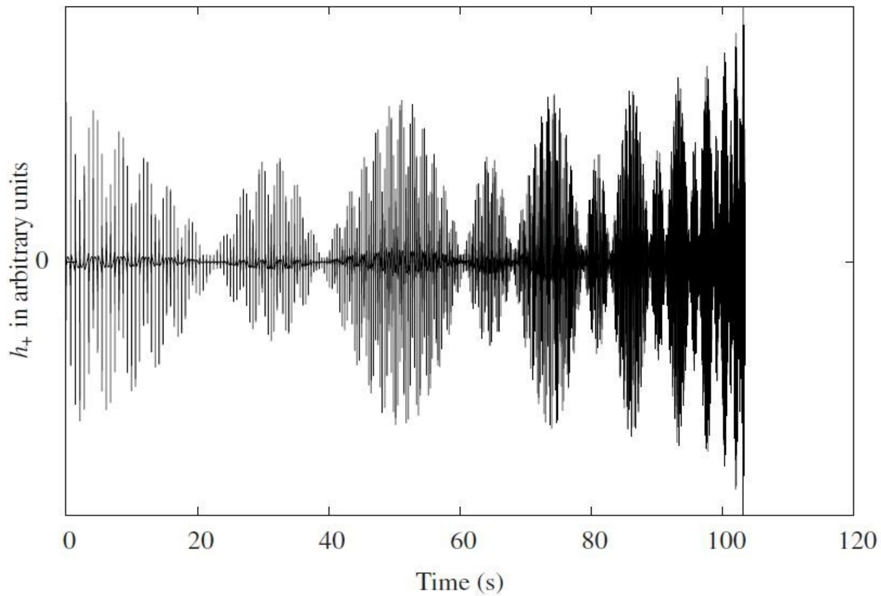
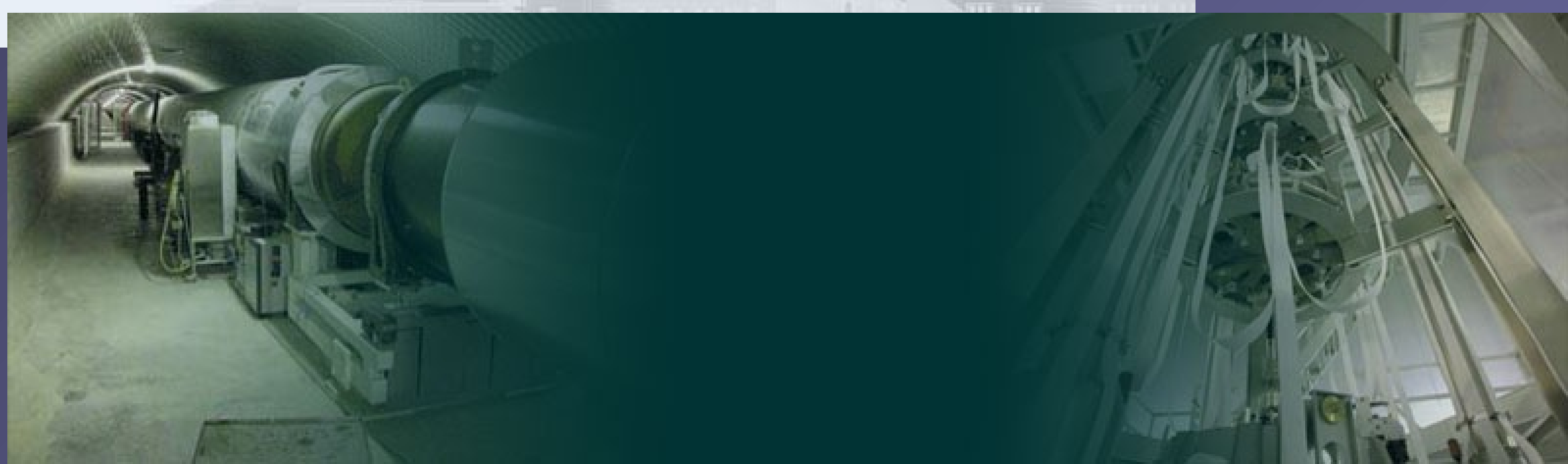


Figure 3.12: Waveform for two objects with a mass ratio of $q = 1/10$ on an orbit with $e = 0.5$ and spins $a_{1,x} = 1.0$, $a_{2,y} = 1.0$.

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)

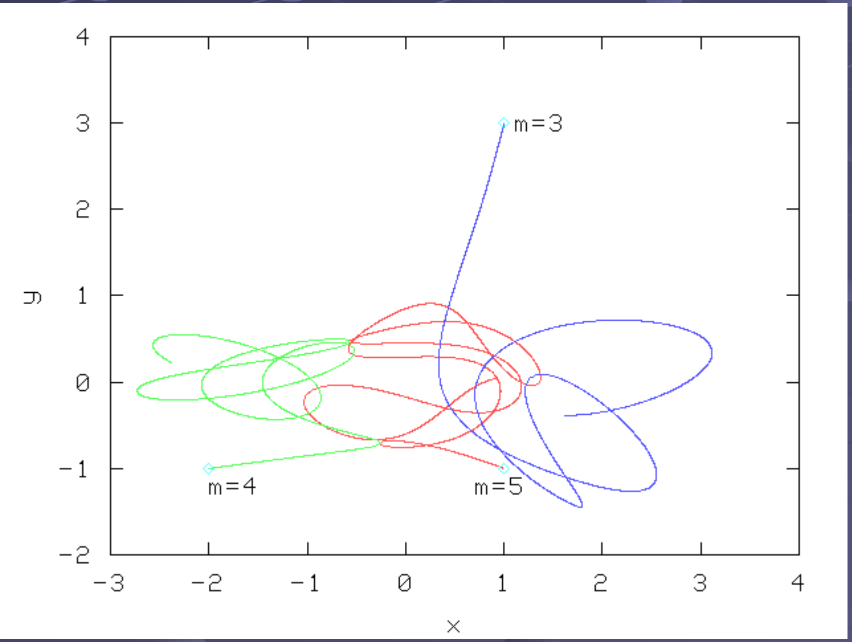
http://www.ligo-la.caltech.edu/
http://www.ego-gw.it
http://www.geo600.uni-hannover.de

Outreach to 50 Millionen light years (Neutron Stars)

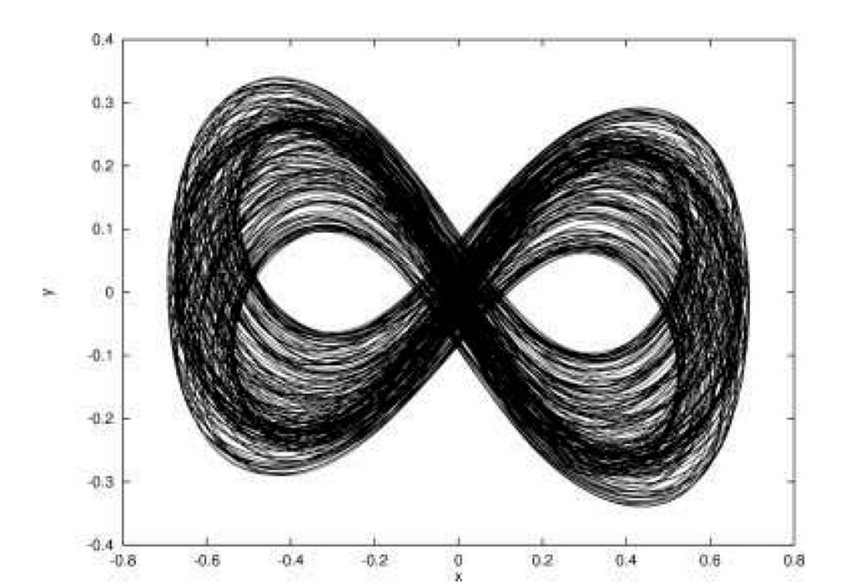
Nonlinear Dynamics and Chaos

3-Body Problems

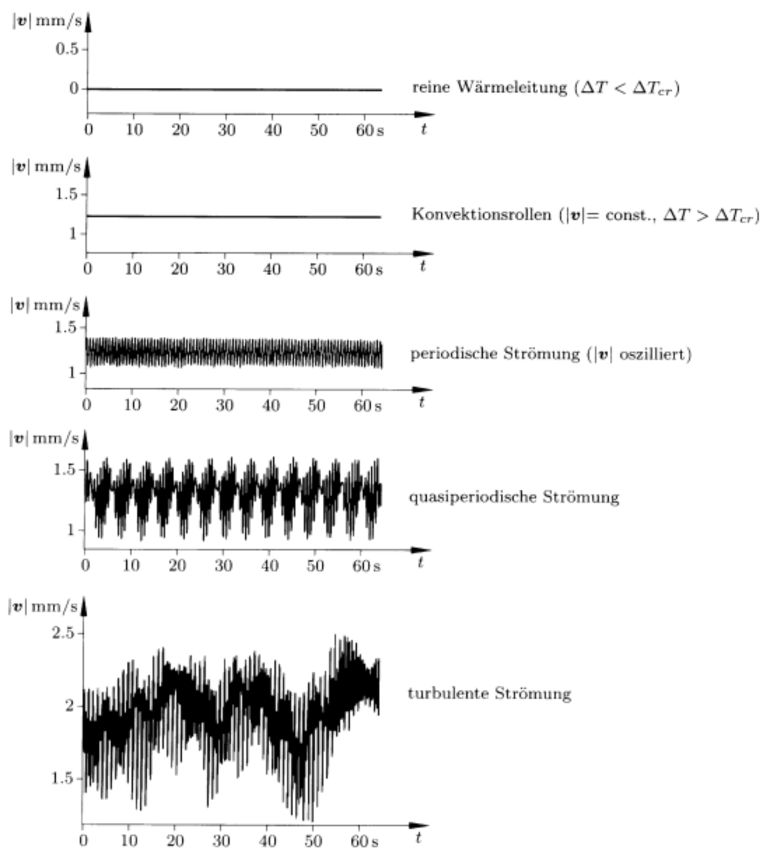
Burrau's Problem



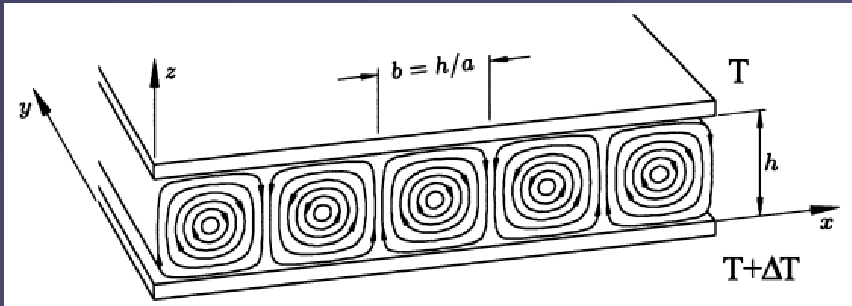
„The Eight"

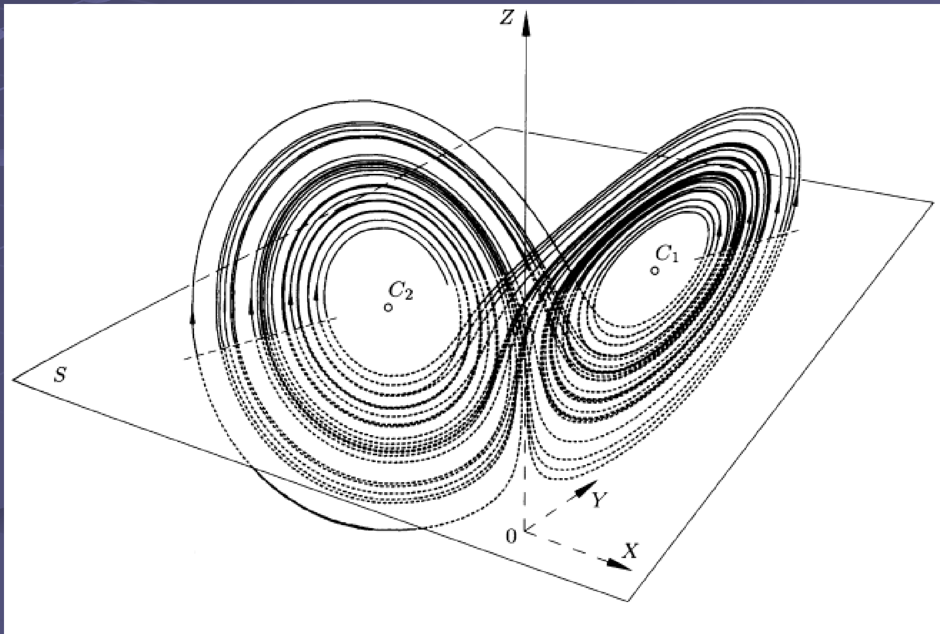


Lorenz-Attraktor



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