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
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

DMMD: molecular dynamics

Trace: groundwater pollution

FIRE: Realtime fMRI

NBODY: star cluster
PEPC: Plasma Simulation

- Simulation of a particle accelerator via Laser pulses:
  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 Magnetic 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?

```

Visualization

VISIT Server API

Tunnel
TCP
File

File-system

ssh-client

Simulation

VISIT Client API

TCP
File

File-system

VTS - proxy

```
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
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
- 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

- 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

Enjoy the Demo
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

UNICORE Client

VISIT Plugin

UNICORE Server

VISIT

Visualisation

SSH

VISIT Proxy

Simulation

October 11th 2005

Th.Eickermann