EUROGRID

Victor Alessandrini

IDRIS - CNRS

va@idris.fr

EUROGRID

Cooperative effort of national HPC centres,
major HPC users and technology providers,
to contribute to the development of
computational grid infrastructures in Europe.

EUROGRID

Forschungszentrum Julich (D) ●

Victoria University of Manchester (UK) ●

CNRS - IDRIS (F) ●

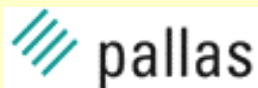Parallab - University of Bergen (N) ●

Warsaw University - ICM (PL) ●

ETH Zurich (SCSC Manno) (CH) ●
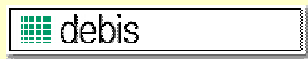
Deutscher Wetterdienst (D) ●

GIE EADS CCR (F) ●

Pallas GmbH (D)   (Project coordination) ●

Associate contractors :

fecit   Fujitsu European Center for Information Technology   (UK) ●

debis   Debis Systemhaus (D) ●

● National HPC Centres   ● Industrial Users   ● Technology Providers

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

EUR⦿GRID

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.

EUROGRID

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)

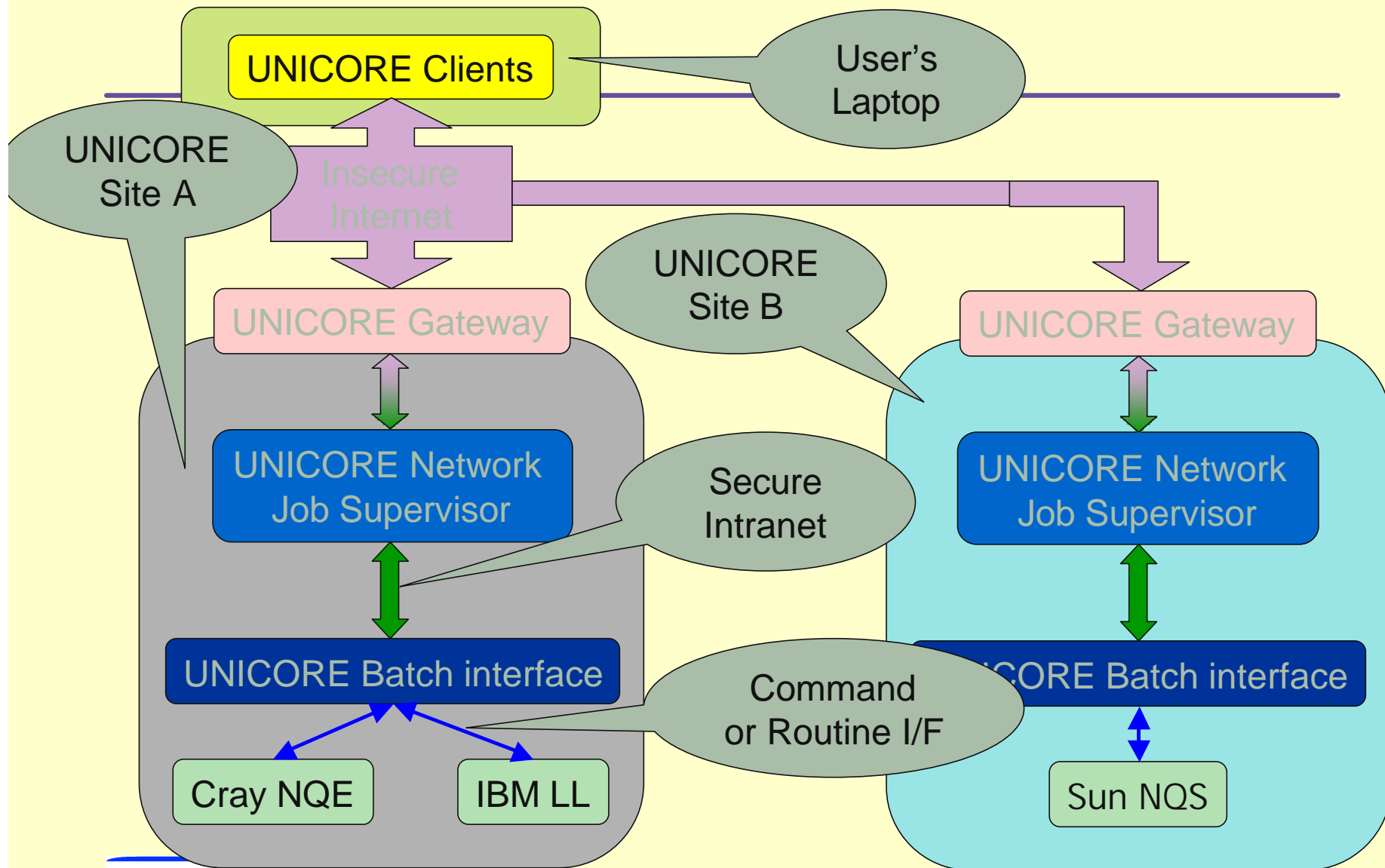**EUR●GRID**

EUROGRID middleware

- <u>CUSTOM</u>

  - UNICORE (German project)

- <u>COMMODITY</u>

  - MPI (scientific standard, soon interoperable)

  - CORBA - JAVA (Internet standards, have significant software engineering advantages).

  - … (others)

EUROGRID

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)

EUROGRID

UNICORE Architecture

UNICORE Clients

User's Laptop

UNICORE Site A

Insecure Internet

UNICORE Gateway

UNICORE Site B

UNICORE Network Job Supervisor

Secure Intranet

UNICORE Network Job Supervisor

UNICORE Gateway

UNICORE Batch interface

Command or Routine I/F

UNICORE Batch interface

Cray NQE

IBM LL

Sun NQS

EUROGRID

ORAP - SPEEDUP meeting, Octobre 2001

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)

EUROGRID

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.

EUROGRID
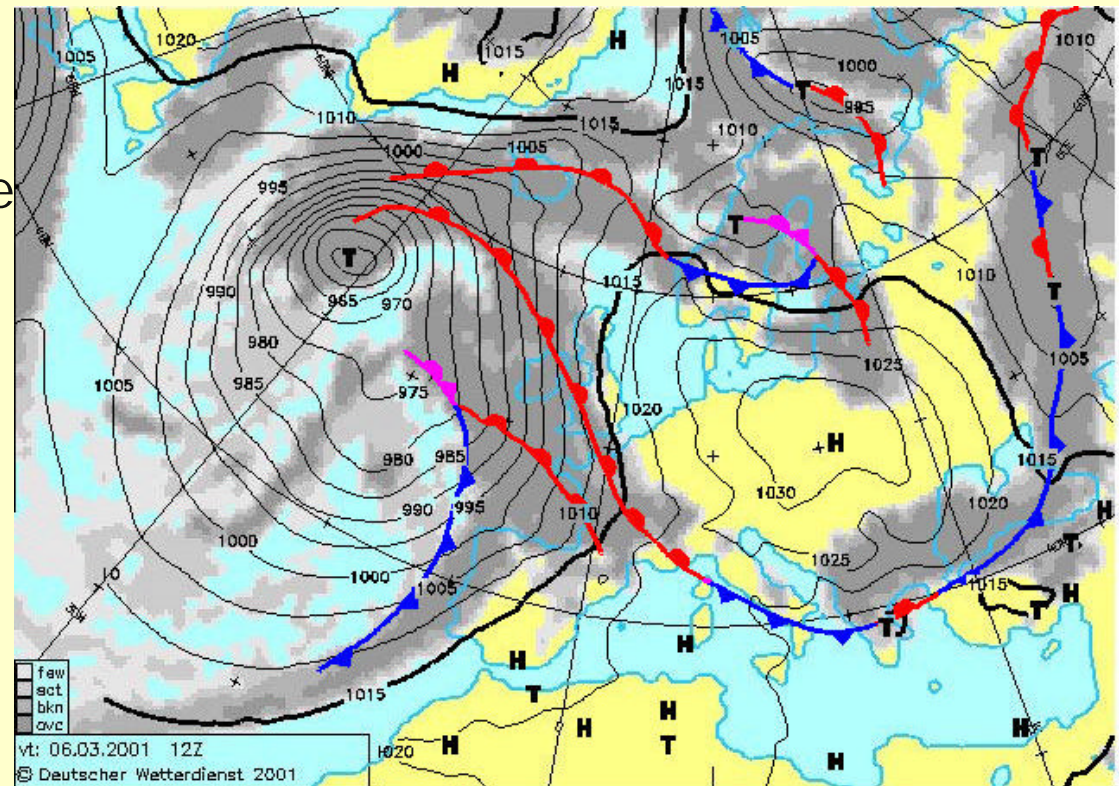
Meteo-GRID

- Develop a relocatable version of local weather prediction model

- ASP solution for on demand localized weather prediction

EUR◉GRID

Meteo-Grid

DWD

Global model Databases

Request global data

HPC-GRID center

Send global data

Request prediction

WAN

Client workstation (somewhere)

GME : mesh 60Km, 31 layers

LM : mesh 25Km x 2 Km typically 48hs

EUR⊕GRID

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

EUR⬤GRID

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.

EUROGRID

HPC - GRID

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

parallab
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)
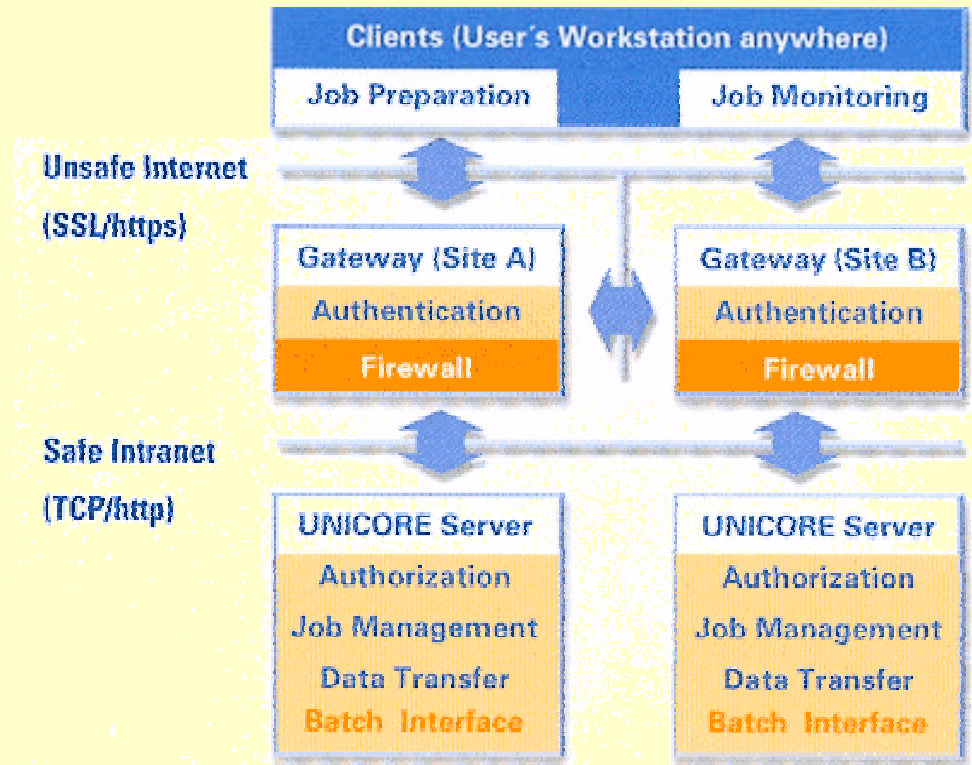SGI O2000 (128 PE)
SGI O3000 (256 PE)

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

EUROGRID

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.

EUR GRID

Applications : turbulence

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

- Coupling fluid - structure (2 dimensional case)

- <u>Status</u> : coupled codes ready and validated

- Under way : execution in UNICORE environment.

EUR⊕GRID

Applications : Cosmology

- <u>Partners</u> J. M. Alimi (LUTH, Meudon), D. Girou, G. Grasseau (IDRIS)

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

- <u>Status</u> : Coupled codes ready and validated.
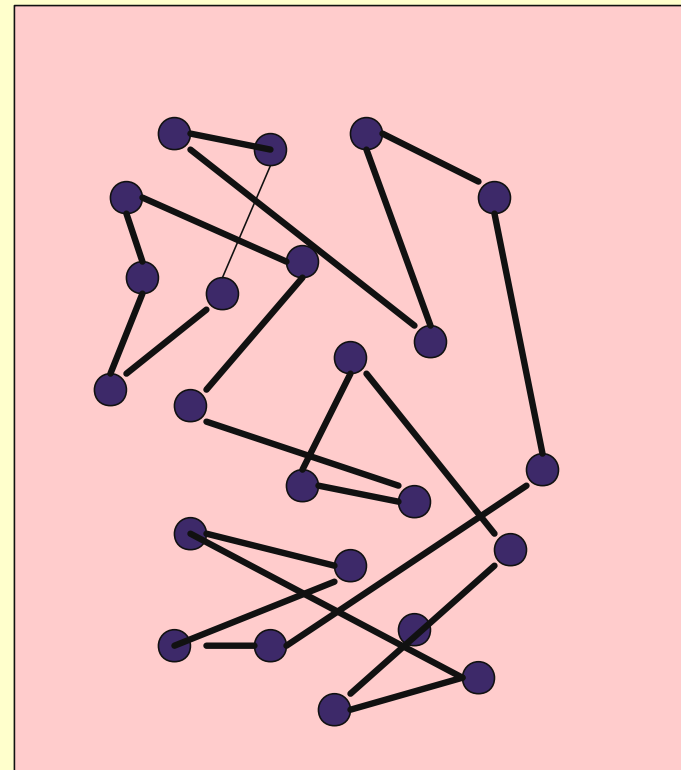
Aplications : Combustion

- <u>Partners</u> : 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

- <u>Status</u> : developments under way
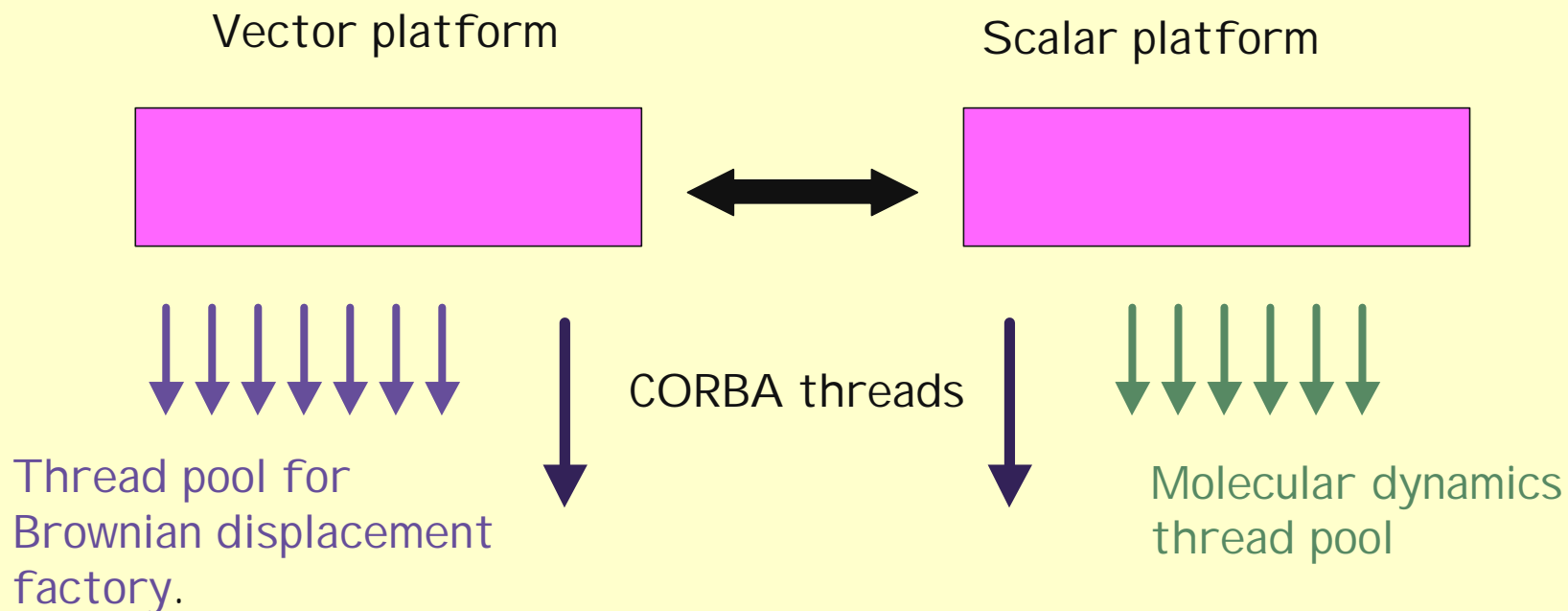
EUR⦾GRID

Applications : Environment

- <u>Partners</u>
  - 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.

- <u>Status</u> developments under way.

EUR⊕GRID

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.

EUR⬤GRID

Supercoiled DNA software

Vector platform

Scalar platform

CORBA threads

Thread pool for
Brownian displacement
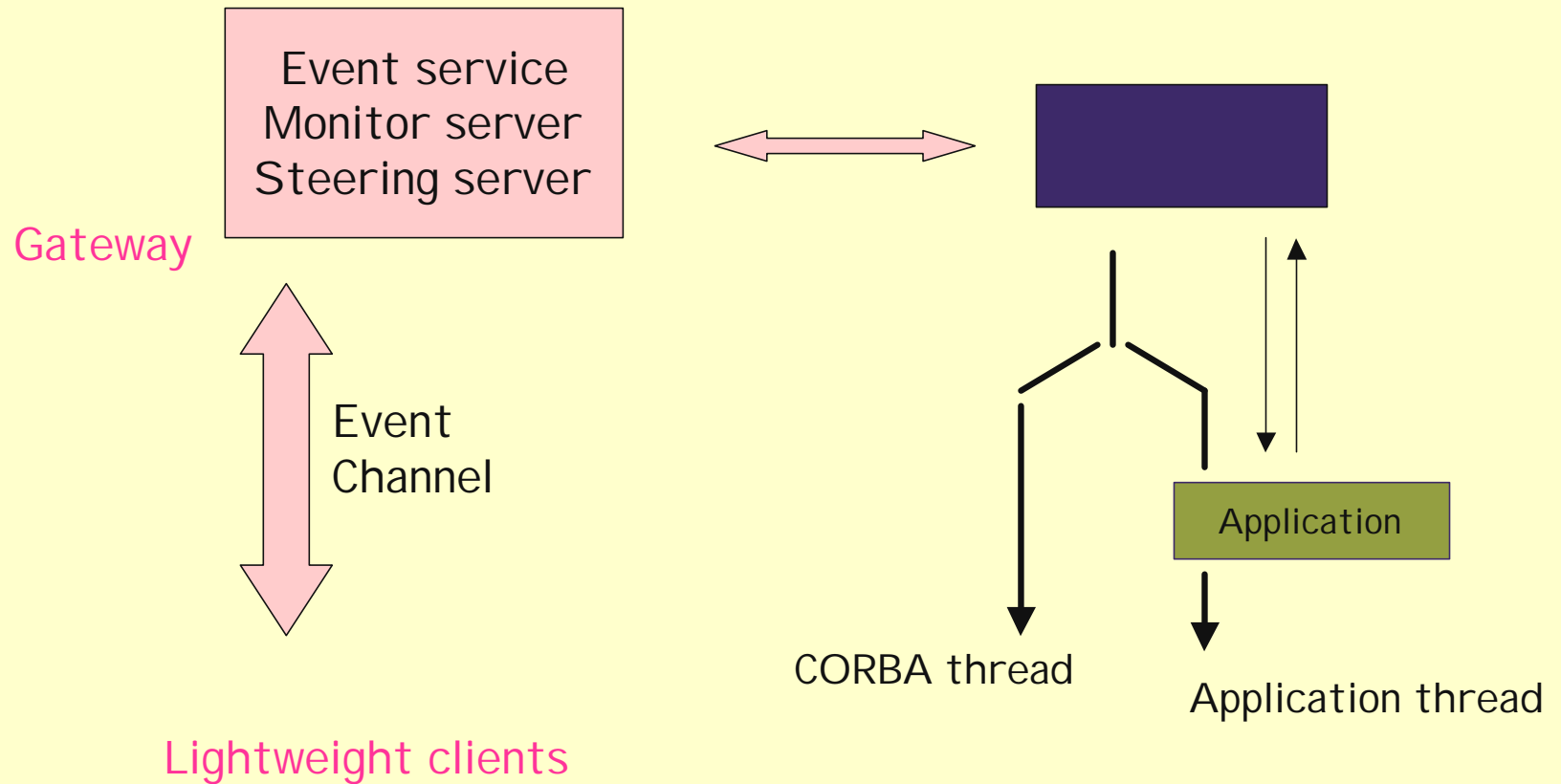factory.

Molecular dynamics
thread pool

Prototype software up and running.

EUR⊕GRID

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.

- <u>Minimal intrusion protocol</u> : 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

Application

CORBA thread

Application thread

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.

EUR**O**GRID