VISIT and UNICORE: Computational Steering meets Grid Computing

Thomas Eickermann
Wolfgang Frings, Anke Visser

NIC - John von Neumann Institute for Computing
Research Centre Jülich, Germany
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)
11 March 2004: 41 x 32 Power4+ 1.7 GHz, 128 GByte, High Performance Switch
8922 Gflops Peak, 5568 Gflops LINPACK

Most powerful computer in Europe!
(until recently)
Content

- Motivation
- UNICORE
- VISIT
- UNICORE - VISIT integration
- Work in progress
- Off-line demonstration
Rationale

• Computational Steering:
  • Gain immediate visual insight into a simulation
  • Speed up the cycle of parameter selection → simulation → post-processing → interpretation
  • Make efficient use of a large scientific instrument: a supercomputer

• Tele-Collaboration:
  • make Computational Steering available to distributed teams

• GRID:
  • Provide the infrastructure and tools for secure and seamless operation of the above
• GRID system developed in German and European projects
• Vertically integrated approach (not bag of services)
• Focus on
  • workflow management of complex batch jobs
  • security: strong authentication, single sign-on, firewall friendly (uses a single TCP-port), ...
• 3-tier architecture: user-client, servers, target systems
• Development towards OGSA/OGSI in European projects GRIP and UniGrids
• Open Source: available at sourceforge
VISIT - Visualisation Interface Toolkit

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

NBODY: star cluster

PEPC: Plasma simulation

Trace: groundwater pollution

DMMD: molecular dynamics

FIRE: Realtime fMRI

CONWIHR: PSE for structural engineering (in progress)

June 15th 2004
UNICORE - VISIT integration

- Implementation issues:
  - Client-Server interchanged
  - Connectionless UNICORE-protocol
UNICORE - VISIT prototype

- UNICORE services:
  - Secure & seamless access
  - Data replication
VISIT / UNICORE Showcase at SC Global 2003
with HLRS (COVISE) & UoM (RealityGrid)
Demo at SC Global '03

JUMP (IBM p690 cluster)

VISIT-Coop Server

UNICORE Server

Juelich

UNICORE Client

visualisation

Access Grid

vic

VNC

UNICORE Client

visualisation

Access Grid

vic

UNICORE Client

visualisation

Stuttgart

Phoenix

Juelich

June 15th 2004

Th. Eickermann
Current Activities

- UniGrids
  - Develop a UNICORE/Grid-Services device
  - Instrument an oil-exploration application (CINECA)
  - Cooperate towards a standard steering API (UoM, ...)
- VIOLA
  (Vertically Integrated Optical testbed for Large Applications)
  - Develop an integrated environment for collaborative exploration of huge atmospheric data-sets in heterogeneous environments
- NIC
  - Dissemination in NIC-user community
  - Provision of an ssh-based device for easy access of non-grid users
Offline-Demo

- Pre-recording:
  - unmodified client

- Replay:
  - uses recorded timing
  - unmodified visualisation
The Application: a Laser-Plasma interaction

- **PEPC** - a tree based plasma simulation code developed at NIC/ZAM (by Paul Gibbon)
- Demonstration example:
  - Simulation of a laser pulse that accelerates electrons to \(~ GeV\) energies:
    envisioned to build extremely effective electron accelerators
    (\(10^2 \ldots 10^5\) x higher electric fields than synchrotrons)
- **VISIT + AVS/Express** integrated into PEPC at early stage of development:
  - Validation/debugging of the code
  - Verification of start-up parameters
  - Perform quick trial runs ahead of full blown simulations
- Online-control of Laser-pulse parameters via VISIT:
  - intensity, duration, width
- **VISIT/UNICORE + Access Grid**:
  - Collaborative exploration of results, discuss qualitative effects
  - Collaborative search for interesting parameters