Cooperative effort of national HPC centres, major HPC users and technology providers, to contribute to the development of computational grid infrastructures in Europe.
<table>
<thead>
<tr>
<th>National HPC Centres</th>
<th>Industrial Users</th>
<th>Technology Providers</th>
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<tbody>
<tr>
<td>Forschungszentrum Julich (D)</td>
<td>Parallab - University of Bergen (N)</td>
<td>Pallas GmbH (D) (Project coordination)</td>
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<tr>
<td>Victoria University of Manchester (UK)</td>
<td>Warsaw University - ICM (PL)</td>
<td>GIE EADS CCR (F)</td>
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<td>CNRS - IDRIS (F)</td>
<td>ETH Zurich (SCSC Manno) (CH)</td>
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<td>Deutscher Wetterdienst (D)</td>
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<td>Fujitsu European Center for Information Technology (UK)</td>
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<td>Debis Systemhaus (D)</td>
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</table>
HPC Centres

- Contribute to the acceleration of scientific discovery, by the use of information technologies
- Provide high performance supercomputing environments for dealing with science’s more challenging problems.
- Act as a technology transfer agent between R&D in information technologies, and computational science
Targets for HPC in next decade

- Capture more physics in the simulation of complex systems
- Complex systems are characterized by multiple time and/or length scales
- Not easy to capture multiple scales in one code
- **Code coupling** for multi-physics applications is viable alternative in some conditions
- This leads naturally to **computational grids**
- Heterogeneous algorithms map naturally to heterogeneous grids.
Project motivations and strategies

- Focus on **heterogeneous**, very high performance supercomputing environments.

- Use of grid technologies to provide a unified image and a transparent access to such environments.

- Deploy an application testbed across Europe by the integration of partner’s HPC environments.

- Provide a major effort to **develop and deploy distributed scientific applications** (EUROGRID is roughly 1/2 applications development, 1/2 technology development).
EUROGRID middleware

- **CUSTOM**
  - UNICORE (German project)

- **COMMODOITY**
  - MPI (scientific standard, soon interoperable)
  - CORBA - JAVA (Internet standards, have significant software engineering advantages).
  - ... (others)
UNICORE goals

- UNICORE develops a **seamless, secure, intuitive** software infrastructure to HPC resources
- Provides **consistent batch access** to heterogeneous remote systems ...
- ... with **minimal intrusion** into the Centers
- Supports **multi-site and multi-systems** applications for one job
- Exploits **existing and emerging** technologies (JAVA, X.509 certificates)
UNICORE Architecture

UNICORE Site A

Insecure Internet

UNICORE Gateway

UNICORE Network

Job Supervisor

UNICORE Batch interface

Cray NQE

IBM LL

UNICORE Site B

Secure Intranet

UNICORE Gateway

UNICORE Network

Job Supervisor

UNICORE Batch interface

Sun NQS

User’s Laptop

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EUROGRID Workpackages

- **WP1 to WP4**: applications development, tests of basic software components.
  - WP1: Bio - Grid (ICM)
  - WP2: Meteo - Grid (DWD)
  - WP3: CAE - Grid (EADS)
  - WP4: HPC - Grid (IDRIS)

- **WP5**: technology developments (UoM)

- **WP6 - WP7**: management and dissemination (Pallas, FJZ)
WP1: Bio-Grid (ICM leading partner)

- Computation portal to bio-molecular applications
- Build interfaces to well known bio-molecular applications, simplify access to databases.
- Integrate interfaces within EUROGRID software.
Meteo-GRID

- Develop a relocatable version of local weather prediction model
- ASP solution for on demand localized weather prediction
Ubiquitous access to local weather prediction software, developed at DWD

**Meteo-Grid**

- **DWD**
  - Global model Databases
  - Send global data
  - Request prediction
- **HPC-GRID center**
  - Request global data
  - Send global data
- **Client workstation (somewhere)**
- **WAN**

**Grid Specifications**

- **GME**: mesh 60Km, 31 layers
- **LM**: mesh 25Km x 2 Km, typically 48hs

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WP3 : CAE Grid (EADS leading partner)

- Focuses on industrial CAE applications
- Code coupling and multi-physics optimisations to improve system design.
- ASP - type services :
  - User interfaces to hide the complexity of HPC systems to industrial users
  - Supercomputing as an e-business : accurate cost prediction of CAE simulations
WP4 : HPC-GRID (IDRIS leading partner)

- Targets:
  - The establishment, by the HPC centres partners of EUROGRID, of an application testbed for general purpose HPC distributed applications
  - The installations and tests of EUROGRID software releases
  - The development of new relevant GRID applications, using existing middlewares, in scientific areas not covered by WP1 to WP3.
HPC - GRID

ibm
- CRAY T3E 900 (32 PE)
- NEC SX4B/2A
- Linux Cluster (4 PE)

paralab
- SGI Onix (4 PE)
- SGI O2000 (128 PE)

FZJ
- Linux Intel Cluster (36 PE)
- CRAY T3E - 600 (512 PE)
- CRAY T3E - 1200 (512 PE)

Manchester Computing
- CRAY T3E - 1200 (816 PE)
- FUJITSU VPP300 (8 PE)
- SGI O2000 (128 PE)
- SGI O3000 (256 PE)

Dias
- IBM SP3 (8 PE)
- NEC SX5 cluster (40 PE)
- IBM Power4 (256 PE, 1.3 TFLOPS)
- COMPAQ Linux Cluster (24 PE)

EUROGRID

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EUROGRID Technology

- Based on UNICORE system (currently V3.5)
- Develop additional GRID components
  - efficient data transfer
  - ASP infrastructure
  - resource broker
  - application coupling
  - interactive access
Applications: strategy

- Main objective is **computational science**.

- **Coupled software modules with:**
  - Location and server transparency: they must run in any heterogeneous grid.
  - Full portability: implementation, architecture, operating system, protocol independence.

- **CORBA on C++ and JAVA.**

- **ONCE** the application exists in its own right, **THEN** we explore the added value provided by UNICORE or GLOBUS metacomputing environments.
Applications : turbulence

- Partners : A. Hadjadj, A.S. Munroval, D. Vandromme (CORIA)
  D. Gorou, G. Grasseau (IDRIS)

- Coupling fluid - structure (2 dimensional case)

- Status : coupled codes ready and validated

- Under way : execution in UNICORE environment.
Applications: Cosmology

- Partners: J. M. Alimi (LUTH, Meudon), D. Girou, G. Grasseau (IDRIS)

- Gravitational N body problem
- Hydrodynamic shocks and adiabatic evolution of baryon gas
- Microscopic cooling processes of primordial chemical elements

- Status: Coupled codes ready and validated.
Applications: Combustion

- **Partners**: D. Veynante (coordinator), S. Ducruix, O. Gicquel, M. Lecanu (EM2C), D. Girou, G. Grasseau (IDRIS)

- **Basic codes for the simulation of reactive flows**, coupled to
  - Production of polluting chemical species
  - Analysis of thermal radiation

- **Status**: developments under way
Applications : Environment

- **Partners**
  - Laboratoire des transferts en hydrologie et environnement, Grenoble (Ch. Messager, coordinator)
  - Laboratoire Hydrosciences, Montpellier
  - IDRIS

- **Coupling of MAR (regional atmospheric model) and ABC (hydrological model) for the simulation of atmospheric and hydrological cycles in West Africa.**

- **Status** developments under way.
Applications: Supercoiled DNA (VA, IDRIS)

- Worm-like chains of elastic segments with torsion are good models for large scale dynamics of macromolecules.
- Brownian motion must be added to describe hidden, fast, degrees of freedom.
- Obtaining the Brownian displacements at each time step constitute today’s computational bottleneck.
Supercoiled DNA software

Prototype software up and running.

Thread pool for Brownian displacement factory.

CORBA threads

Molecular dynamics thread pool
ASP environment (VA, IDRIS)

- Internet monitoring and steering of complex simulation running in protected environments.
- ASP services to users who want to avoid direct access to HPC centers.
- **Minimal intrusion protocol**: the application is practically not modified, and it is not Internet aware.
- Uses public domain CORBA - JAVA middleware.
- Prototype up and running.
- Security compliance (X.509 certificates) under way.
- When security OK, will start beta testing on Compaq Linux cluster.
ASP software architecture.

- Event service
- Monitor server
- Steering server
- Gateway
- Event Channel

Lightweight clients

CORBA thread

Application thread

Application

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Conclusions:

- Integration of modern grid software technologies in European supercomputing infrastructures
- Major effort in distributed application development in science and technology
- Strong commitment from national HPC Centers to participate to the deployment of computational grid infrastructures in Europe.