

Computational Steering with VISIT in UNICORE

Thomas Eickermann Sonja Dominiczak, Wolfgang Frings, Morris Riedel (th.eickermann@fz-juelich.de)

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

> 1st UNICORE Summit October 11th 2005 14:30 - 15:00

October 11th 2005

Content



- Motivation Computational Steering
- VISIT a toolkit for Computational Steering

UNICORE - VISIT integration

Work in progress

Motivation

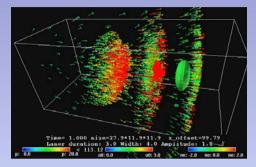


- Online visualization and Computational steering:
 - Visualize intermediate results of a simulation as they are created
 - Change simulation parameters of a running simulation on the fly
- Benefits:
 - Gain immediate visual insight into the simulated system
 - Speed up the cycle of parameter selection \rightarrow simulation \rightarrow post-processing \rightarrow 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

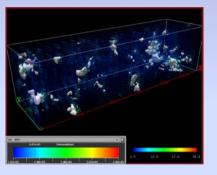
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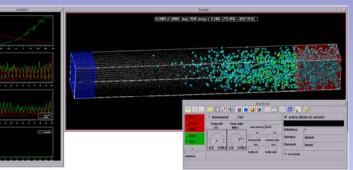
Computational Steering Examples



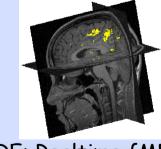


PEPC: Plasma simulation



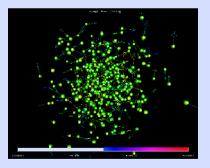


DMMD: molecular dynamics



FIRE: Realtime fMRI

Trace: groundwater pollution

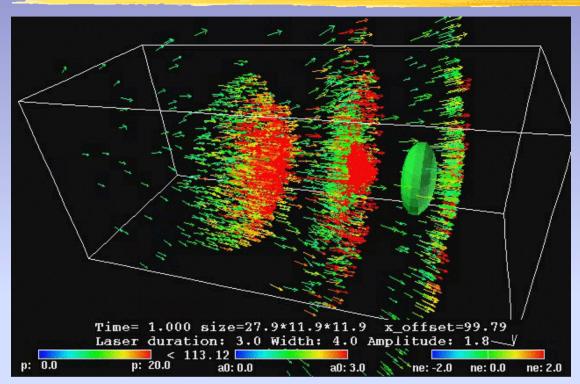


NBODY: star cluster

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PEPC: Plasma Simulation



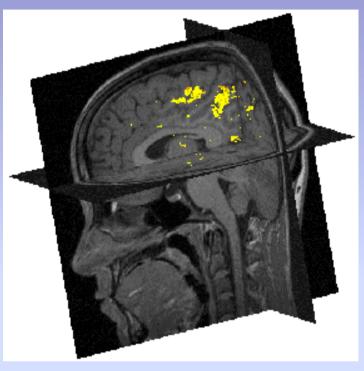


- Simulation of a particle accelerator via Laser pluses: modify e.g. laser beam parameters on the fly
- Online visualization and steering included during code development: debugging
- Education: give students immediate visual insight

(Paul Gibbon, NIC, FZ-Jülich) October 11th 2005

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)

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VISIT - Visualization Interface Toolkit

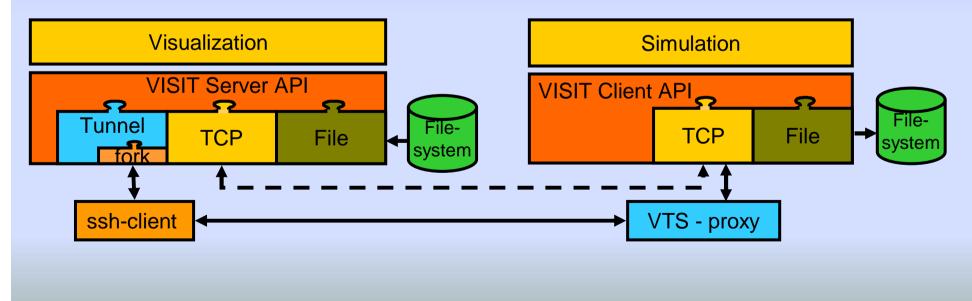


- Light-weight library for Online-Visualisation and Computational Steering
- Functionality:
 - Dynamic attachment/detachment of visualization(s) to/from simulation
 - Bi-directional data transport, transparent conversion
 - Dynamic resource discovery via directory service (SEAP)
- Various language bindings
 - 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



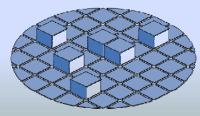
- lean API towards application
- Internal device API to support different transport mechanisms:
 - TCP/IP
 - File I/O
 - Fork: parent-child communication
 - Tunnel: firewall-friendly by tunnelling through ssh-connection seamless establishment of ssh-connection ?



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:





Morris Riedel Wolfgang Frings Thomas Eickermann

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First demonstration at **UNICORE** Server UniGrids Review in September Th.Eickermann

plugin: Creates key-pair

VISIT / UNICORE Implementation

places & removes public

UNICORE Client

Other

Plugins

Transfer key details using

SW - Resources

GATEWAY

VISIT

Plugin

NJS

TSI

VTS Proxy Simulation

Uses VISIT's ssh-tunnel with public-key authentication UNICORE-VISIT client

- TSI-extension:
 - key on target system



Visualisation

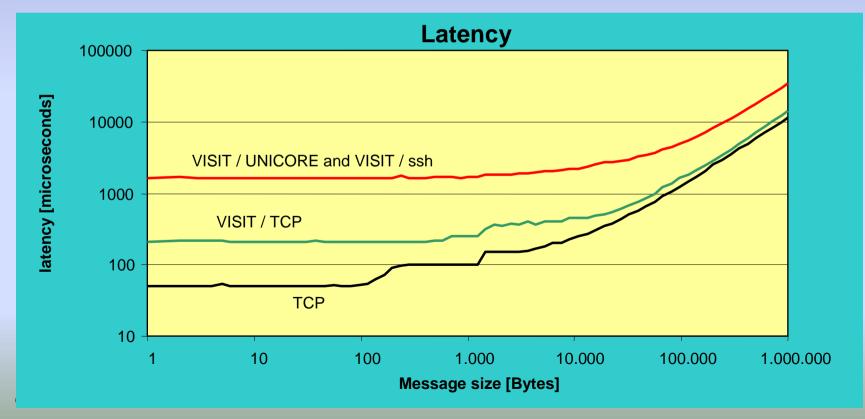
VISIT

SSH

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 / UNICORE to communicate with nbody

Xnbody Demo at UNICORE-Summit



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



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Summary and Outlook



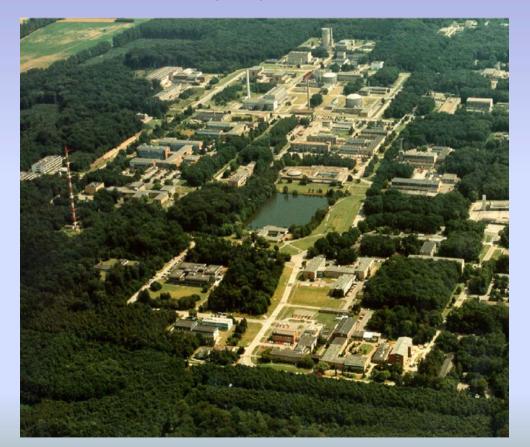
- VISIT / UNICORE provides:
 - Online visualization and computational steering of UNICORE jobs
 - Uses UNICORE's security and single-sign-on
 - Is firewall-friendly by using ssh for data transfer
 - Delivers good performance
 - Is the basis for a new UNICORE client-plugin for interactive shell access
- 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)



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) /

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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

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Th.Eickermann

NIC

Implementation Details



