

The Scientific Profile of the NIC

Prof. Dr. G. Münster

Chairman of the Scientific Council

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A Bit of History

1987: Foundation of HLRZ (Höchstleistungsrechenzentrum)
by KFA Jülich, DESY and GMD

H. Rollnik, F. Hoßfeld

1990: KFA → FZ Jülich

1994: DESY Zeuthen, with parallel computers (APE)

1998: HLRZ → John von Neumann Institute for Computing
founded by FZJ and DESY

A Bit of History

Computers (partial list)

1987 - 88:	Cray X-MP
1989 - 95:	Cray Y-MP
1994 -	Quadrics/APE
1996 - 2004:	Cray T3E, Cray T90/Cray SV1
2004 -	IBM JuMP
2005 -	IBM Blue Gene/L

Organization of NIC

Supported by FZJ and DESY, + GSI soon

Machines operated by

ZAM in Jülich, Director Prof. Dr. Dr. Th. Lippert,
and DESY Zeuthen

- Management Board of Directors
- Scientific Council
- Resource Allocation Committee (RAC)

Organization of NIC

NIC Research Groups

- Elementary Particle Physics
Zeuthen, K. Jansen
- Computational Biology and Biophysics
Jülich, U. Hansmann

Present Computers

- JuMP: IBM p690, 1312 proc., 8.9 TFlop/s → 44.8 TFlop/s
- IBM Blue Gene/L, 2048 proc., 5.7 TFlop/s
- APEmille (Zeuthen), 1104 proc., 0,58 TFlop/s
- apeNEXT (Zeuthen), 1024 proc., 1.6 TFlop/s → 3 TFlop/s

JuMP:



Activities

- **Workshops, Symposia**
~ 3 / year
algorithms, science, machines
- **User Courses**
~ 3 / year
parallel programming, usage of JuMP, ...
- **Guest student program**
2.5 months, 13 participants

Activities

- Winter School
1 week, ~ 40 participants
- Research at NIC/ZAM
Grid Computing, UNICORE, ...

European Activities

European users have access to the facilities in the framework of the programs

- **I3HP**
- **DEISA**
- **SCSE** (Strengthening Computational Science in Europe):
the current **initiative towards new EU member states**

European Activities

I3HP (Integrated Infrastructure Initiative on Hadron Physics)

Supported by the EU

presently

4 groups from DESY, Glasgow, Edinburgh, Cyprus

European Activities

DEISA (Distributed European Infrastructure for Supercomputing Applications)

Amsterdam, Barcelona, Bologna, Edinburgh,
Espoo, Garching, Jülich, München, Orsay,
Reading, Stuttgart

European Activities

DEISA (Distributed European Infrastructure for Supercomputing Applications)

DECI (DEISA Extreme Computing Initiative)

51 project applications in 2005

From NIC, approved:

- tmQCD, Jansen et al., Zeuthen
- IQCS (Quantum Computer Simulations)
De Raedt et al., Groningen
- Black Holes, Spurzem, Heidelberg

Research Proposals

Computing periods: 01.07. - 30.06.

Proposals can be filed by any scientist

Deadline: 30.04.

No deadlines in the SCSE initiative

Form of proposals: see www.fz-juelich.de/nic

Evaluation by the RAC, based on a peer review process

Grant of computer time based on a monthly budget

Application Fields

JuMP, present period

	#	CPUh
Condensed Matter	46	32%
Elementary particles	7	28%
Chemistry	28	17%
Astrophysics	8	10%
Others	25	13%
Materials Science		5%
Comp. Fluid Dynamics		2%
Geosciences		1%
Plasma Physics		1%
Miscellaneous		4%

Project Sizes

~ 150 projects

Exponential distribution

From 44.000 CPUh/month (elementary particles)
to ~ 500 CPUh/month

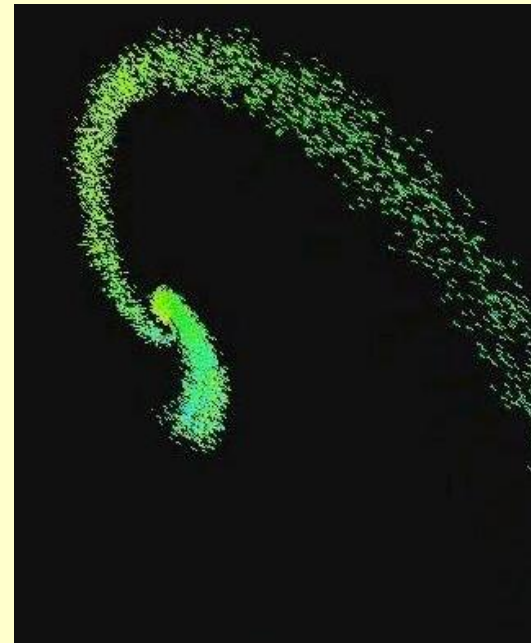
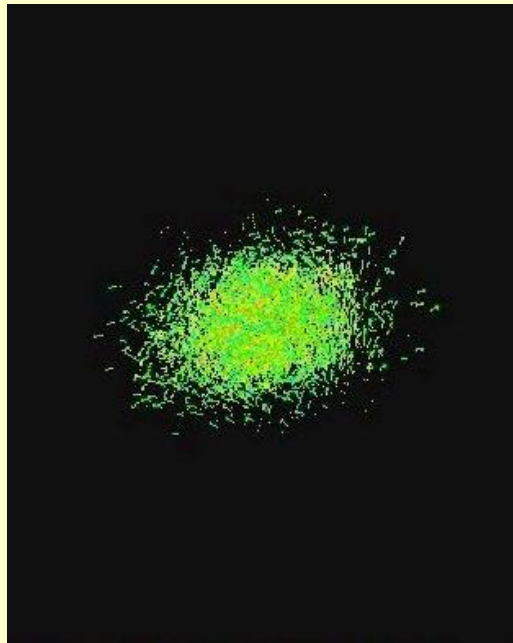
Scientific Fields

Examples from current projects

see also [NIC brochure online](#)

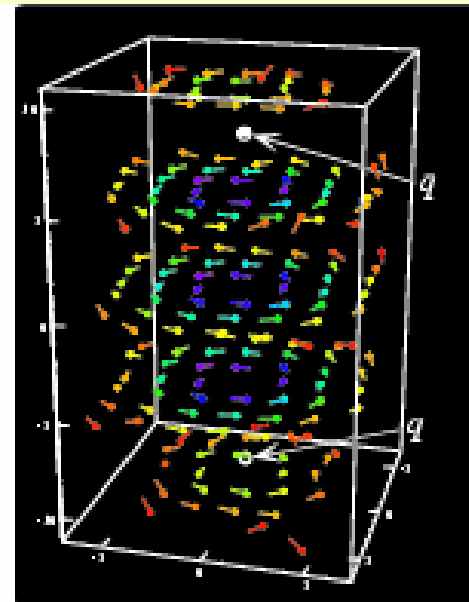
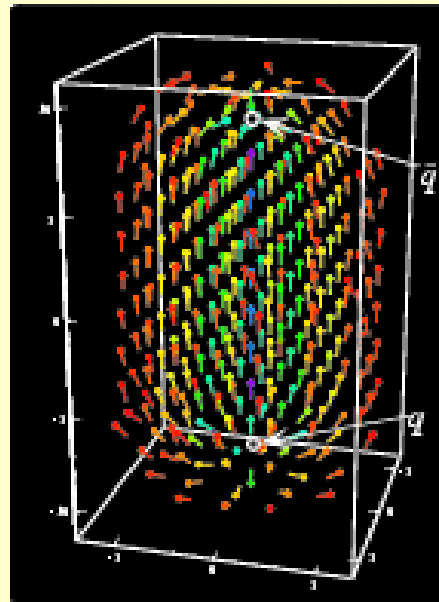
Astrophysics

- Solar eruptions
- Simulations of supernova explosions
- Simulation of astrophysical many-body systems
(star clusters, galaxies)



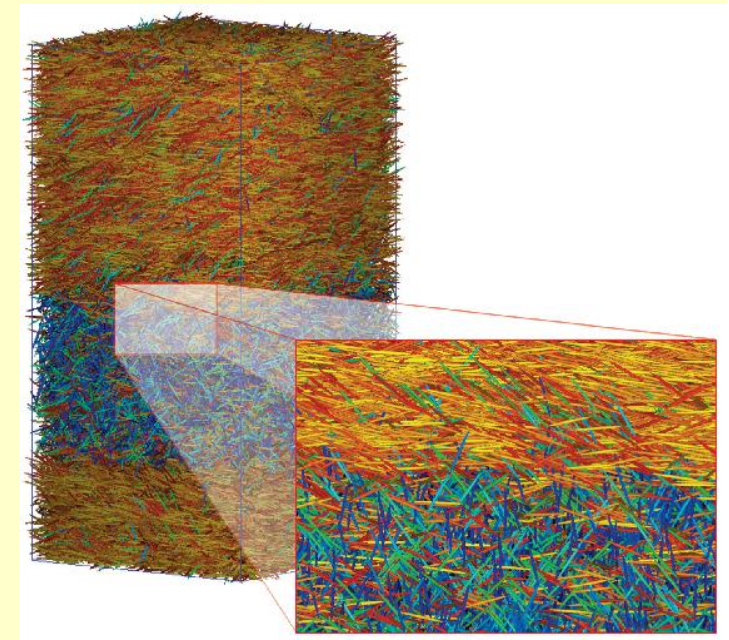
Elementary Particle Physics

- Hadron spectrum
- Structure of nucleons, hadronic matrix elements
- Quark masses
- String breaking in QCD
- Quark confinement



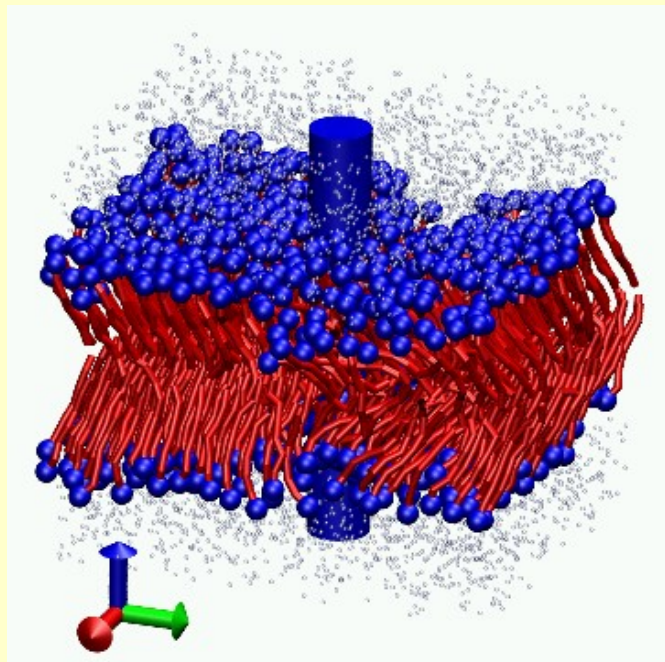
Condensed Matter Physics

- Molecular dynamical simulation of silicates
- High-temperature superconductivity
- Reactions in biological systems
- Quantum Monte Carlo studies of correlated systems
- Microscopic properties of surfaces
- Properties of nanowires
- Rodlike liquid crystalline molecules



Polymers - Soft Matter

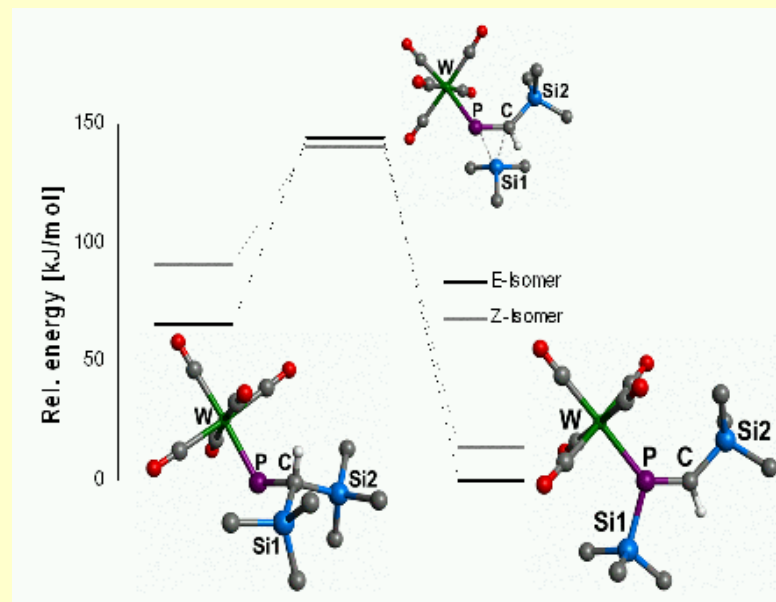
- Simulations of branched polymers
- Orienting liquid crystals
- Lipid-protein interactions



lipid-gel phase

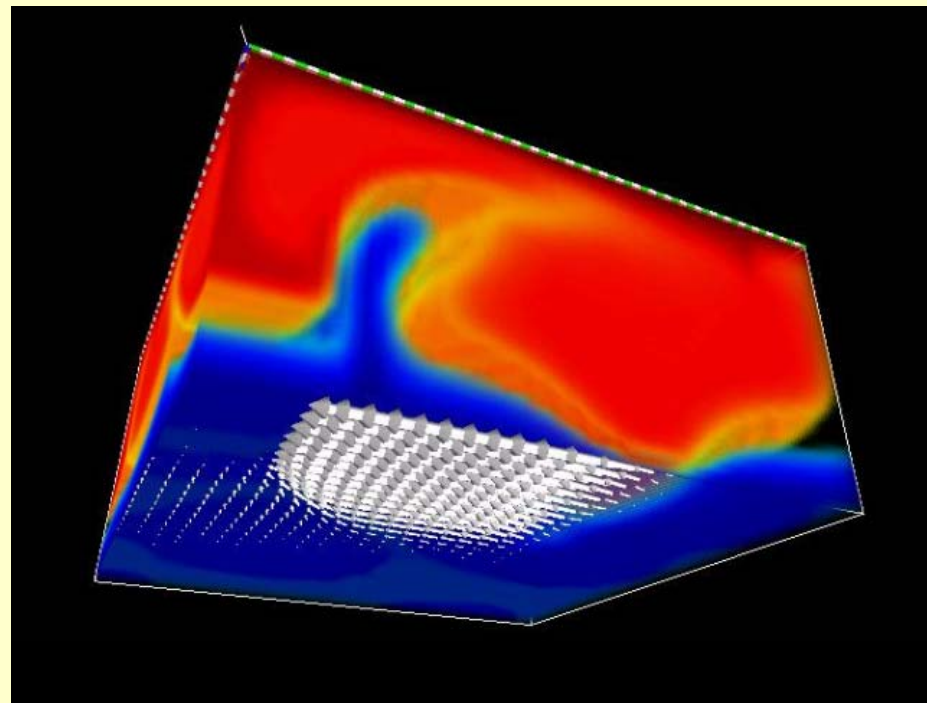
Chemistry

- Nanostructured clusters of transition metal oxides
- Chromophores in nonlinear optics
- Photostability of DNA
- Electronic conduction on the molecular scale
- Rearrangements of molecular complexes - the Compliance Matrices Method



Earth and Environment

- Transport of contaminants in the soil
- Viscosity of the earth's mantle
- Origin of the earth's magnetic field
- Mantle convection and plate tectonics



Others

- Nonlinear EEG analysis of epilepsy patients
- Spatio-temporal patterns of ion channels in biomembranes
- Compact Laser-driven ion sources
- Molecular mechanism of conduction in ion channels
- Synchronisation processes in the brain

