Computational Steering with VISIT in UNICORE

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NIC - John von Neumann Institute for Computing
Research Centre Jülich, Germany

1st UNICORE Summit
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14:30 – 15:00

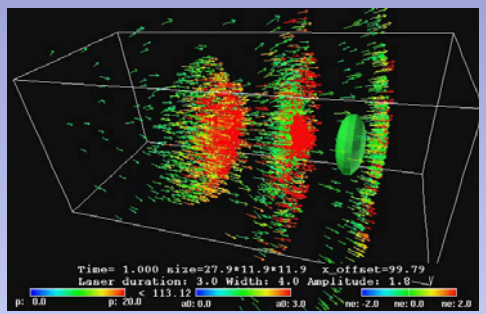
Content

- Motivation - Computational Steering
- VISIT – a toolkit for Computational Steering
- UNICORE – VISIT integration
- Work in progress

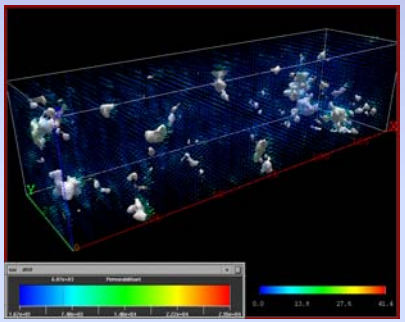
Motivation

- Online visualization and Computational steering:
  - Visualize intermediate results of a simulation as they are created
  - Change simulation parameters of a running simulation on the fly
- Benefits:
  - Gain immediate visual insight into the simulated system
  - Speed up the cycle of
    parameter selection → simulation → post-processing → interpretation
  - Make more efficient use of valuable resources:
    supercomputers & researchers time
- GRID:
  - Provide the infrastructure and tools for secure and seamless operation of the above

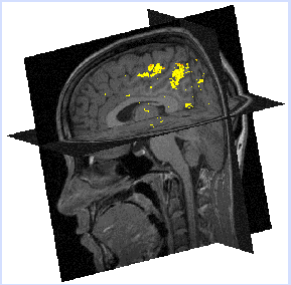
Computational Steering Examples



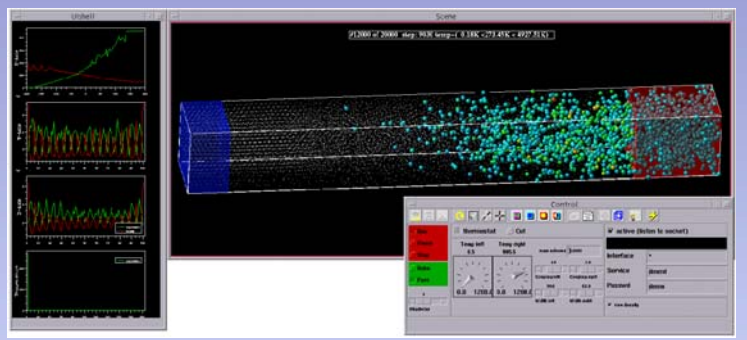
PEPC: Plasma simulation



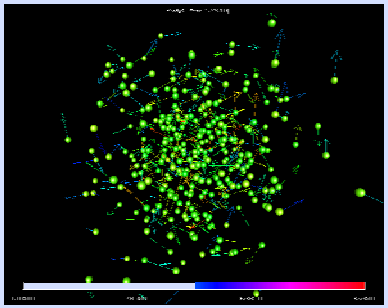
Trace: groundwater pollution



FIRE: Realtime fMRI

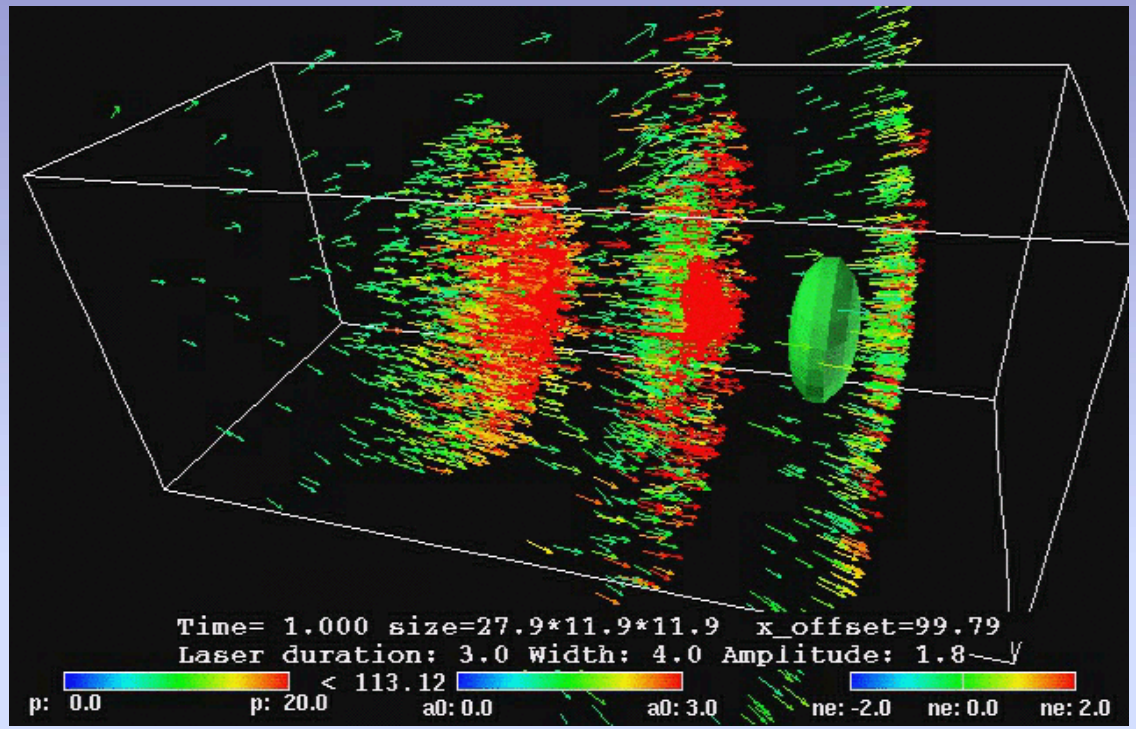


DMMD: molecular dynamics



NBODY: star cluster

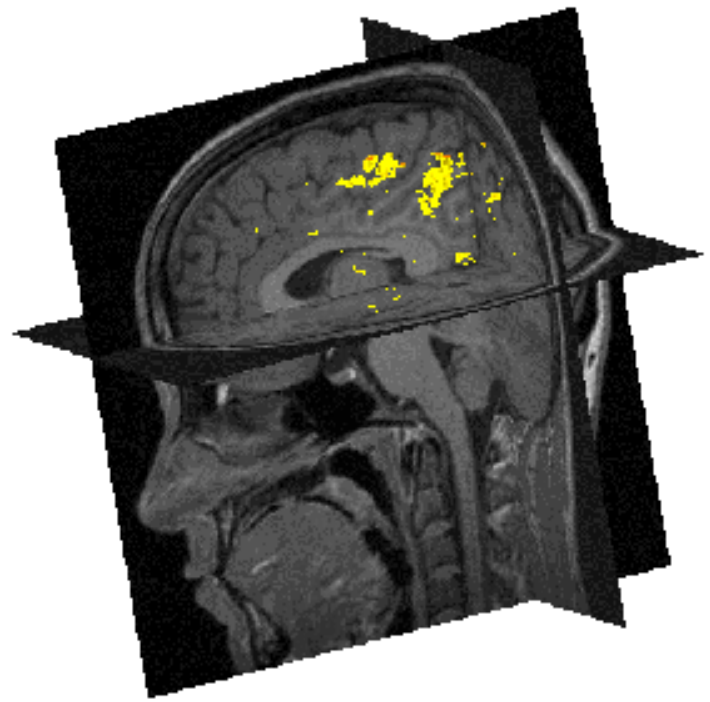
PEPC: Plasma Simulation



- Simulation of a particle accelerator via Laser pluses:
  modify e.g. laser beam parameters on the fly
- Online visualization and steering included during code development:
  debugging
- Education: give students immediate visual insight

(Paul Gibbon, NIC, FZ-Jülich)

FIRE: Realtime fMRI



- functional Mangetic Resonance Imaging - Online monitoring of brain activity:
  MRI + Parallel Computer + Visualization
- Optimize / modify experimental parameters
  while the test person is in the scanner

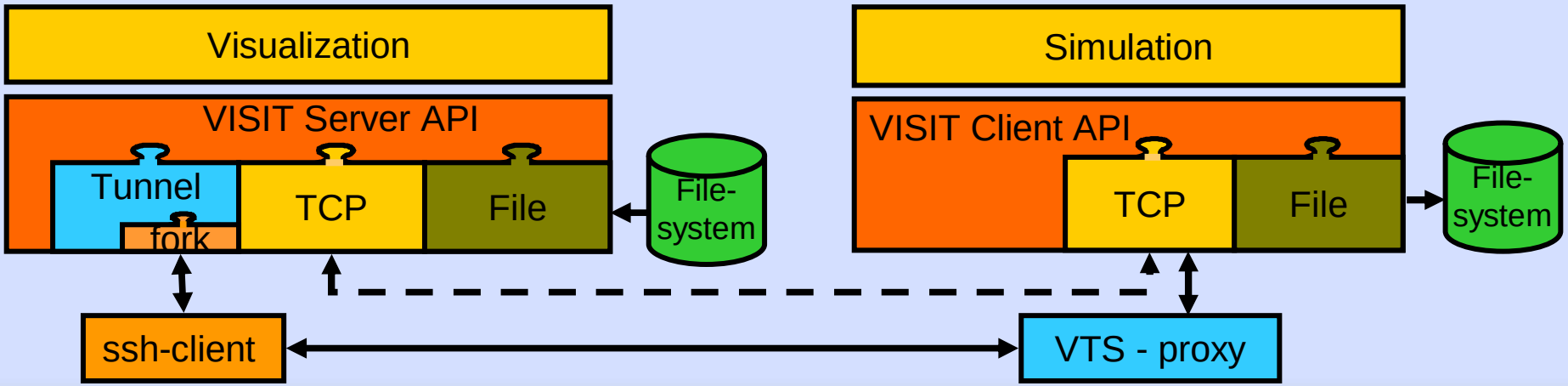
(Stefan Posse, Institute for Medicine, FZ Jülich)

VISIT – Visualization Interface Toolkit

- Light-weight library for Online-Visualisation and Computational Steering
- Functionality:
  - Dynamic attachment/detachment of visualization(s) to/from simulation
  - Bi-directional data transport, transparent conversion
  - Dynamic resource discovery via directory service (SEAP)
- Various language bindings
  - Supports C, FORTRAN, Perl, Java for simulation
  - Supports C, Perl, AVS/Express, IDL, Java for visualisation
- Support for large applications via add-on library LVISIT
  - parallel simulations and data-reduction
  - higher-level API and code generator
- Open Source, available at: www.fz-juelich.de/zam/visit

VISIT - Design

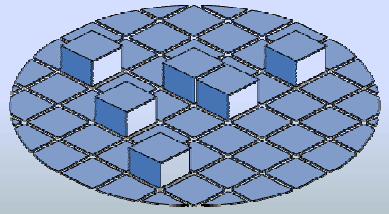
- lean API towards application
- Internal device API to support different transport mechanisms:
  - TCP/IP
  - File I/O
  - Fork: parent-child communication
  - Tunnel: firewall-friendly by tunnelling through ssh-connection
    seamless establishment of ssh-connection ?



VISIT extension for UNICORE

- Goals:
  - Support online visualization and computational steering of UNICORE jobs
  - Make use of UNICORE's security and single-sign-on model, further simplifying VISIT handling
  - No performance compromise
  - No modification of core components of current production version of UNICORE V5
  - No modification of VISIT client API
    Use existing applications (almost) without modification
  - Concept "upgradeable" to UNICORE/GS

- Work carried out in FP6-STREP UniGrids:

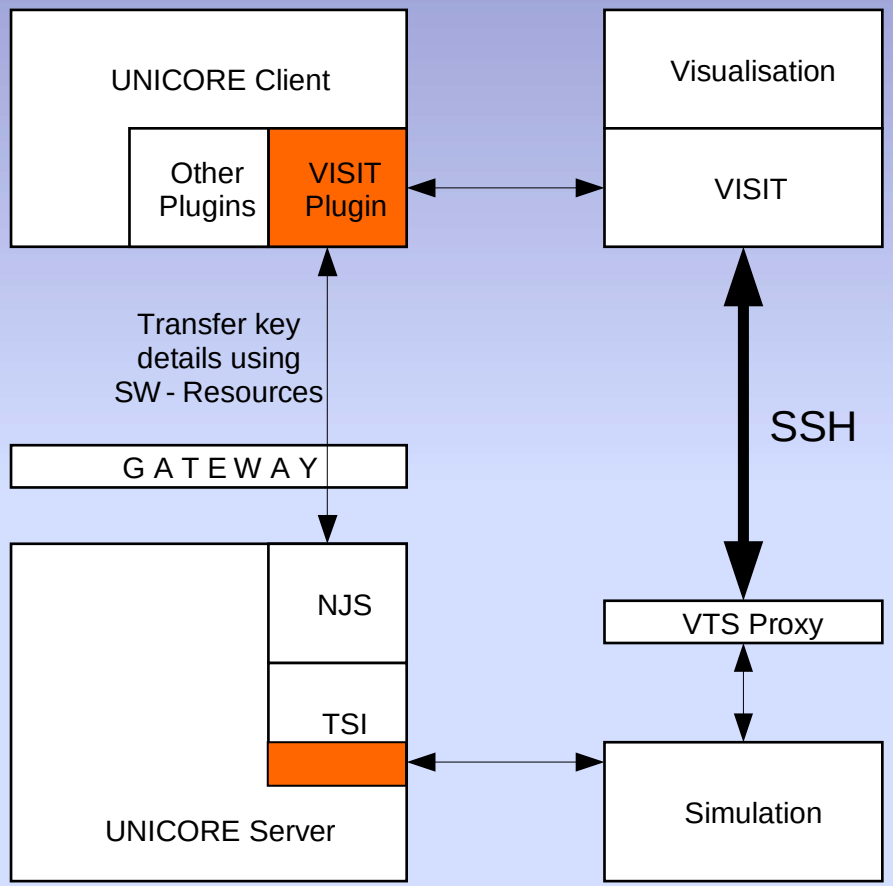


UniGrids

Morris Riedel
Wolfgang Frings
Thomas Eickermann

VISIT / UNICORE Implementation

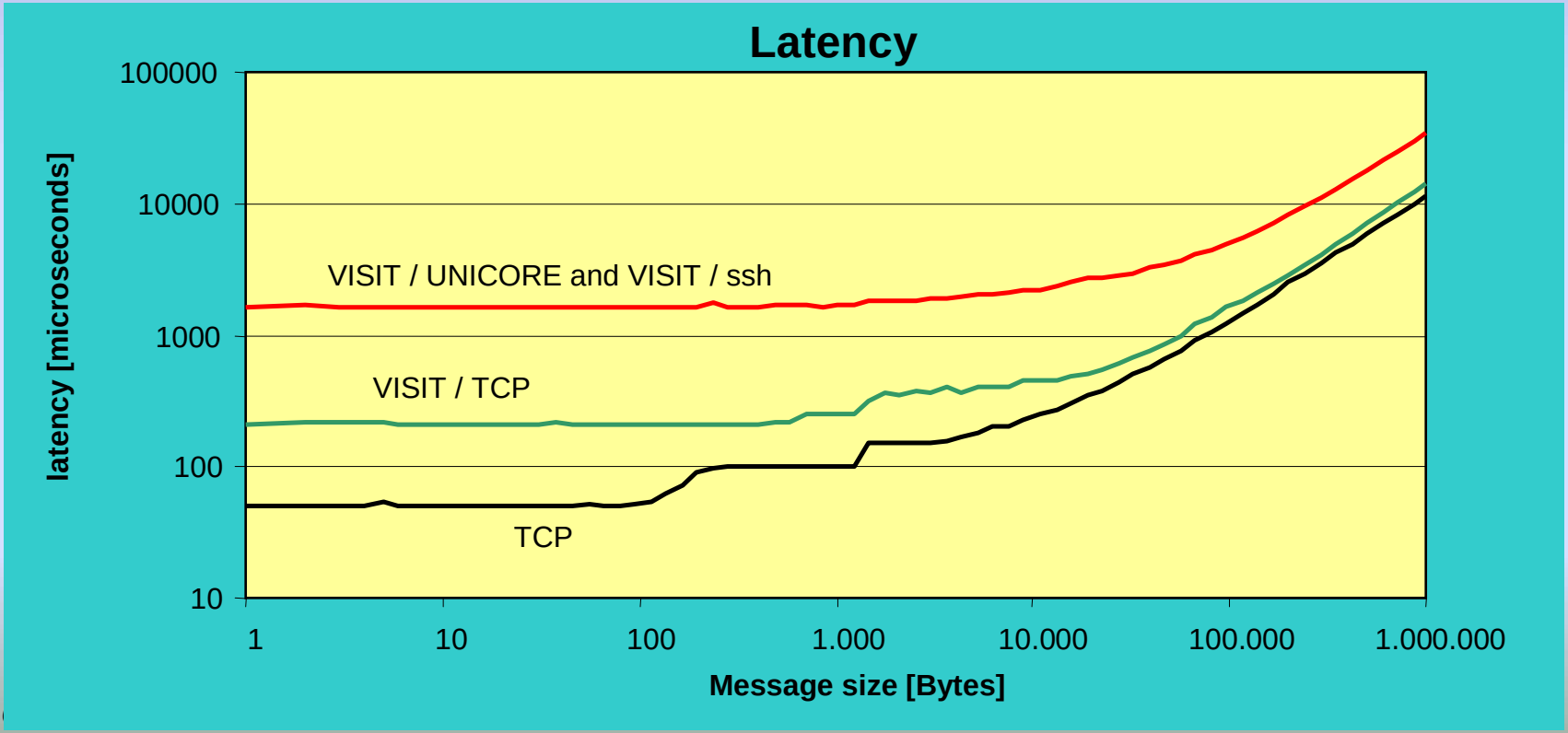
- Uses VISIT's ssh-tunnel with public-key authentication
- UNICORE-VISIT client plugin:
  - Creates key-pair
- TSI-extension:
  - places & removes public key on target system
- First demonstration at UniGrids Review in September



VISIT / UNICORE Performance

- Setup: Two Dual-Pentium Linux-PCs with Gigabit-Ethernet connections

- Throughput VISIT/UNICORE: 220 Mbit/s
  (TCP: 660 Mbit/s, VISIT/TCP: 540 Mbit/s)
- No performance penalty through UNICORE (compared to plain VISIT-ssh)

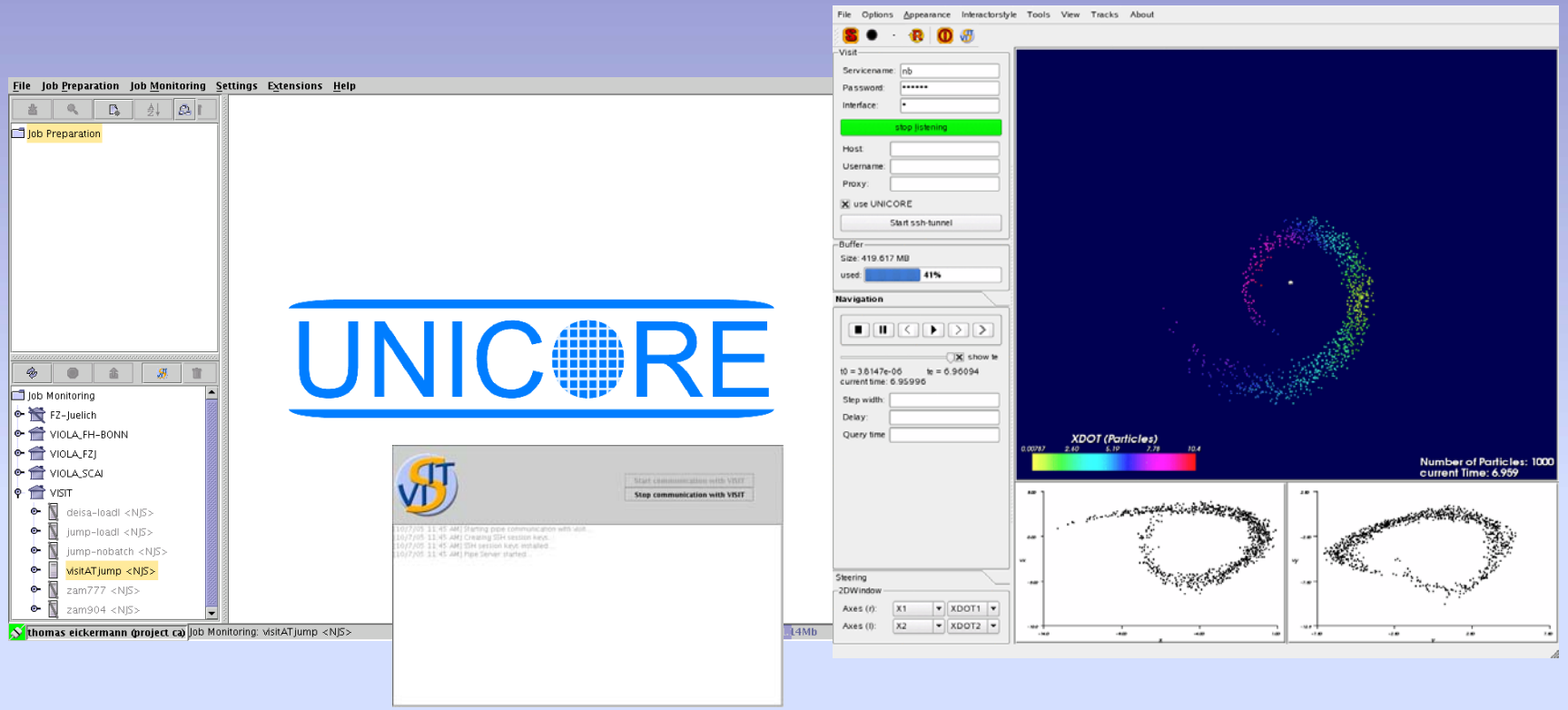


Application Example: nbody

- **nbody** is a well-known parallel simulation tool in the astrophysics community
  - Star cluster simulations
  - Planetary dynamics
  - Models of active galactic nuclei containing black holes
  - Extension for VISIT is available
    (by Andreas Ernst, ARI Heidelberg)

- **Xnbody**, an online visualization and steering tool for nbody6++
  (by Sonja Dominiczak, NIC FZ Jülich)
  - Visualize the internal dynamical evolution of stellar systems
  - Based on Qt and VTK
  - Uses VISIT / UNICOREto communicate with nbody

Xnbody Demo at UNICORE-Summit



- Run and steered via VISIT / UNICORE:
  - Client on a Laptop here
  - 16 CPU Job at NIC's 9 TFLOPS Supercomputer JUMP in Jülich

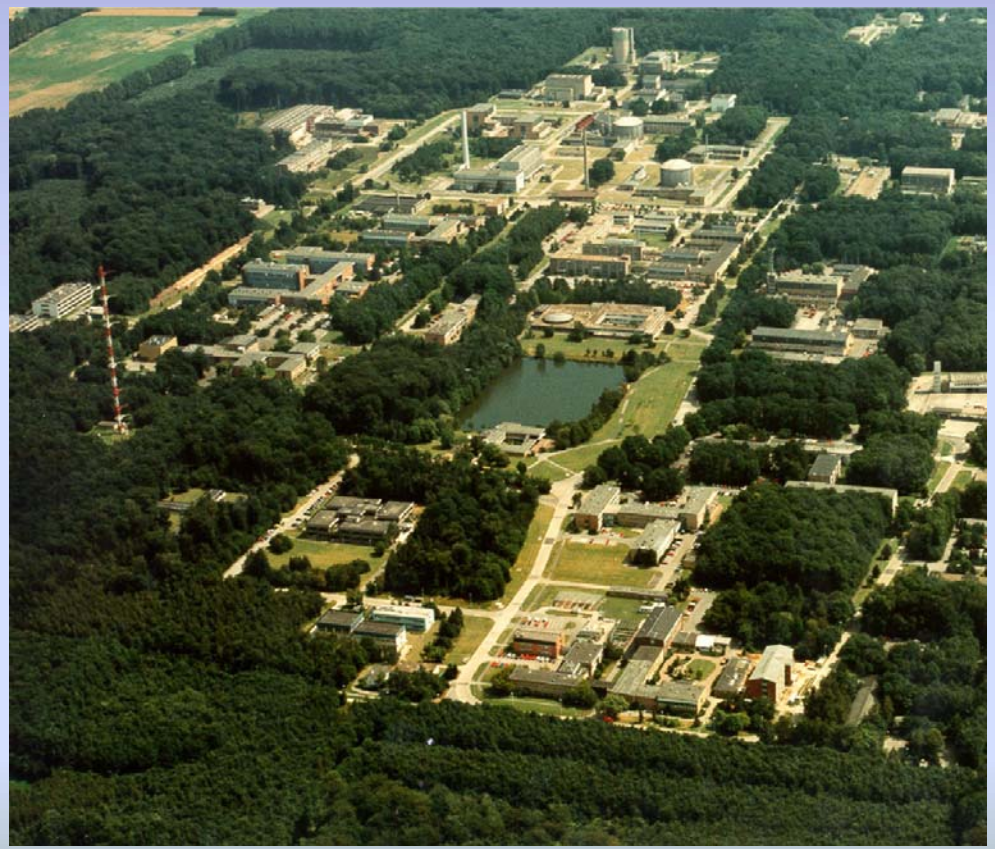
Summary and Outlook

- VISIT / UNICORE provides:
  - Online visualization and computational steering of UNICORE jobs
  - Uses UNICORE's security and single-sign-on
  - Is firewall-friendly by using ssh for data transfer
  - Delivers good performance
  - Is the basis for a new UNICORE client-plugin for interactive shell access
- Next steps:
  - Migrate to UNICORE/GS
  - Add support for collaborative visualization
  - Deploy more applications:
    - Geo-Dynamics by Uni Münster is almost done (Summer Student)
    - Huge atmospheric data sets is under way (VIOLA)

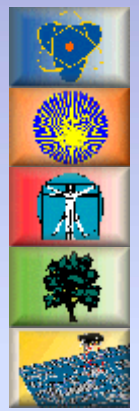
Finally

About Research Centre Jülich

- Member of Helmholtz-Society
- ~ 4200 Employees / 1000 Scientists



5 Work areas:



Matter,

Energy,

Life,

Environment

Information

Central Institute for Applied Mathematics (ZAM) /

John von Neumann Institute for Computing (NIC)

JUMP – Jülich Multi Processor

11 March 2004: 41 x 32 Power4+ 1.7 GHz,
128 GByte, High Performance Switch
8922 Gflops Peak, 5568 Gflops LINPACK

Implementation Details