# General Information

## Venue

Auditorium of Forschungszentrum Jülich.

## Oral Presentations

The Auditorium is equipped with overhead projectors, slide projectors and a video beamer.

## Poster Session

We invite contributions in the form of poster presentations. The posters will be mounted on movable walls provided by the organisers. The maximum size of a single poster should not exceed 90 cm width and 145 cm height (portrait format).

## Registration

Please register before **7 February 2008** under the following link http://www.fz-juelich.de/nic/symposium/

## Accommodation

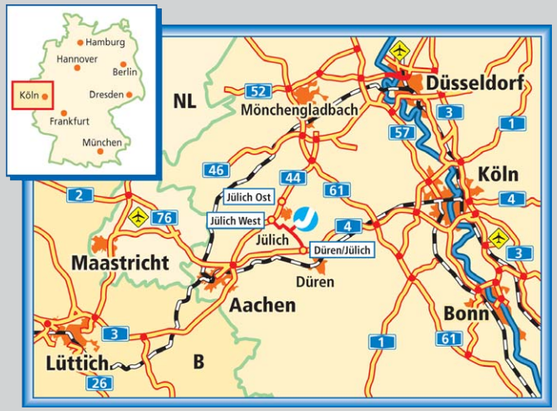
We have booked a number of rooms at hotels in Jülich, which will be held for NIC-Symposium until **7 February 2008**. Please use the Online-Registration form to reserve a room.

You will receive a confirmation of your room reservation from Ms. Erika Wittig immediately.

Reservations received after that date will be accepted on a space available basis.

Shuttle service will be provided from the Hotel „Am Hexenturm“ to the conference site.

**How to find us:**




## How to get to Jülich

Jülich can be reached

*By train:* go to Düren main station (Hauptbahnhof), then take the local train (Rurtalbahn) to Jülich.

*By plane:* Düsseldorf or Cologne airport. Individual transportation to Jülich upon request.

*By car:* via Autobahn A4, A44 and A61 (see map).

**We are looking forward to seeing you in Jülich**

## Further Information

Additional information is available on the web at

**http://www.fz-juelich.de/nic/symposium/**

or contact the conference service:

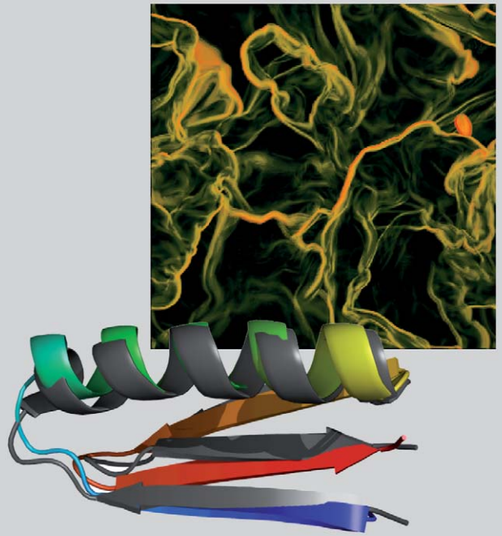

Forschungszentrum Jülich GmbH
Ms. Erika Wittig
D-52425 Jülich

Telefon: 02461-61-3833
Fax: 02461-61-5333
E-Mail: e.wittig@fz-juelich.de


John von Neumann Institute for Computing

# NIC Symposium 2008

**20 – 22 February 2008**
**Forschungszentrum Jülich, Germany**



**Invitation and Registration**

This fourth NIC symposium will give an overview of the activities and the results obtained in the last two years at the John von Neumann Institute for Computing (NIC). The great progress in supercomputing is also highlighted by the fact that the newly installed Blue Gene/P system in Jülich currently ranks number two in the Top 500 List. This will open new dimensions in supercomputing for researchers in Germany and Europe.

NIC – a joint institute of Forschungszentrum Jülich, Deutsches Elektronen-Synchrotron (DESY) and Gesellschaft für Schwerionenforschung (GSI) – supports with its supercomputer facilities about 130 research groups at universities and national labs which work on computer simulations in various fields of science.

Fifteen invited lectures will cover selected topics in the following fields:

- Astrophysics
- Biophysics
- Chemistry
- Condensed Matter
- Material Science
- Elementary Particle Physics
- Polymers
- Environmental Research
- Nuclei, Atoms, Plasmas, and Patterns

The talks are intended to inform a broad audience of scientists and the interested public about the research activities at NIC.

The proceedings of the symposium will cover a larger range of projects that have been supported by the IBM JUMP And IBM Blue Gene/L supercomputers in Jülich and the APE topical computer at DESY Zeuthen.

This symposium will be the fourth in a series intended to document regularly the activities at NIC.

## Organizing Committee

G. Münster
D. Wolf
M. Kremer

Ms Helga Frank (Symposium Secretary)
Ms Erika Wittig (Conference Service)

# Programme

## Wednesday, 20 February 2008 (Auditorium)

| | |
|---|---|
| 8.30 | Transfer from Jülich |
| 9.00 | Registration |
| 9.30 | Opening |
| 9.45 | Th. Lippert, Forschungszentrum Jülich<br>The Status of Supercomputing: Technical and Political Developments |
| 10.30 | Coffee |
| 11.00 | Z. Fodor, NIC, DESY Zeuthen<br>Phase Transitions and the Mass of the Visible Universe |
| 11.45 | G. Schierholz, NIC, DESY Zeuthen<br>The Transverse Spin Structure of the Nucleon |
| 12.30 | Lunch |
| 14.00 | M. Gruner, Universität Duisburg-Essen<br>Large-Scale First-Principles Calculations of Magnetic Nanoparticles |
| 14.45 | R. Jones, Forschungszentrum Jülich<br>Structural Patterns in Ge/Sb/Te Phase-change Materials |
| 15.30 | Coffee |
| 16.00 | E. Koch, Forschungszentrum Jülich<br>Realistic Description of TTF-TCNQ – a Strongly Correlated Organic Metal |
| 16.45 | J. Harting, Universität Stuttgart<br>Boundary Effects in Microfluidic Setups |
| 17.30 | Poster Session and Reception |
| 19.00 | Transfer to Jülich |

## Thursday, 21 February 2008 (Auditorium)

| | |
|---|---|
| 8.30 | Transfer from Jülich |
| 9.00 | S. Jahn, GFZ Potsdam<br>Fluids under Extreme Conditions of Pressure and Temperature and their Role in Geological Processes |
| 9.45 | R. Spurzem, Universität Heidelberg<br>Formation and Evolution of Black Holes in Galactic Nuclei and Star Clusters |
| 10.30 | Coffee |
| 11.00 | U.H.E. Hansmann, NIC Jülich<br>Protein Simulations on Massively Parallel Computers |
| 11.45 | W. Plass, Universität Jena<br>Transition Metal Centers in Biological Matrices: Why Nature Has Chosen Vanadate as Cofactor for Haloperoxidase |
| 12.30 | Lunch |
| 14.00 | D. Marx, Universität Bochum<br>Glycine at the Pyrite Water Interface: An *ab initio* Metadynamics Study |
| 14.45 | F. Müller-Plathe, TU Darmstadt<br>Molecular Dynamics Simulations of PVA/Pt(111) Interfaces |
| 15.30 | Coffee |
| 16.00 | B. Metsch, Universität Bonn<br>Coarse Grid Classification: AMG on Parallel Computers |
| 16.45 | M. Behr, RWTH Aachen<br>Towards Shape Optimization for Ventricular Assist Devices Using Parallel Stabilized FEM |
| 17.30 | Transfer to Jülich |

## Friday, 22 February 2008

| | |
|---|---|
| 8.30 | Transfer from Jülich |
| 9.00 | Jutta Docter, Michael Stephan, Forschungszentrum Jülich<br>Introduction to JUGENE at Forschungszentrum Jülich (Lecture Room at JSC) |
| 10.00 | Christoph Pospiech, IBM<br>Porting Applications to Blue Gene/P (Lecture Room at JSC) |
| 11.30 | Inauguration of the Blue Gene/P System (Auditorium) |
| 13.30 | Transfer to Jülich |

More details are available at:
**http://www.fz-juelich.de/nic/symposium/**