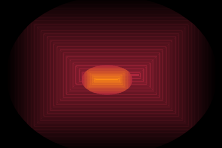




Computer Physik

Computational Physics



Volker Springel, Heidelberg Institute for Theoretical Studies
Rainer Spurzem, Astronomisches Rechen-Institut Zentrum für
Astronomie, Universität Heidelberg

spurzem@ari.uni-heidelberg.de, volker.springel@h-its.org

<http://www.ari.uni-heidelberg.de/mitarbeiter/spurzem/>

<http://www.h-its.org/english/homes/springel/index.php>

Computerphysik - Vorlesung

Warum Computerphysik notwendig?

- Differentialgleichungen (DGL) – keine analytische Lösung!
Zusammenhang: Nichtlineare Dynamik, Chaostheorie
- Gewöhnliche zeitabh. DGL – Teilchensimulationen
Plasmaphysik, Moleküldynamik, Stelldynamik...
- Partielle zeitabh. DGL – Gittermethoden
Hydrodynamik, Relativitätstheorie, Quantenmechanik
- Zeitunabh. DGL – Mittelwerte, stationäre Zustände
Quantenmechanik, statistische Mechanik, Monte-Carlo Verfahren.
- Spezialfall Computermathematik-komplexe analytische Lösungen, konventionell praktisch unlösbar.
Mathematica, Maple, MatLab, ...

Geschichte

● Erik Holmberg (1908-2000)

Dissertation Univ. Lund (Schweden) (1937):

``A study of double and multiple galaxies``

Galaxien oft in Gruppen und Paaren

Satellitengalaxien ungleichmäßig verteilt (Holmberg-Effekt)



● **Vater der numerischen Astrophysik....**

● **...mit 200 Glühbirnen**

Geschichte



LUMA METALL

The Astrophysical Journal, Nov. 1941

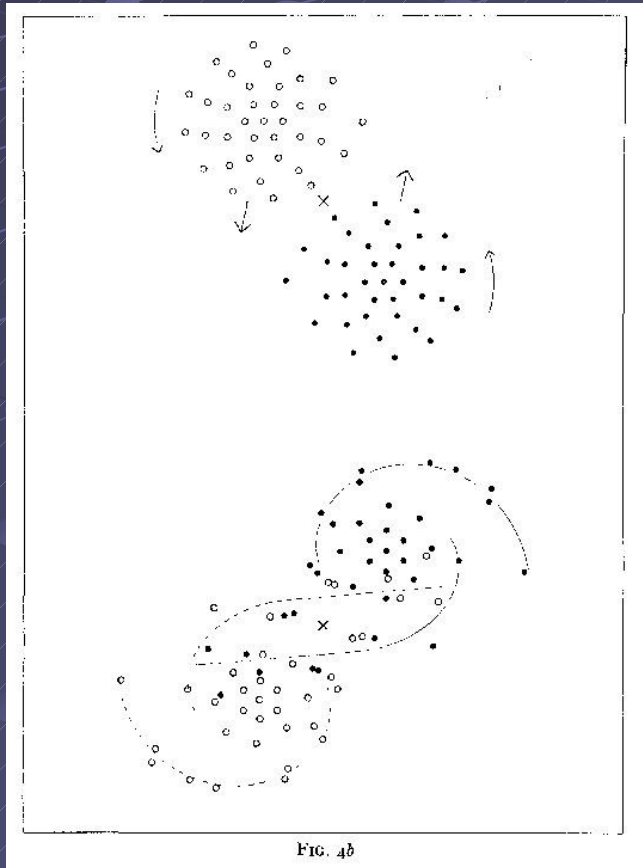


FIG. 4b

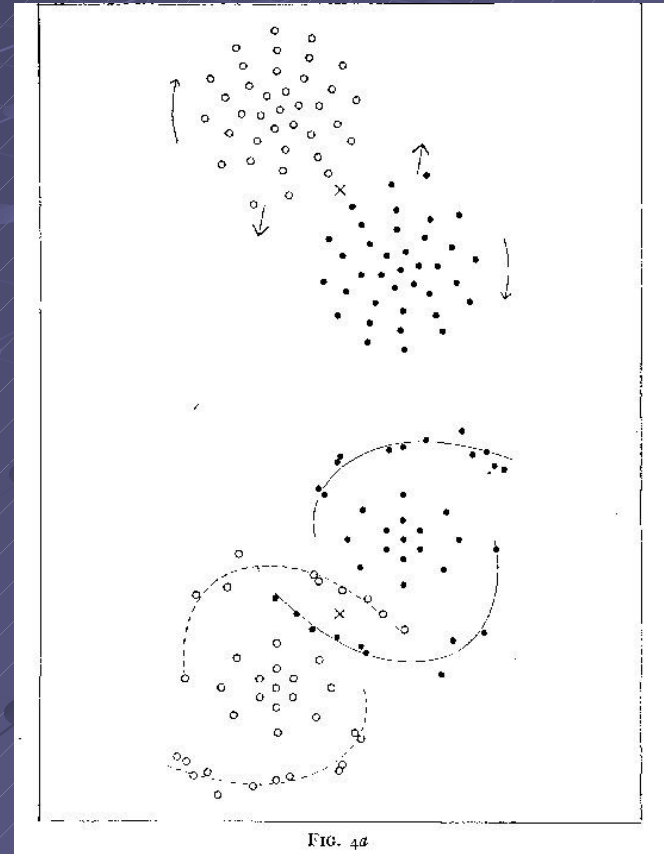


FIG. 4a

Geschichte

● Konrad Zuse (1910-1995) Berlin

Erfinder des frei programmierbaren Rechners



Z1 in der elterlichen Wohnung 1936



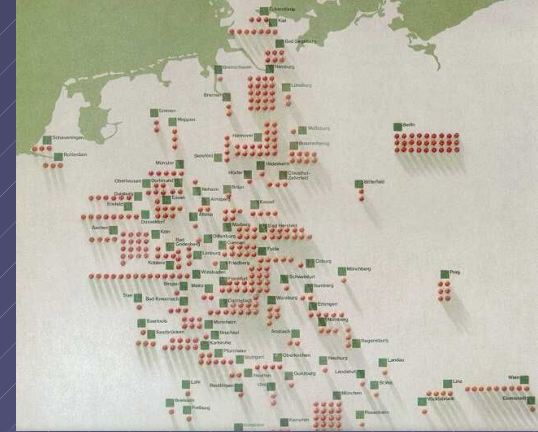
RT-Distribution

Schwingungen

Geschichte

0.03 Mflops

<http://www.rtd-net.de/Zuse.html>



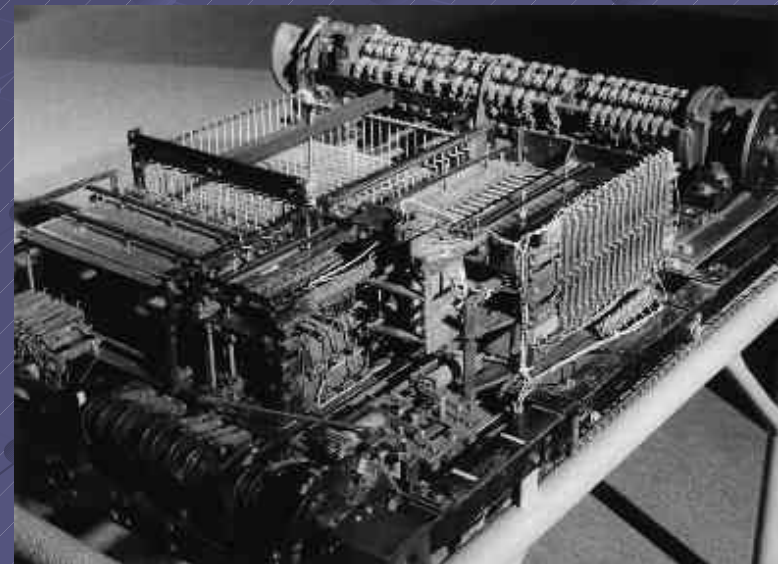
Zuse Z4: 1944 Berlin, 1950 Zürich

1954 Frankreich

1959 Deutsches Museum München



Rechenanlage 0.03 MHz



Speicher 256 byte

Geschichte

● Grundprinzipien des elektronischen Rechners

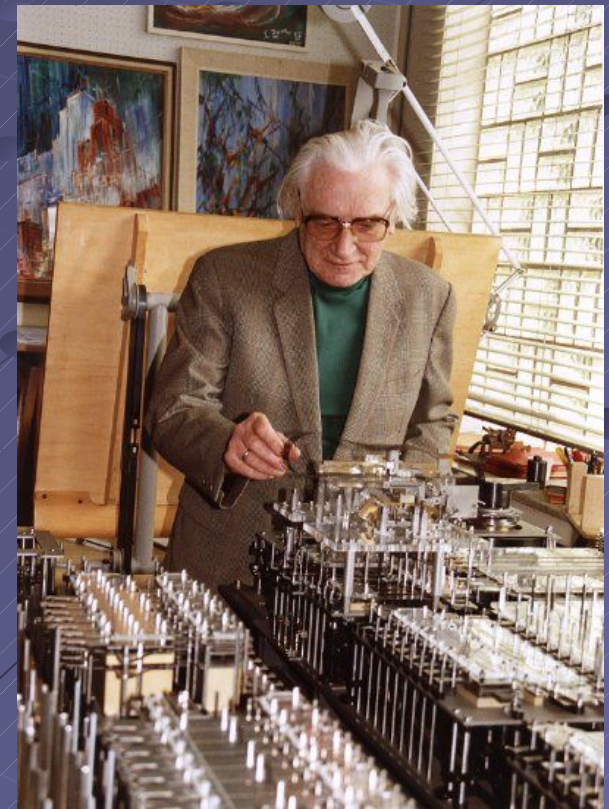
Verwirklicht bei Zuse, Theorie von Neumann

Freie Programmierbarkeit

Binäres Zahlenformat

Speicher

Gleitkommaarithmetik



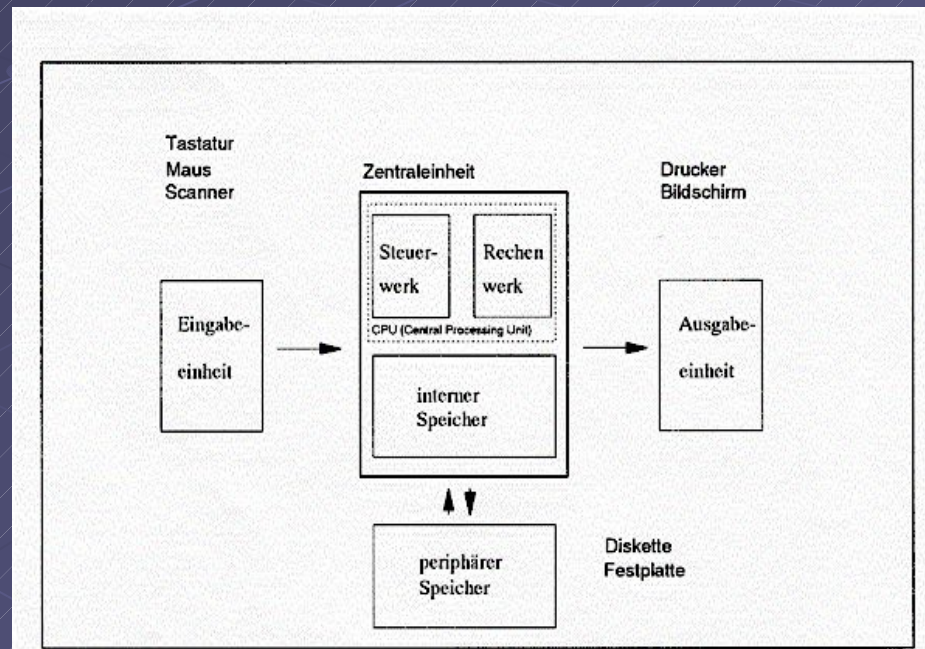
Geschichte

● John von Neumann (1903-1957)

Geb. Budapest, Dozent Berlin,

ab 1930 Princeton Univ. NJ USA Princeton

„Requirements for an electronic computing machine“ (1946)



Geschichte

Astronomisches Rechen-Institut in Heidelberg
Mitteilungen Serie A Nr. 14

Die numerische Integration des n -Körper-Problemes für Sternhaufen I

Von

SEBASTIAN VON HOERNER

Mit 3 Textabbildungen

(Eingegangen am 10. Mai 1960)

Astronomisches Rechen-Institut in Heidelberg
Mitteilungen Serie A Nr. 19

Die numerische Integration des n -Körper-Problems für Sternhaufen, II.

Von

SEBASTIAN VON HOERNER

Mit 10 Textabbildungen

(Eingegangen am 19. November 1962)

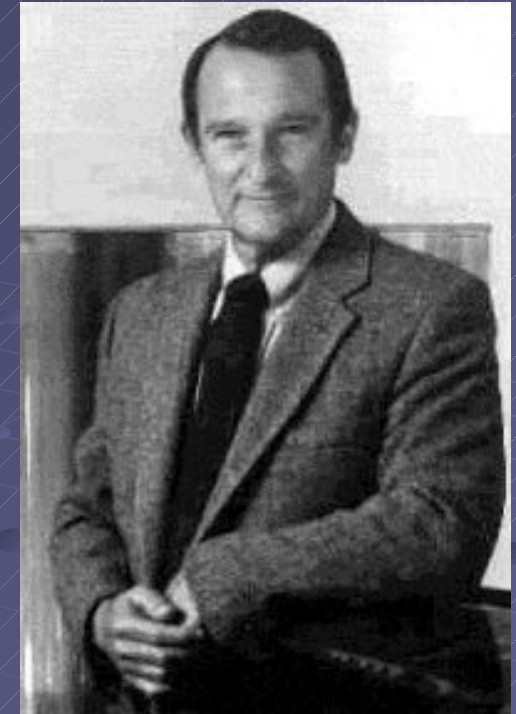


S.v. Hoerner,
1919 – 2003

Z.f.Astroph. 1960, 63

Sebastian von Hoerner, 2001: How it all started, in: Dynamics of Star Clusters and the Milky Way, ASP Conference Series, Vol. 228. Edited by S. Deiters, B. Fuchs, R. Spurzem, A. Just, and R. Wielen. San Francisco: Astronomical Society of the Pacific. ISBN: 1-58381-060-9, 2001.

Geschichte



● Seymour Cray (1925-1996)

● "The father of supercomputing"

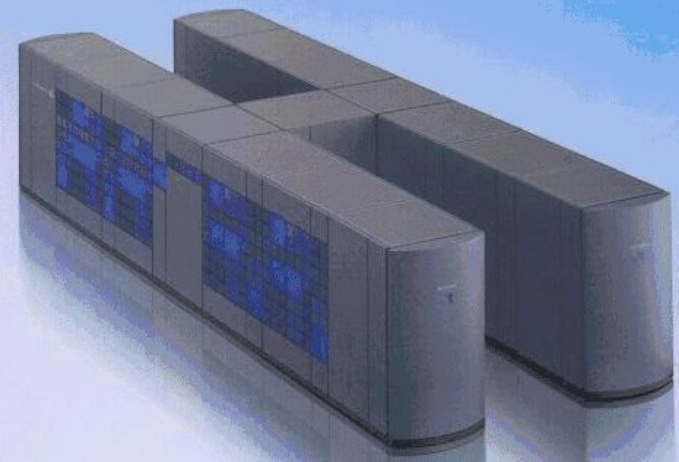


CRAY1: Vektorregister (1976)

160 Mflop, 80 MHz, 8 MByte RAM

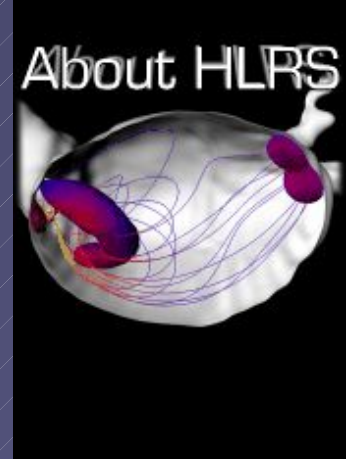
CRAY2: (1984)

1Gflop, 120MHz, 2GByte RAM



Geschichte

Hitachi SR8000 LRZ München
6 Tflops, TByte Memory

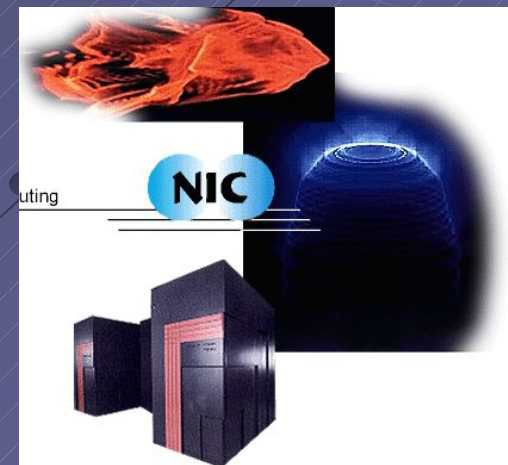


HLRS Stuttgart

● Für welche Zwecke?

- Autos, Flugzeuge, ..., Weltraumforschung
- Meteorologie, Klimaforschung, Wetter
- Elementar-Teilchen, Astro-Teilchen,
Hochenergiephysik
- Astrophysik
- Geisteswissenschaften, Datenbanken,
Wissensarchivierung
- (Krieg – Militär)

NIC Jülich





Leibniz-Rechenzentrum München,
Jülich Supercomputing Centre, HLRS Stuttgart
Europäisches Netzwerk der Höchstleistungsrechner
<http://www.deisa.org>

SGI Altix 4700
62 Tflop/s



Einführung

Superrechner

JUGENE

IBM Blue Gene

Jülich

Supercomputing

Centre (JSC)

223 Tflop/s

...Petaflop/s...

2015: Exaflop/s

Prototype with IBM

2019: Exaflop/s System

(...Trillion...)



Eröffnet mit J. Rüttgers Juni 2008



Über Petaflop/s zu Exaflop/s?

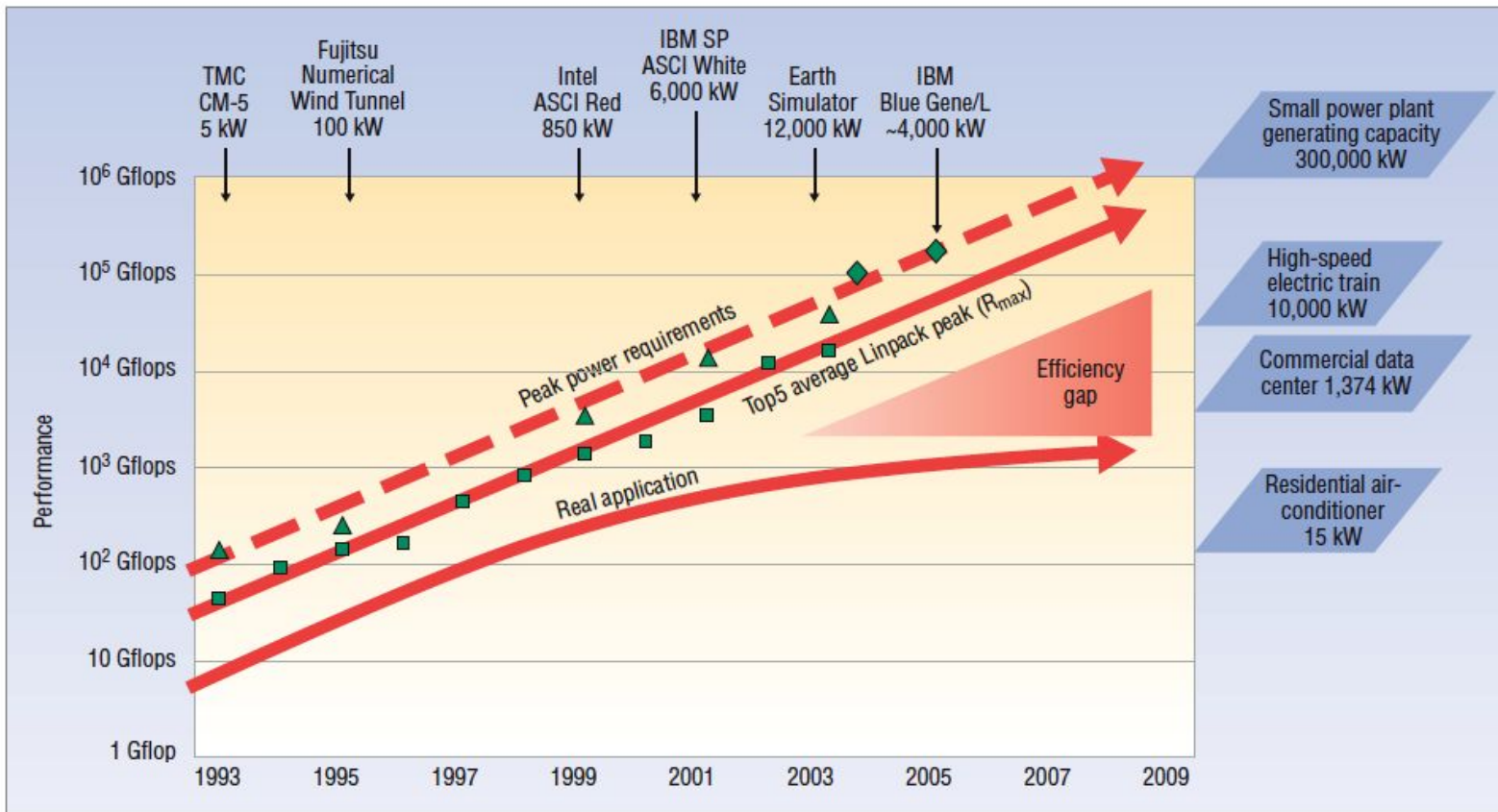


Figure 1. Rising power requirements. Peak power consumption of the top supercomputers has steadily increased over the past 15 years.

Neue Lösungen dringend! Green Flash – Power Efficient Supercomputing at the Exaflop/s Scale – UC Berkeley and Lawrence Berkeley, and Univ. of Heidelberg!
http://www.citris-uc.org/events/green_flash_power_efficient_scientific_computing_exascale

HARDWARE



2007...

GeForce 8800 GTX, 128 Stream Proc., 768 MB

GeForce 8800 GTS, 128 Stream Proc., 512 MB

GeForce 8800 GT, 112 Stream Proc., 512 MB

2008...

GeForce 9800 GTX, 128 Stream Proc., 512 MB

GeForce 9800 GX2, 256 Stream Proc., 1 GB

GeForce 9800 GT, 64 Stream Proc., 512 MB

<http://www.nvidia.com>



GPU Computing



PCI
Express 2.0



GPU

- Number of processor cores: 240
- Processor core clock: 1.296 GHz
- Voltage: 1.1875 V
- Package size: 45.0 mm × 45.0 mm 2236-pin flip-chip ball grid array (FCBGA)

Board

- Fourteen layer printed circuit board (PCB)
- PCI Express 2.0 ×16 system interface
- Physical dimensions: 4.376 inches × 10.50 inches, dual slot
- Board power dissipation: 187.8 W

External Connectors

- None

Internal Connectors and Headers

- One 6-pin PCI Express power connector
- One 8-pin PCI Express power connector
- 4-pin fan connector

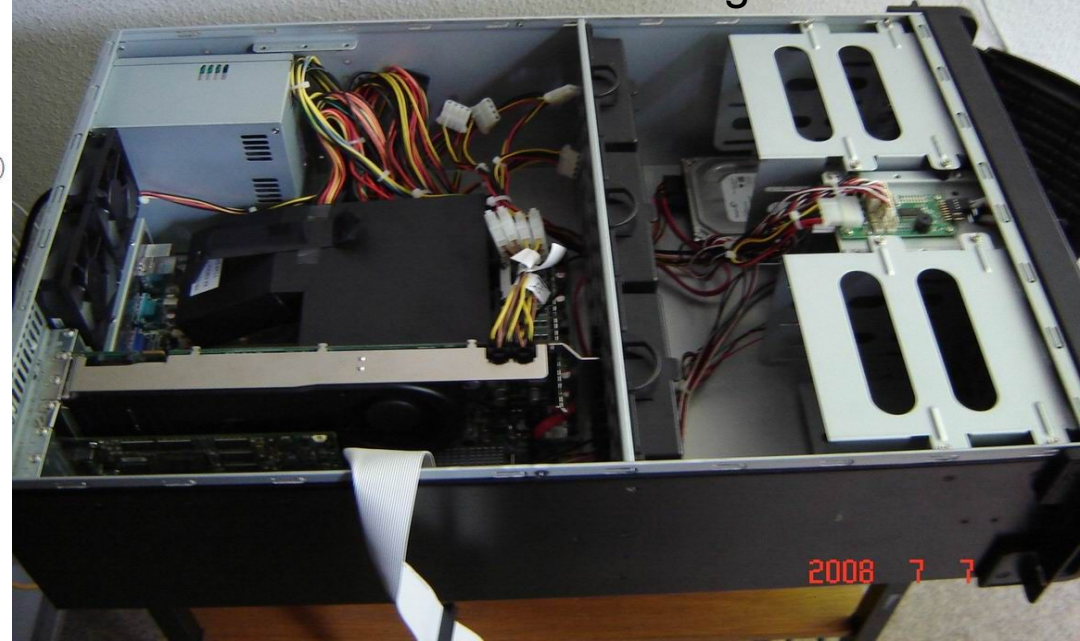
General Purpose GPU Supercomputing (GPGPU)

<http://www.nvidia.com>

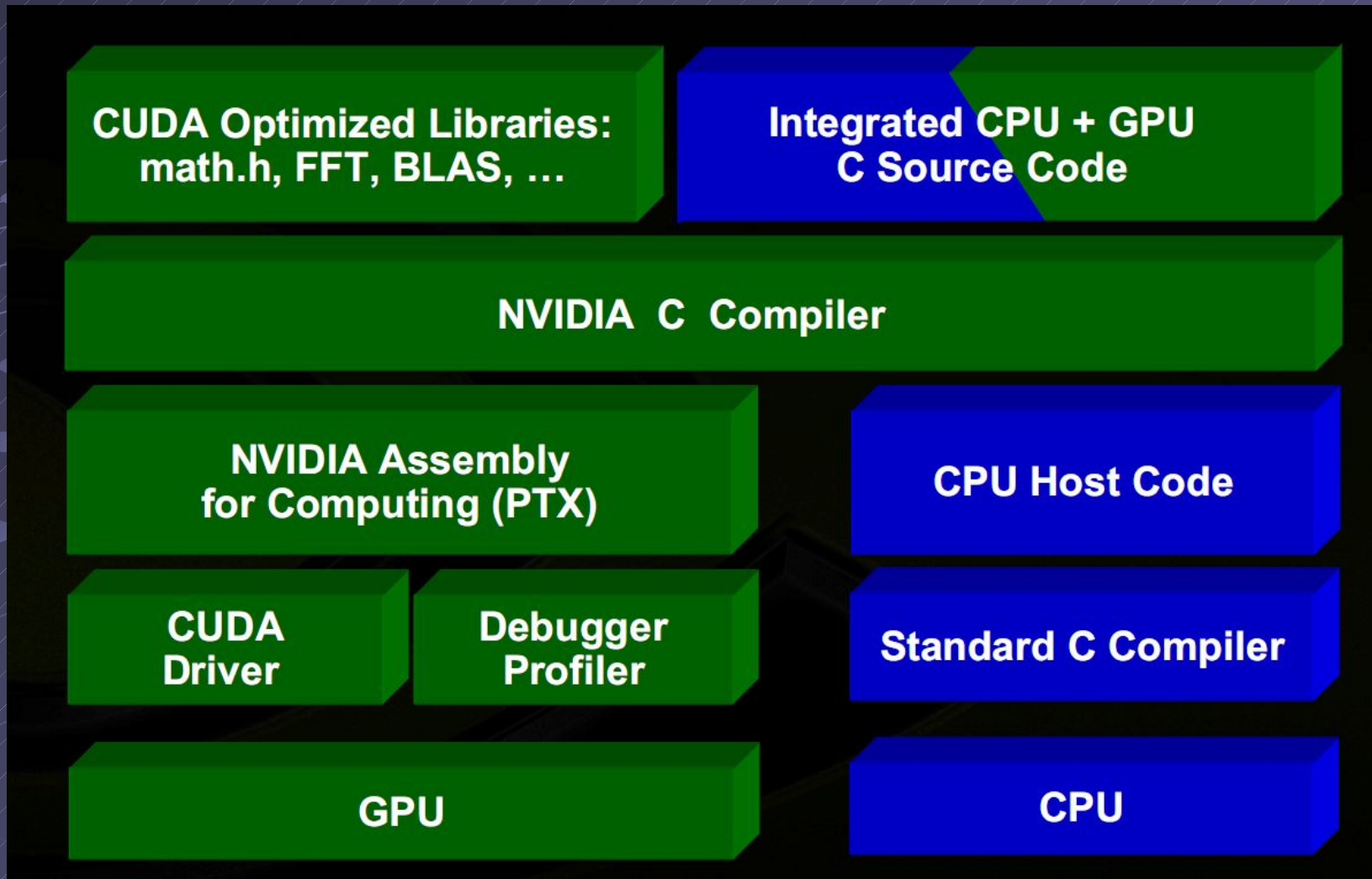
<http://www.astrogpu.org>

<http://gpgpu.org>

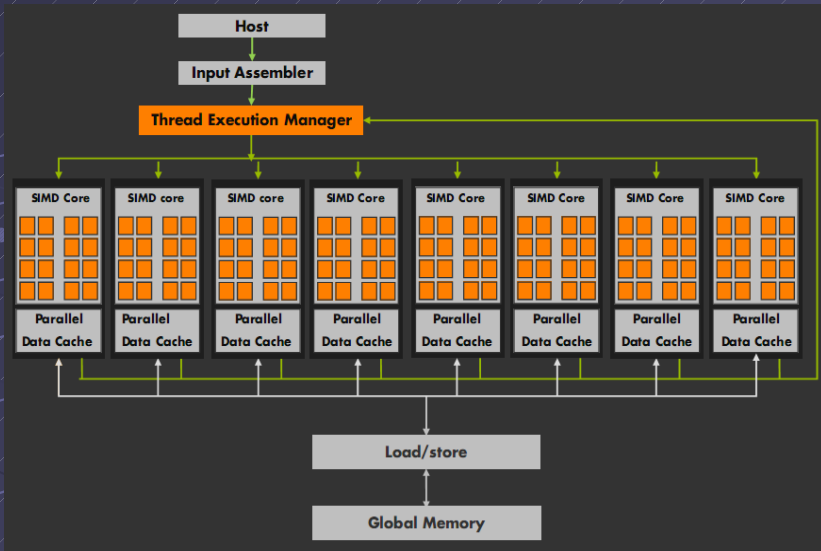
NVIDIA Tesla C1060
in kolob cluster Heidelberg Univ.



CUDA



Hardware



Each core

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

Parallel Data Cache

Total #threads/chip
 $16 * 512 = 8K$

NVIDIA Tesla C1060 :

1.3 GHz * 240 processors * 3 flopclock = 930 Gflops



Towards Peta-Scale Green Computation

— applications of the GPU supercomputers in CAS

<http://www.nvidia.com/gtc2010-content>



GPU TECHNOLOGY CONFERENCE

GTC 2010 | Sept 20-23, 2010

San Jose Convention Center, San Jose, California

Watch the Keynote Recordings

[Algorithms & Numerical Techniques](#)

[Astronomy & Astrophysics](#)

[Audio Processing](#)

[Cloud Computing](#)

[Computational Fluid Dynamics](#)

[Computer Graphics](#)

[Computer Vision](#)

[Databases & Data Mining](#)

[Digital Content Creation](#)

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[General Interest](#)

[GPU Accelerated Internet](#)

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[Mobile & Tablet & Phone](#)

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[Neuroscience](#)

[Physics Simulation](#)

[Programming Languages &](#)

[Techniques](#)

[Quantum Chemistry](#)

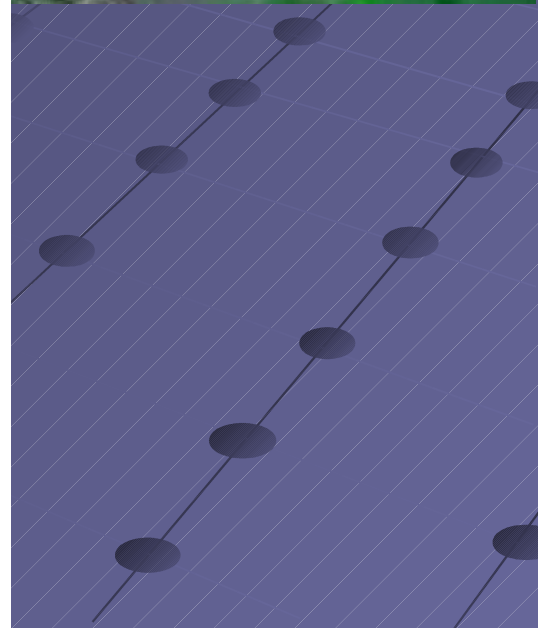
[Ray Tracing](#)

[Signal Processing](#)

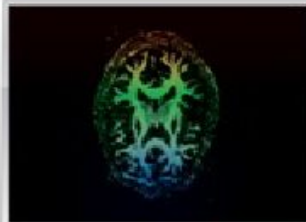
[Stereoscopic 3D](#)

[Tools & Libraries](#)

[Video Processing](#)

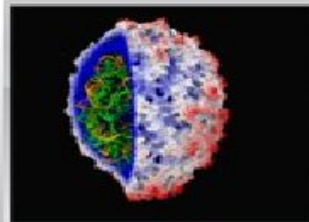


Speedups using GPU vs. CPU



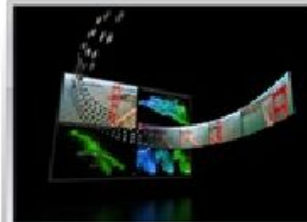
146X

Interactive visualization of volumetric white matter connectivity¹



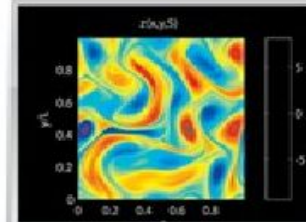
36X

Ionic placement for molecular dynamics simulation on GPU²



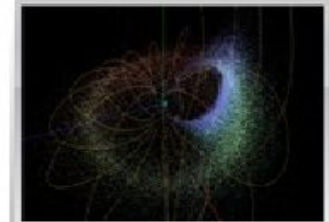
18X

Transcoding HD video stream to H.264 for portable video³



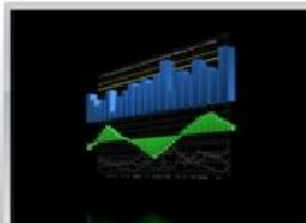
17X

Simulation in Matlab using .mex file CUDA function⁴



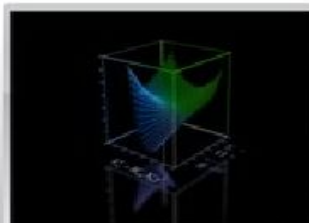
100X

Astrophysics N-body simulation⁵



149X

Financial simulation of LIBOR model with swaptions⁶



47X

GLAME@lab: M-script API for linear Algebra operations on GPU⁷



20X

Ultrasound medical imaging for cancer diagnostics⁸



24X

Highly optimized object oriented molecular dynamics⁹

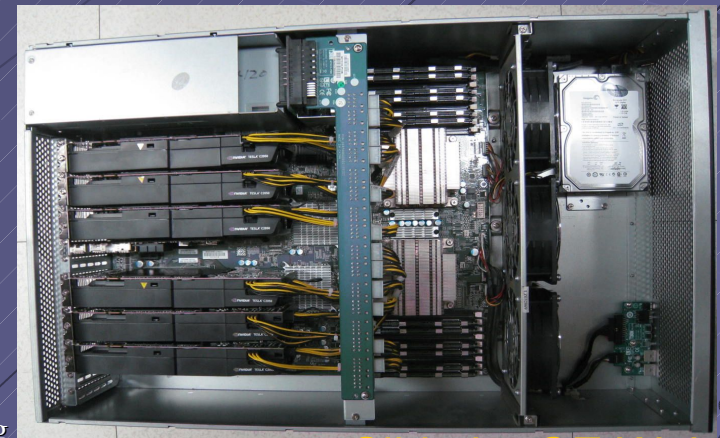


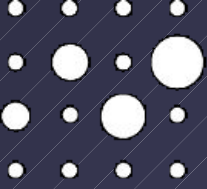
30X

Cmatch exact string matching - find similar proteins & gene sequences¹⁰

Fermi-based GPU supercomputer IPE (2010.04.24) China HPC System

Rpeak SP : 2Pflops
Rpeak DP : 1Pflops
Linpack: 207.3T (Top500 19th)
Mflops/Watt: 431 (Green500 8th)
Total RAM : 17.2TB
Total VRAM : 6.6TB
Total HD : 360TB
Inst. Comm. : H3C GE
Data Comm. : Mellanox QDR IB
Occupied
area : 150 sq.m.
Weight : 12.6 tons
Max Power : 600kW(computing)
200kW(cooling)
System : CentOS 5.4, PBS
Monitor : Ganglia, GPU monitor
Languages : C, C++, CUDA 3.1 , OpenCL





**MPRACE Card, ZITI
Zentrales Inst. Techn. Informatik
Univ.Heidelberg in Mannheim**

NAOC Beijing (**CAS and Silk Road Project**)

Bottom Right: NAOE Cluster

86x8 Cores, 170 Tesla C1060



HARDWARE

Custom PC Clusters

with manycore accelerator hardware:

Heidelberg (2x, GRAPE, FPGA, GPU)

Rochester, NY (only GRAPE)

Kiev, Ukraine (2x, GRAPE, GPU)

NAOC Beijing (**CAS and Silk Road Project**)

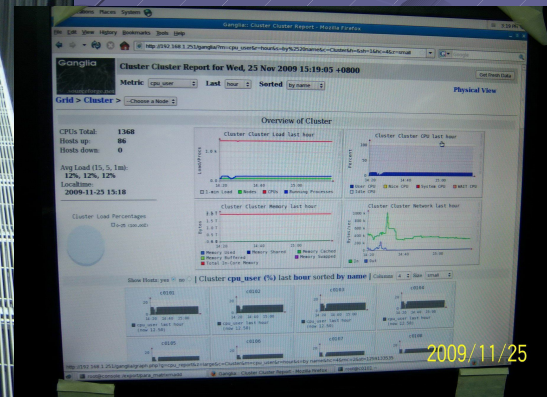
Bottom Right: NAOC Cluster

86x8 Cores, 170 Tesla C1060



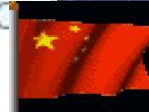
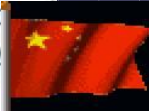
Top: Frontier Cluster

41x8=328 Cores, 40 Tesla GPU
Klessen, Banerjee,
Spurzem, Männer et al.



TOP 10 Systems - 11/2010

- 1 Tianhe-1A - NUDT TH MPF X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C
- 2 Jaguar - Cray XT5-HE Opteron 6-core 2.6 GHz
- 3 Nebulae - Dawning TC3600 Blade, Intel X5650, NVidia Tesla C2050 GPU
- 4 TSUBAME 2.0 - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows
- 5 Hopper - Cray XE6 12-core 2.1 GHz
- 6 Tera-100 - Bull bullx super-node S6010/S6030
- 7 Roadrunner - BladeCenter QS22/LS21 Cluster, PowerXCell 8i 3.2 Ghz / Opteron DC 1.8 GHz, Voltaire Infiniband
- 8 Kraken XT5 - Cray XT5-HE Opteron 6-core 2.6 GHz
- 9 JUGENE - Blue Gene/P Solution
- 10 Cielo - Cray XE6 8-core 2.4 GHz



From www.top500.org - list of fastest supercomputers in the world...

► 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).

New Supercomputing in China....

... use GPU (Graphical Processing Unit)

Ranking the World's Most ENERGY-EFFICIENT SUPERCOMPUTERS



www.green

Green500 Rank	MFLOPS/W	Site*	Computer*	Total Power (kW)
1	1684.20	IBM Thomas J. Watson Research Center	NNSA/SC Blue Gene/Q Prototype	38.80
2+	1448.03	National Astronomical Observatory of Japan	GRAPE-DR accelerator Cluster, Infiniband	24.59
2	958.35	GSIC Center, Tokyo Institute of Technology	HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows	1243.80
3	933.06	NCSA	Hybrid Cluster Core i3 2.93Ghz Dual Core, NVIDIA C2050, Infiniband	36.00
4	828.67	RIKEN Advanced Institute for Computational Science	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect	57.96
5	773.38	Universitaet Wuppertal	QPACE SFB TR Cluster, PowerXCell 8i, 3.2 GHz, 3D-Torus	57.54
5	773.38	Universitaet Regensburg	QPACE SFB TR Cluster, PowerXCell 8i, 3.2 GHz, 3D-Torus	57.54
5	773.38	Forschungszentrum Juelich (FZJ)	QPACE SFB TR Cluster, PowerXCell 8i, 3.2 GHz, 3D-Torus	57.54
8	740.78	Universitaet Frankfurt	Supermicro Cluster, QC Opteron 2.1 GHz, ATI Radeon GPU, Infiniband	385.00
9	677.12	Georgia Institute of Technology	HP ProLiant SL390s G7 Xeon 6C X5660 2.8Ghz, nVidia Fermi, Infiniband QDR	94.40
10	636.36	National Institute for Environmental Studies	GOSAT Research Computation Facility, nvidia	117.15
11	635.15	National Supercomputing Center in Tianjin	NUDT YH Cluster, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C	4040.00
12	628.13	Lawrence Livermore National Laboratory	Appro GreenBlade Cluster Xeon X5660 2.8Ghz, nVIDIA M2050, Infiniband	160.00
13	555.50	CSIRO	Supermicro Xeon Cluster, E5462 2.8 Ghz, Nvidia Tesla s2050 GPU, Infiniband	94.60
14	492.64	National Supercomputing Centre in Shenzhen (NSCS)	Dawning TC3600 Blade, Intel X5650, Nvidia Tesla C2050 GPU	2580.00

www.green500.org



“天河一号” 超级计算机系统 TH-1 supercomputer



Landmark result of the important project "High Efficient Supercomputer and Grid Service Environment" supported by National 863 Program.

- ▶ Built by National University of Defense Technology, with the cooperation of National Supercomputer Center in Tianjin (NSCC -TJ) and Inspur (Beijing) Electronic Information Industry Co., Ltd.

Host system of NSCC-TJ, installed in Tianjin Binhai New Area.

A backbone node of the national grid of China.



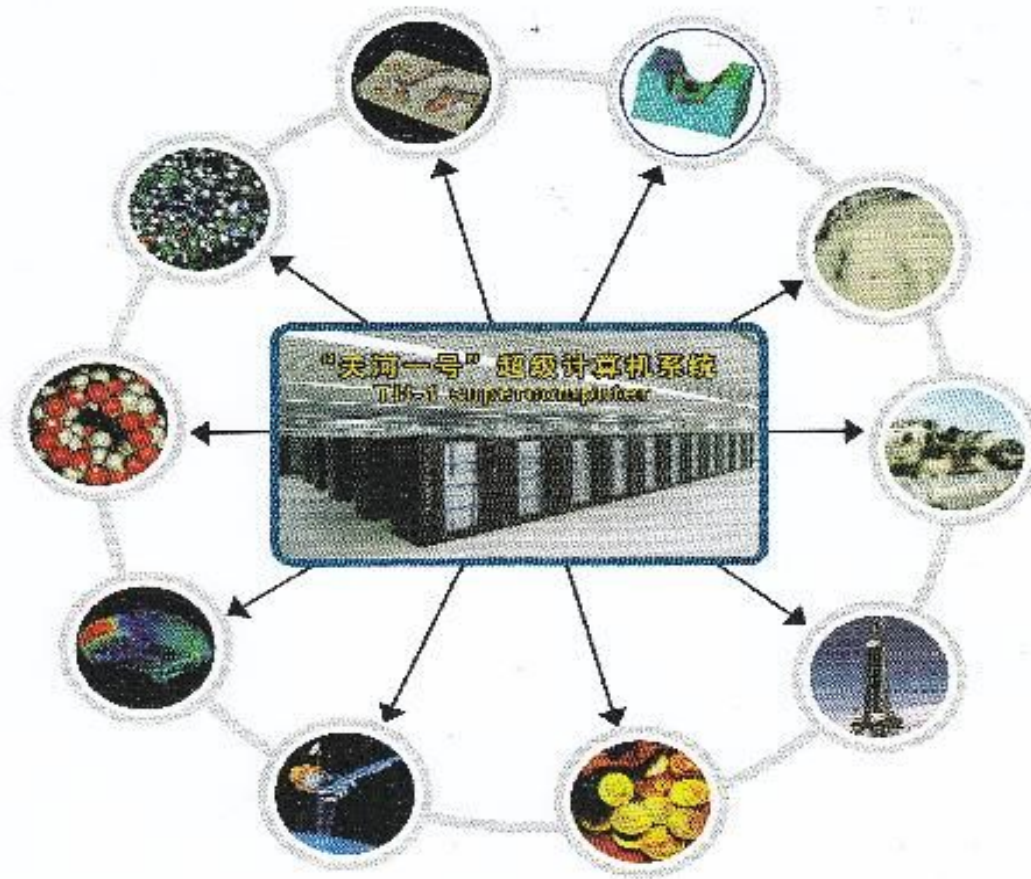
系统配置 System Configuration

- CPU和GPU相结合的异构融合计算体系结构
- 14336个商用处理器, 7168个加速处理器和2048个自主飞腾-1000处理器
- 内存总容量262TB
- 链路双向通信带宽达到160Gbps
- 共享磁盘总容量2PB, Lustre全局分布共享并行I/O结构
- 计算机柜112个、服务机柜8个、通信机柜6个、I/O存储机柜14个

- Hybrid architecture of heterogeneous integration with CPUs and GPUs
- 14336 commercial CPUs, 7168 accelerators, 2048 domestic FT-1000 CPUs
- 262TB total memory
- Bi-directional bandwidth of 160Gbps
- 2PB disk capacity, Lustre global shared file system with parallel I/O architecture
- 112 computing cabinets, 8 service cabinets, 6 communication cabinets, and 14 I/O cabinets

- Oil exploration
- High-end equipment development
- Bio-medical research
- Animation design
- Exploitation of new energy sources

- New materials research
- Engineering design and simulation analysis
- Weather forecast
- Remote sensing data processing
- Financial risk analysis



NCSA director: GPU is future of supercomputing

by Brooke Crothers



Font size



Print



E-mail



Share



6 comments

Tweet

99



Share

25

2

Digg ↑

The director of the National Center for Supercomputing Applications has seen the future of supercomputing and it can be summed up in three letters: GPU.

Thom Dunning, who directs the NCSA and the Institute for Advanced Computing Applications and Technologies at the famed supercomputing facilities on the campus of University of Illinois at Urbana-Champaign, says high-performance computing will begin to move toward graphics processing units or GPUs. Not coincidentally, **this is exactly what China has done to achieve the world's fastest speeds with its "Tianhe-1A"** supercomputer. That computer combines about 7,000 Nvidia GPUs with 14,000 Intel CPUs: the only hybrid CPU-GPU system in the world of that scale.

"What we're really seeing in the efforts in China as well as the ones we have in the U.S. is that GPUs are what the future will look like," said Dunning in a phone interview Thursday. "What we're seeing is the beginning of something that's going to be happening all over the world."

NCSA already has a small CPU-GPU hybrid system. "It's something we have been working on for a number of years. We have a CPU-GPU cluster for the NCSA academic community. Made up of Intel CPUs and Nvidia GPUs. A 50 teraflop machine," he said. (Note that **Oak Ridge National Laboratories is also installing a hybrid system now.**)



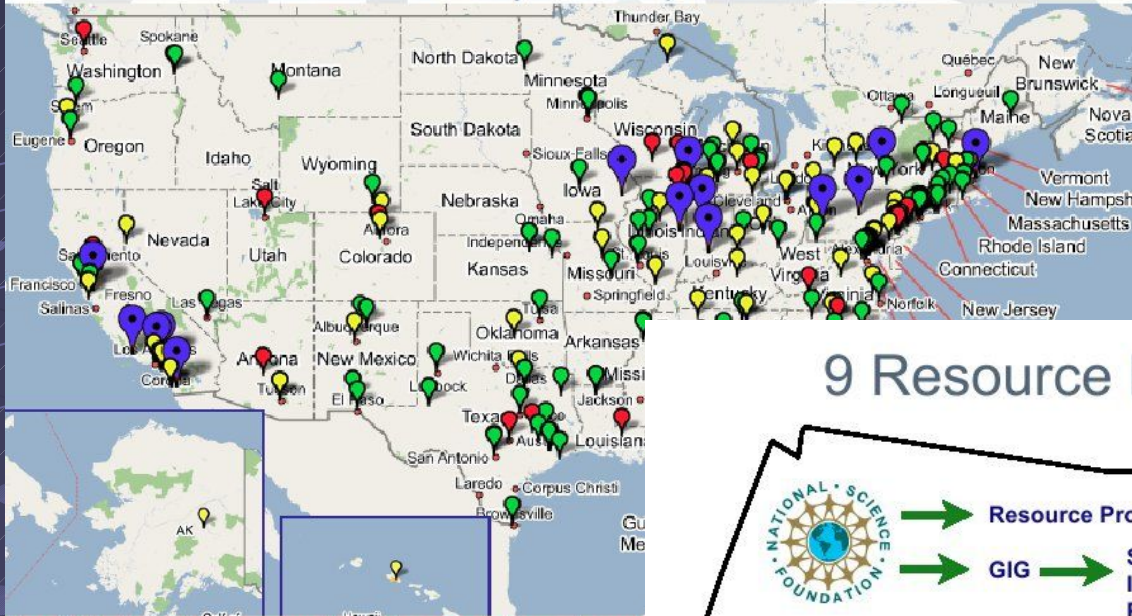
Thom Dunning directs the Institute for Advanced Computing Applications and Technologies and the NCSA.

The GRID....

- DEISA – Europe www.deisa.org
- Teragrid – USA www.teragrid.org
- NAREGI – Japan www.naregi.org
- D-Grid – Deutschland www.d-grid.de
- Astrogrid-D Deutschland www.astrogrid-d.de

Teragrid – Science Grid in the USA

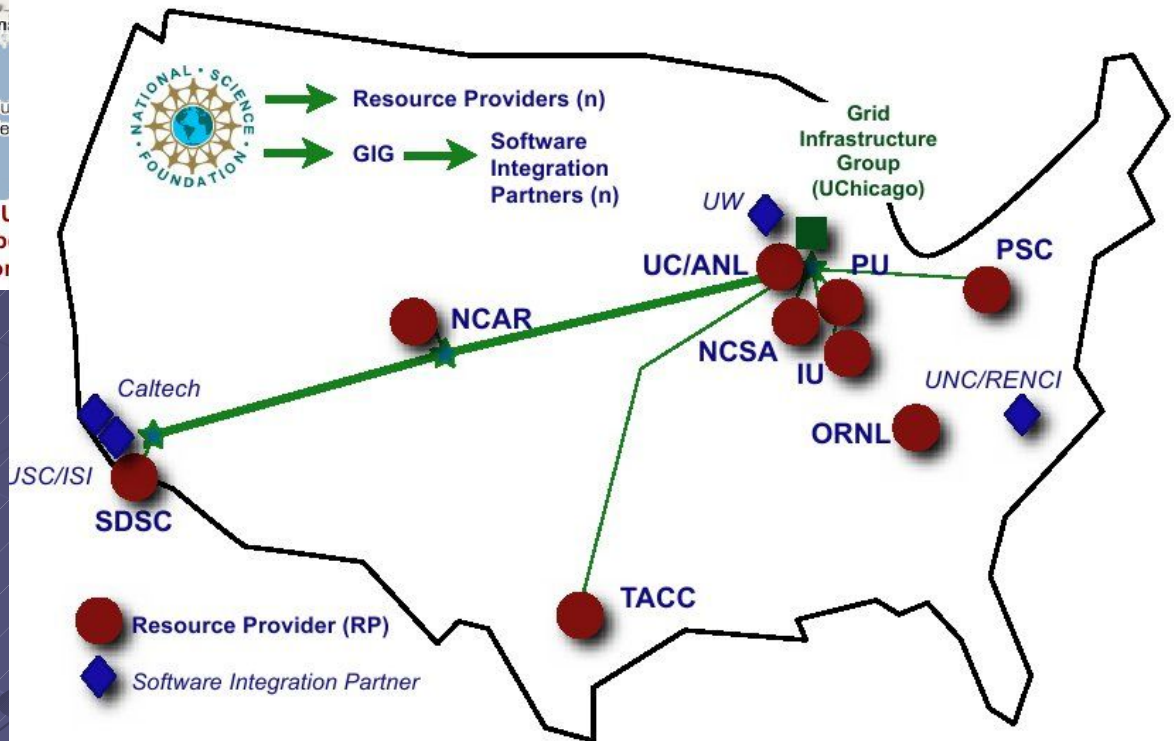
TeraGrid Projects by Institution



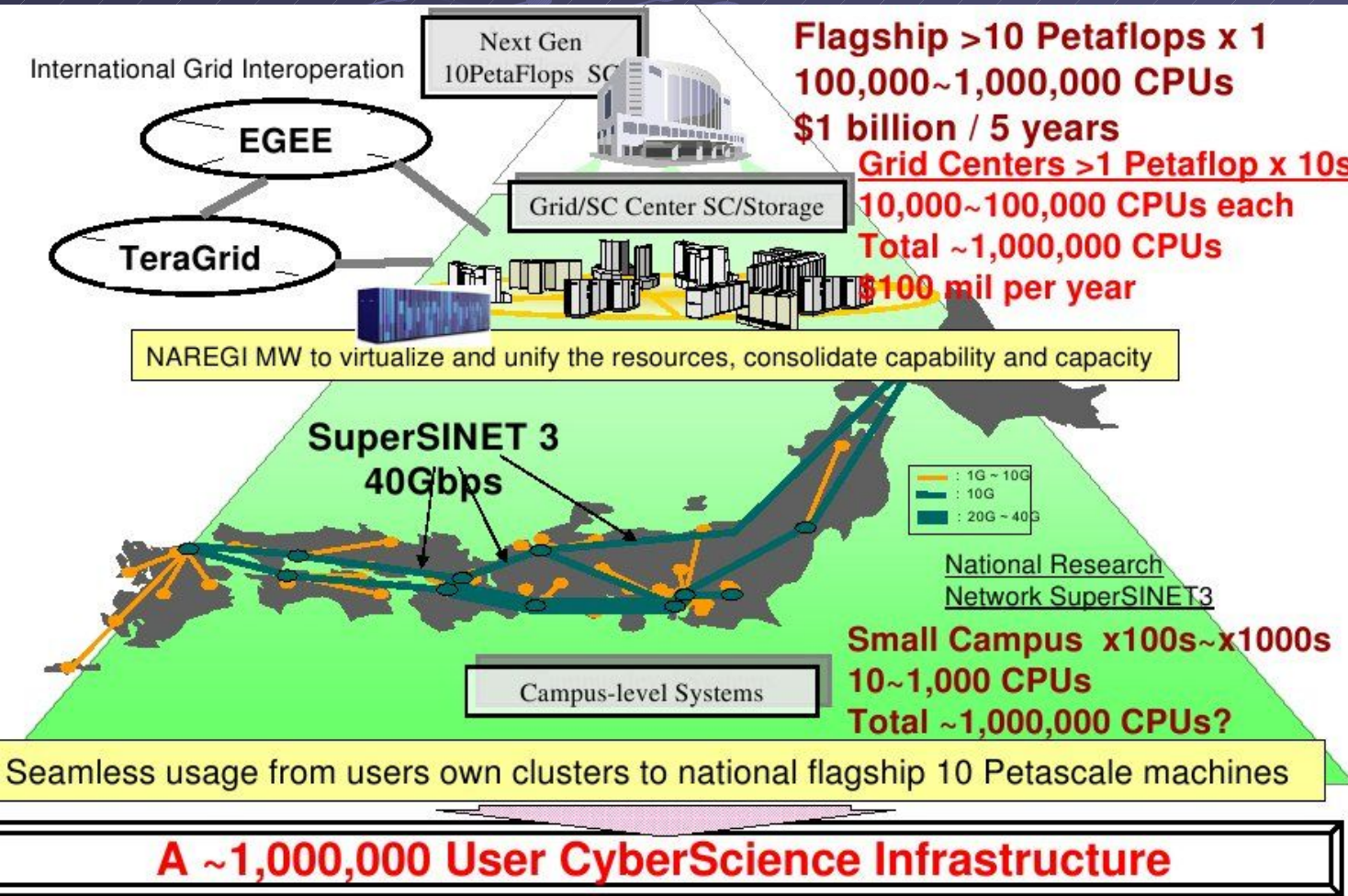
TeraGrid allocations are available to researchers at any US institution by peer review. Exploratory allocations can be through a biweekly review process. See www.teragrid.org

1000 projects (VOs),
4000 Users

9 Resource Providers, One Facility



NAREGI – Japanese Grid - the other example...



Seamless Network

Vertically (user to Supercomputing)

Horizontally (international connection)

With EGEE And Teragrid

Via GIN Grid Interface Network



Computer Physics - Examples

Computerphysik

• Traditionell:

Theorie

Experiment/Beobachtung

• Modern:

Theorie

Computer-Experiment

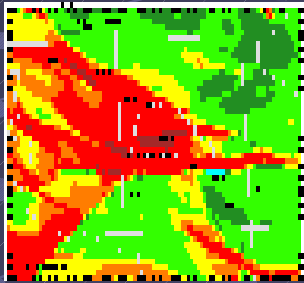
Beobachtung

Beobachtungen, die direkt nicht möglich sind!
Beobachtungen nicht existierender Objekte!

Computerphysik

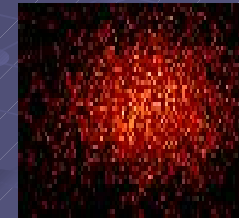
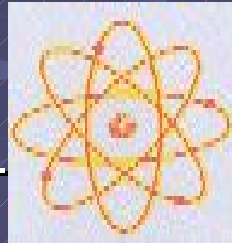
<http://www.fz-juelich.de/nic/Publicationen/Broschuere/Broschuere-d.html>

● Projekte am Jülich Supercomputing Centre (JSC)



Umwelt

Elementar-
Teilchen



Astrophysik



Vielteilchen

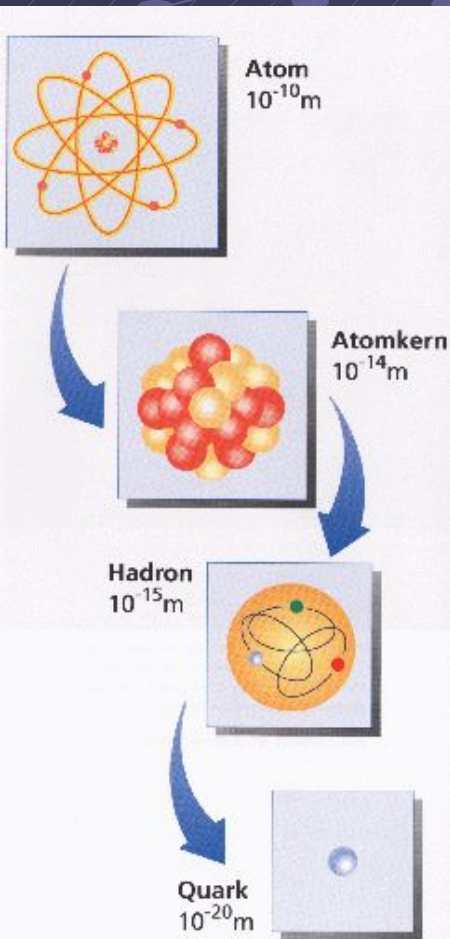
Polymere



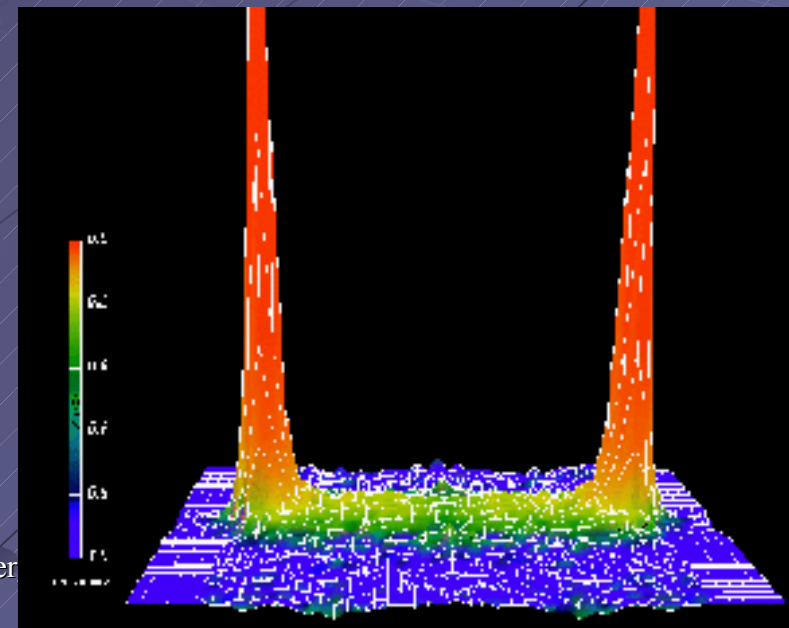
Chemie

Computerphysik - Teilchenphysik

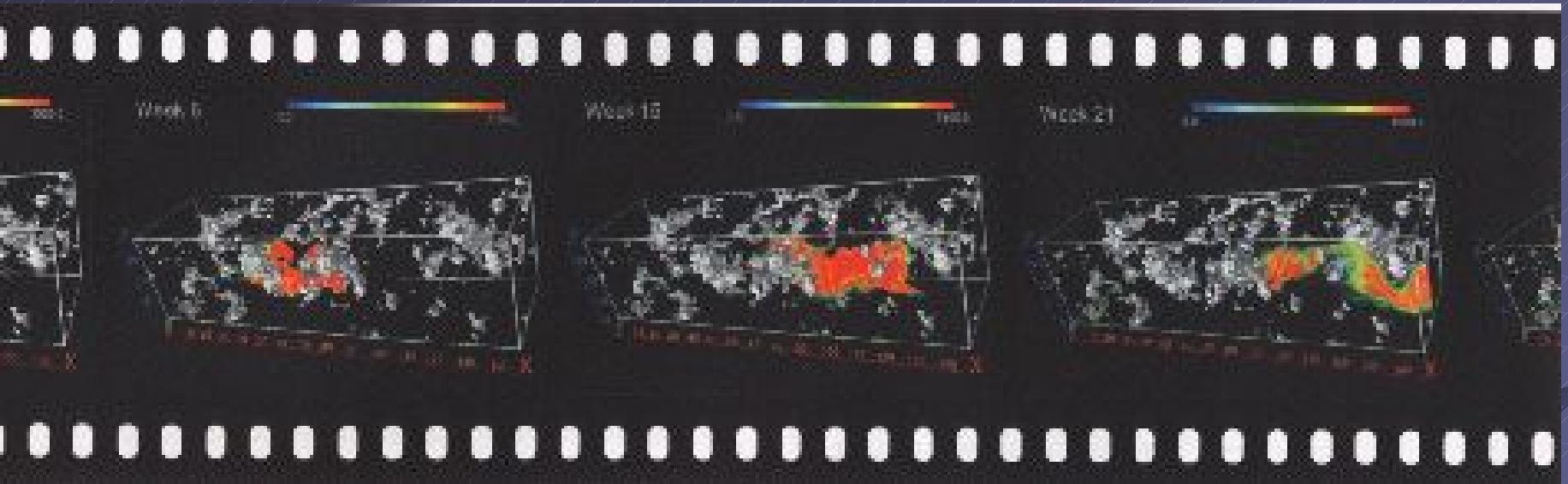
Nahezu die gesamte Masse der Atome ist im Atomkern konzentriert, der aus Protonen und Neutronen besteht und durch die starke Wechselwirkung zusammengehalten wird. Protonen und Neutronen (Hadronen) selbst sind wiederum aus drei Quarks aufgebaut, die durch den Austausch von Gluonen (glue = Klebstoff) zusammengehalten werden. Soweit heute bekannt ist, haben Quarks und Gluonen keine weitere Substruktur. **(Klaus Schilling, NIC-FG Elementarteilchenphysik)**



Man erkennt, daß die statische Wechselwirkung zwischen Quark und Antiquark durch Ausbildung eines engen Flußschlauches erfolgt. Er verhindert, daß Quarks von Antiquarks isoliert werden können.



Computerphysik - Umweltphysik



In Jülich wurde ein Software-Paket entwickelt, mit dem sich die Schadstoffausbreitung im Grundwasser voraussagen läßt. Während mehrjähriger Labor- und Feldarbeit wurden Bodenproben in einem Feld bei Krauthausen nahe Jülich genommen und auf ihre Wasserleitfähigkeit und Speicherkapazität untersucht. Um den Wasserfluß im Böden zu verfolgen, setzten die Forscher ungiftige Fluoreszenz-Farbstoffe ein und analysierten regelmäßig ihren Verbleib. Aus den gewonnenen Daten konnte ein Computer-Modell erarbeitet werden, das die Mobilität von Schadstoffen vorausberechnet. Das Programmpaket besteht aus drei Teilen: "Trace" berechnet den Wasserfluß im Erdboden; das Programm läuft auf einem Parallelrechner. Aufbauend auf den Ergebnissen berechnet "Partrace" die Ausbreitung der Schadstoffpartikel auf dem Vektorrechner CRAY T90. Anschließend werden die Ergebnisse auf einem Graphikrechner visualisiert. Das Bild zeigt die Ausdehnung einer Schadstoffwolke (rot) im Verlauf mehrerer Wochen. Wasserundurchlässige Gesteinsschichten sind grau dargestellt.

(Harry Vereecken, Institut für Erdöl und Geochemie, Forschungszentrum Jülich)

Computerphysik - Astrophysik

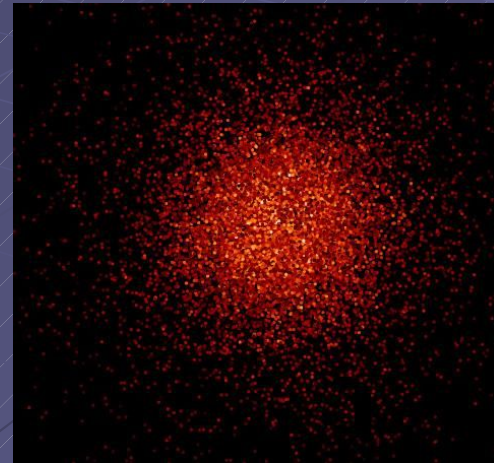
● Theorie:
Differentialgleichung

● Modell:
Diskretisierung

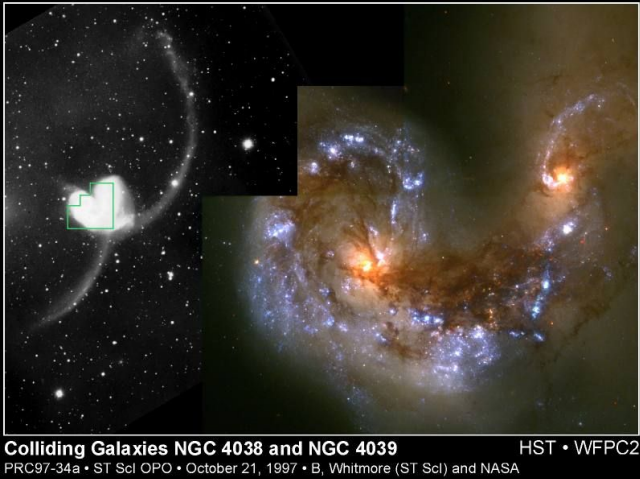
● Simulation:
Zeitablauf

● Ergebnisse:
Vergleich mit Beobachtung oder Theorie

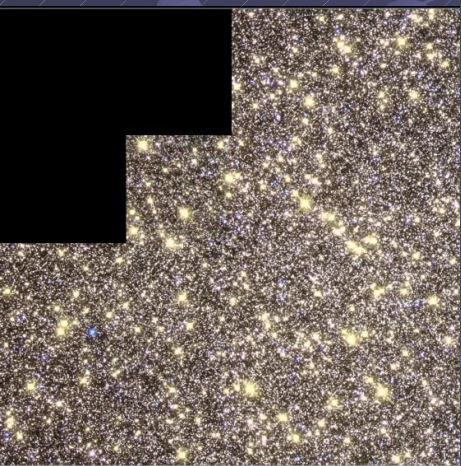
$$\vec{a}_0 = \sum_j Gm_j \frac{\vec{R}_j}{R_j^3} ; \quad \vec{a}_0 = \sum_j Gm_j \left[\frac{\vec{V}_j}{R_j^3} - \frac{3(\vec{V}_j \cdot \vec{R}_j)\vec{R}_j}{R_j^5} \right]$$



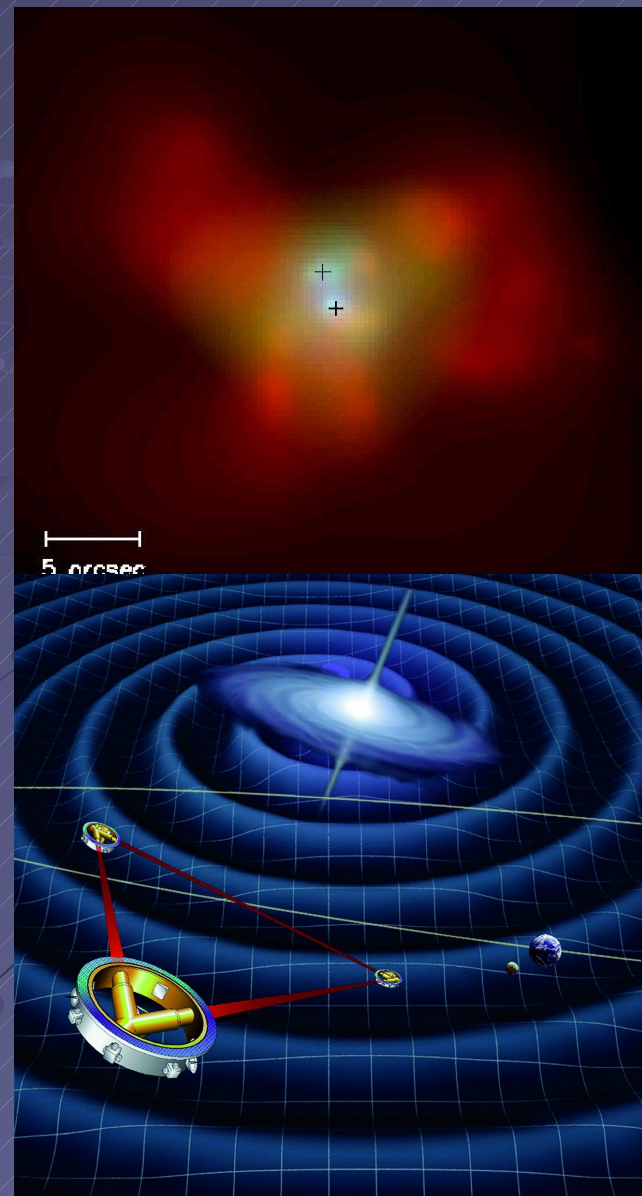
Computerphysik - Relativitätstheorie



Colliding Galaxies NGC 4038 and NGC 4039
HST • WFPC2
PRC97-34a • ST ScI OPO • October 21, 1997 • B, Whitmore (ST ScI) and NASA



Verschmelzung Massereicher Schwarzer Löcher Gravitationswellen

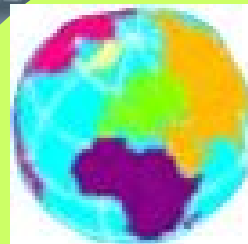
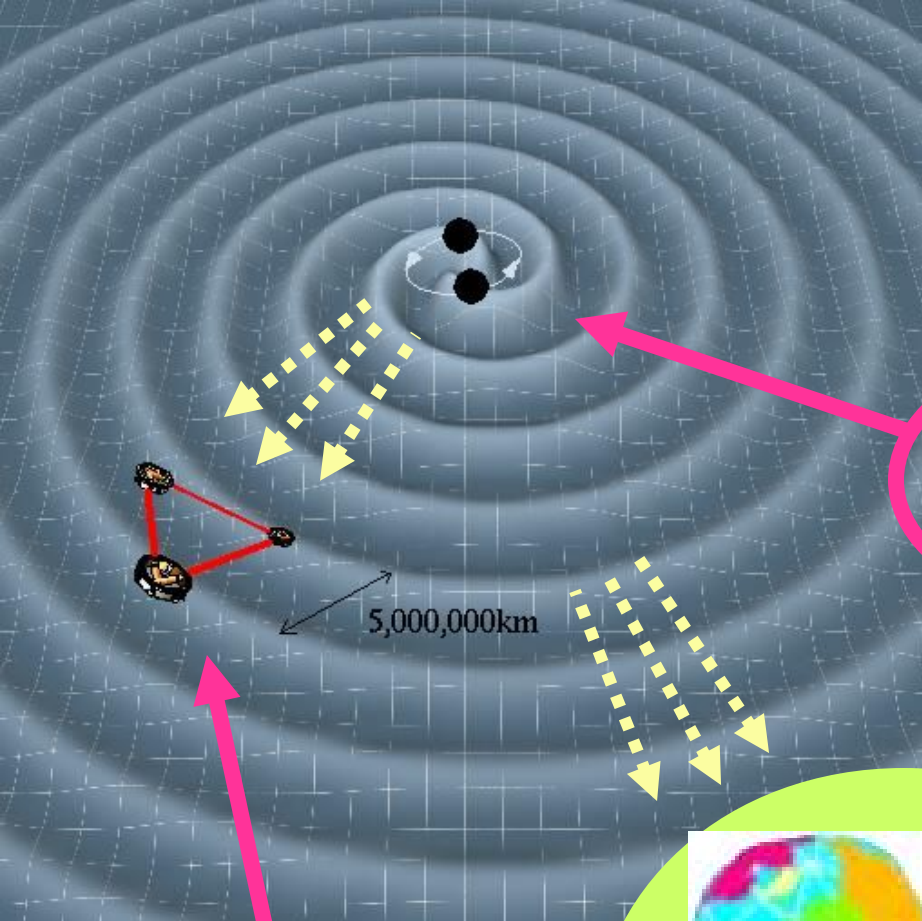


Direct Proof
still waiting

**Astrophysical
Sources**

**Terrestrial Detectors
VIRGO, LIGO, TAMA, AIGO**

**Space detectors
LISA**



EUROPEAN GRAVITATIONAL OBSERVATORY

EGO



Example: VIRGO Detector in Cascina near Pisa, Italy

Consortium of



Computerphysik - Relativitätstheorie

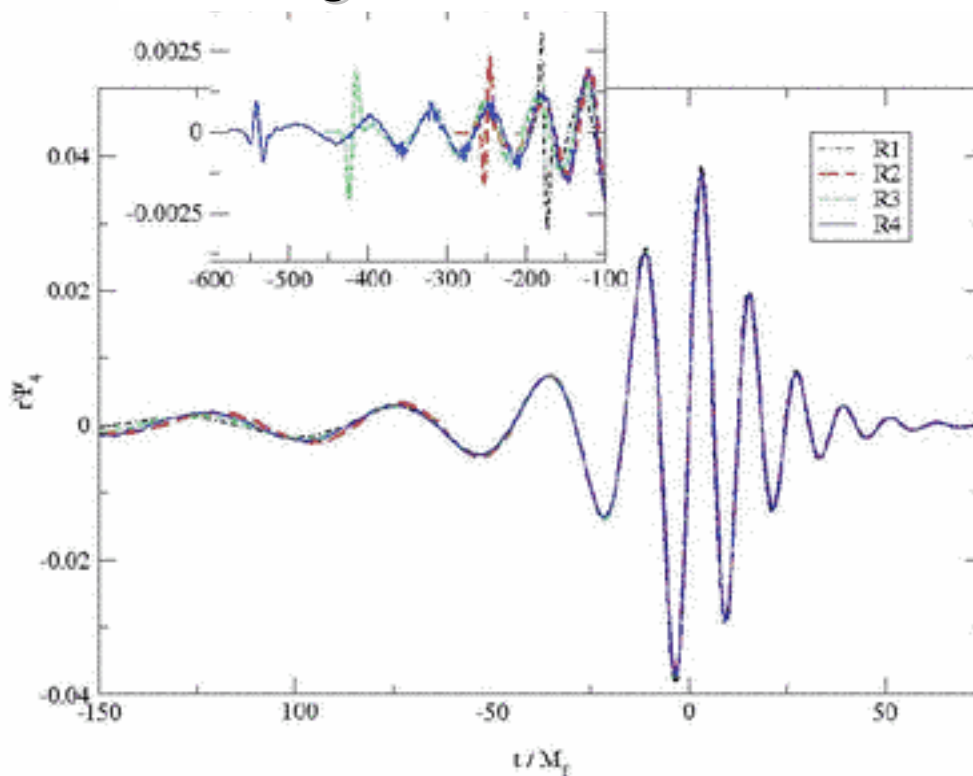


VIRGO – Pisa 3km
LIGO – Livingston, LA
Hanford, WA
1km
GEO600 – Hannover
600m
AIGO – Australien
(planned, 5 km)

<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)

Gravitationswellen-Spur der Verschmelzung Zweier Schwarzer Löcher – direkte Computer -Lösung der Einstein'schen Feldgleichungen!



Initial separations:

R1 = 6.5 M

R2 = 7.6 M

R3 = 8.5 M

R4 = 9.6 M

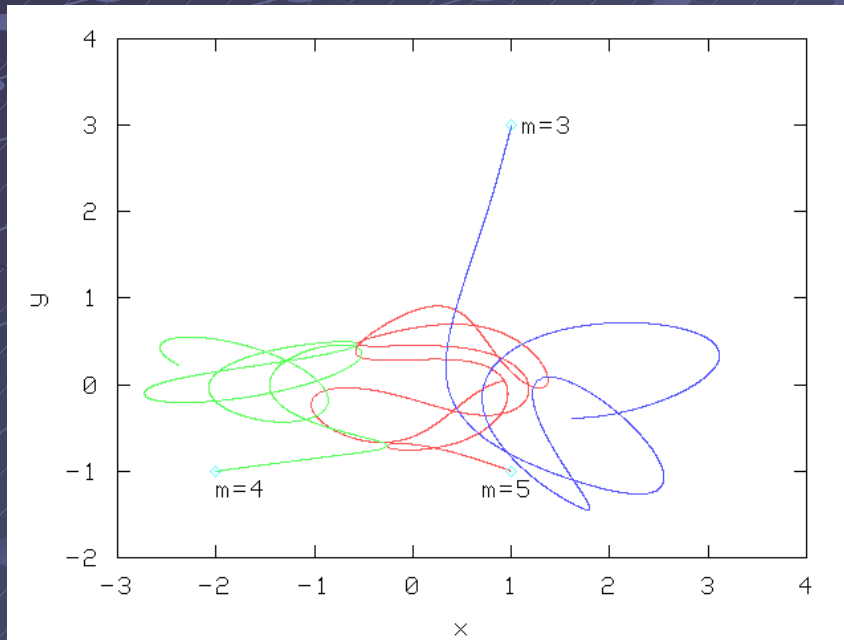
NASA-GSFC

Baker, Centrella, Choi, Koppitz, van Meter

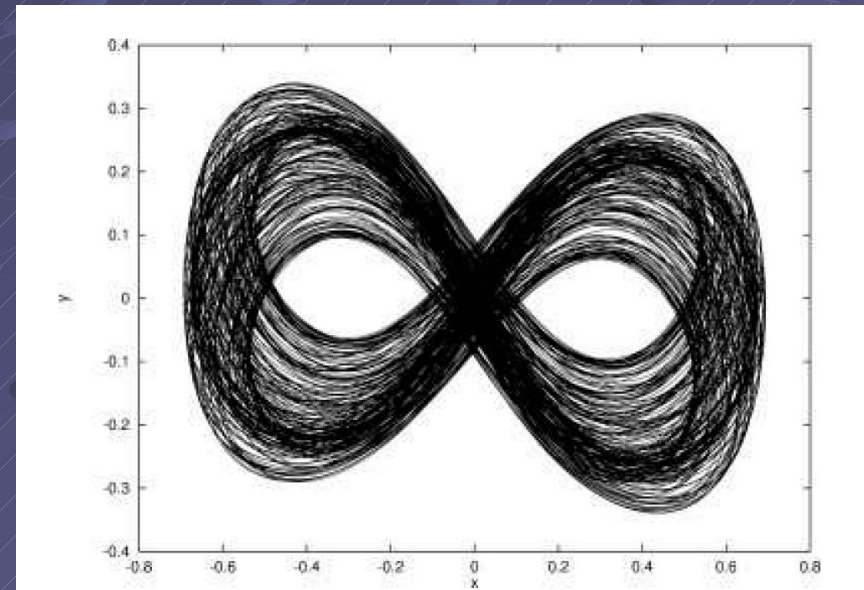
Phys.Rev. D73 (2006) 104002

3-Body Problems

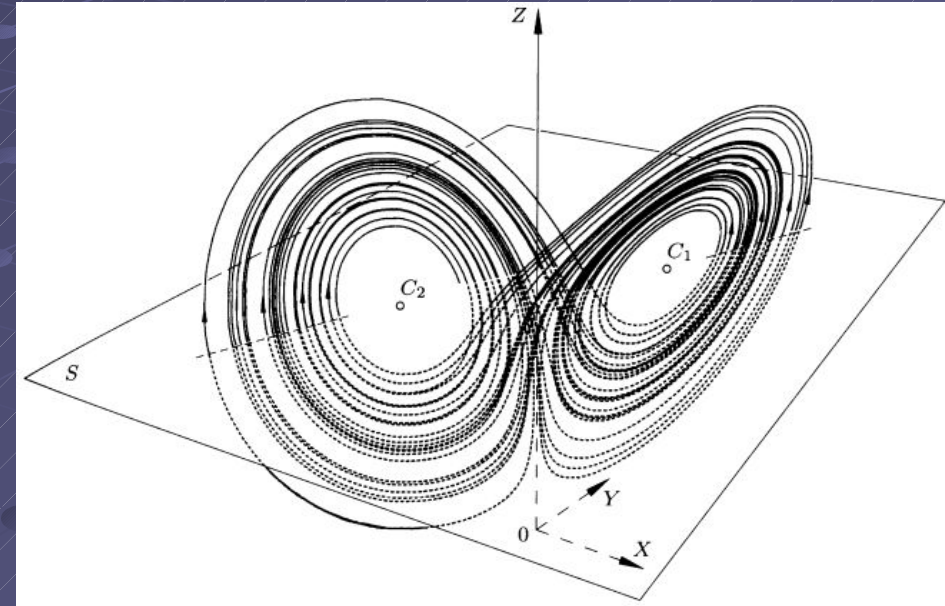
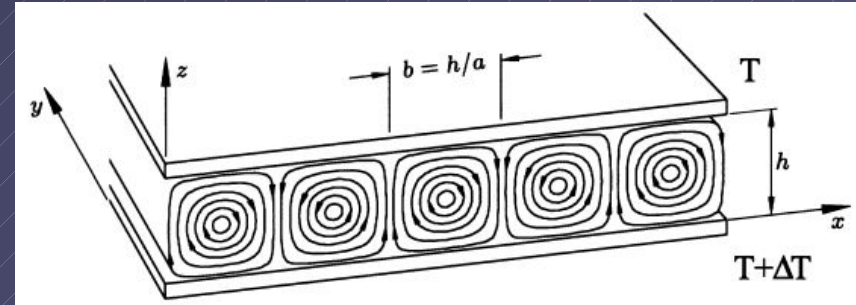
Burrau's Problem



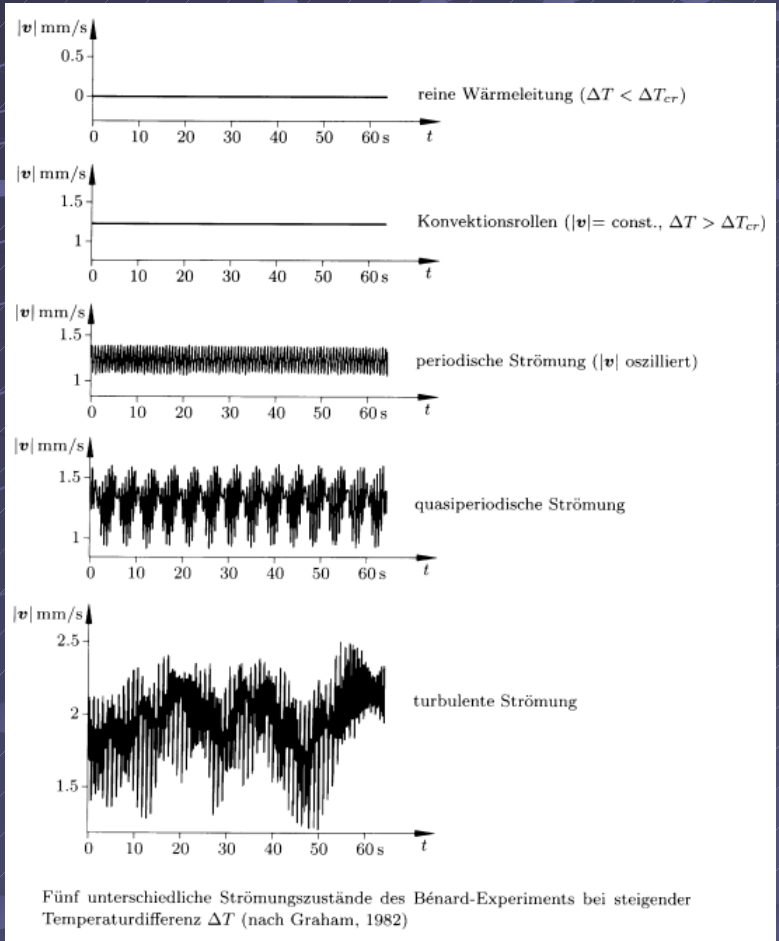
„The Eight“



Lorenz-Attraktor



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

