

Due to the emergence of Grid computing, numerical simulations are becoming more and more complex — it is not uncommon to find different models and codes coupled. Our purpose is to analyse, to design and to develop a software environment for steering distributed parallel simulations from the visualization. This computational steering environment should combine the facilities of scientific visualization with the capabilities of existing high performance simulations. The simple integration of an existing simulation should allow the end user to visualize the intermediate results and to directly interact with the simulation during its execution.

Context and Crucial Issues

Parallel & distributed numerical simulations

- Aiming the most common codes (C/C++/Fortran with MPI/PVM)
- Each step of a simulation can generate very huge data

Parallel scientific visualization

- Complex and intensive visualization processing
- Promising evolution of the parallel visualization (clustering, tiled display)

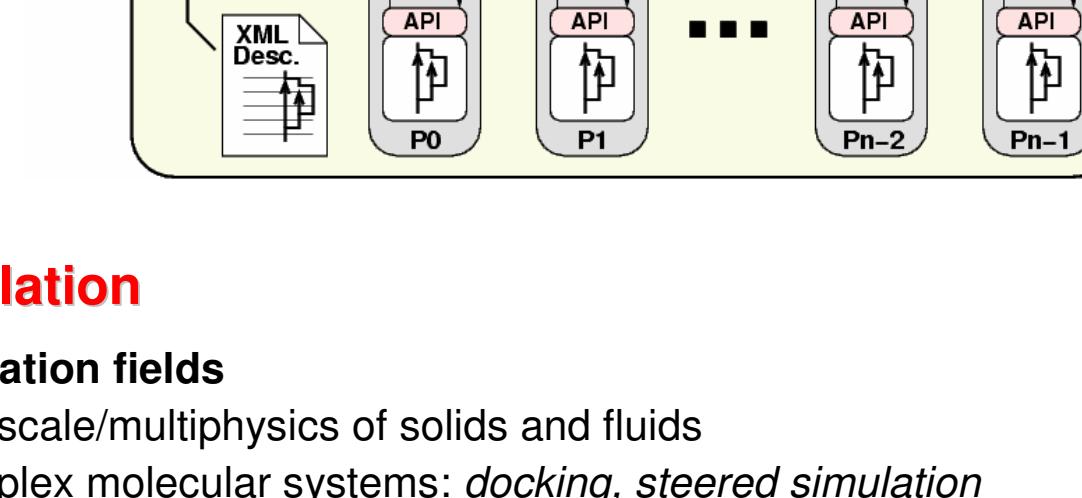
⇒ The coupling of parallel simulations and parallel visualization systems leads to several open and crucial issues.

- ✗ How to transfer data distributed on a parallel application directly to another parallel application ?
- ✓ EPSN uses a **M-by-N redistribution library RedGRID** (locally developed).
- ✗ How to assign precise dates in a complex simulation (e.g. nested loops) ?
- ✓ EPSN uses a **hierarchical task model** of the steerable simulations.
- ✗ How to ensure the steering treatments to occur at the same date in all the parallel processes without strongly synchronizing them ?
- ✓ EPSN **schedules** the treatments with a **weak synchronization** and the parallel processes execute them independently.

Architecture

Communication infrastructure based on CORBA

- Support of heterogeneous distributed system
- CORBA server encapsulated in a thread
- Use of CORBA fully hidden to the end-user



Simulation

Application fields

- Multiscale/multiphysics of solids and fluids
- Complex molecular systems: *docking, steered simulation*
- Environment: *population dynamics, epidemiology and prophylaxis*

Supported simulations

- Parallel SPMD applications
- Complex simulations : multiple tasks/loops, nested tasks/loops
- Distributed complex data : data fields (generic block decomposition), particles, structured grids, unstructured meshes

User Interface

Visualization

- Data collection for the on-line visualization of intermediate results
- Generic client adapted to any simulation
- AVS/Express (sequential) or VTK (parallel) data source modules
- EPSN client API to develop customized user interfaces

Interaction

- Remote control of the simulation execution (play/stop)
- Modification of parameters and data on-the-fly
- Invocation of actions in the simulation code

Contact

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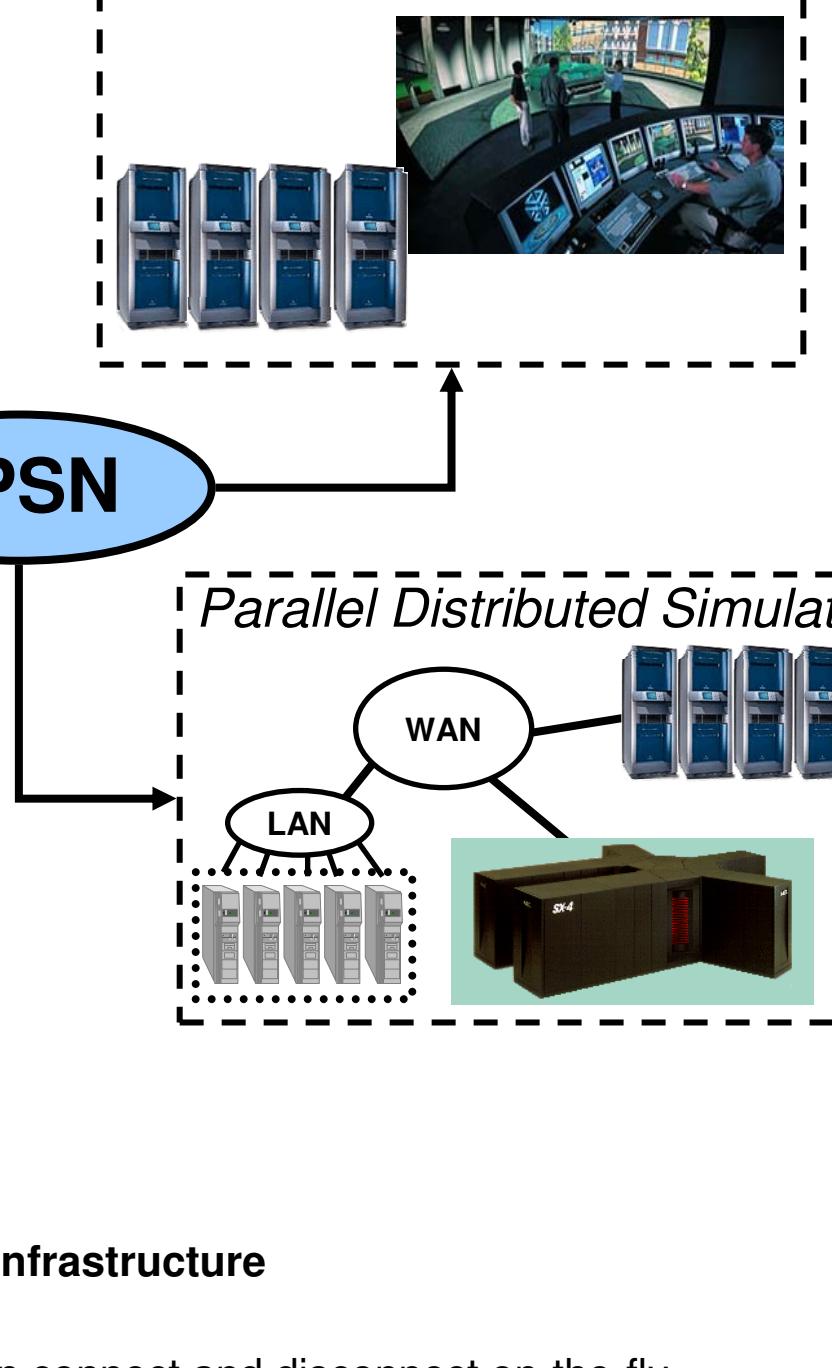
Web sites

EPSN <http://www.labri.fr/epsn>
RedGRID <http://www.labri.fr/Perso/~esnard/RedGRID>
CoICOWS <http://colcows.sourceforge.net>

Publications

ParCo 2003, Toward a Computational Steering Environment based on CORBA. O. Coulaud, M. Dussere, A. Esnard.

EuroPar 2004, A Time-Coherent Model for the Steering of Parallel Simulations. A. Esnard, M. Dussere, O. Coulaud.



Key Points

Distributed and dynamic infrastructure

- Client/server relationship
- Several remote clients can connect and disconnect on-the-fly
- Concurrent client-directed requests

Instrumentation of legacy simulation

- Annotations of the sources with EPSN C++ API (C/Fortran bindings)
- Description of the simulation structure (data and tasks)

Performance design

- Low perturbation instrumentation (no request ⇒ no overhead)
- Communication overlapping of the and zero-copy sending
- Few synchronizations between the simulation and the steering applications

Infrastructure

Simulation source-code

```
struct Particle { double x, y, z, vx, vy, vz, ax, ay, az, mass, charge; };
Particle particles[MAX_PARTICLES];
...
init_particles(particles, my_offset, particles_number)
for (count = 0; count < N_OF_ITERATIONS; count++) {
    exchange_particles(particles, my_offset, particles_number)
    compute_acceleration(particles, my_offset, particles_number)
    move_particles(particles, my_offset, particles_number)
}
MPI_Finalize();
```

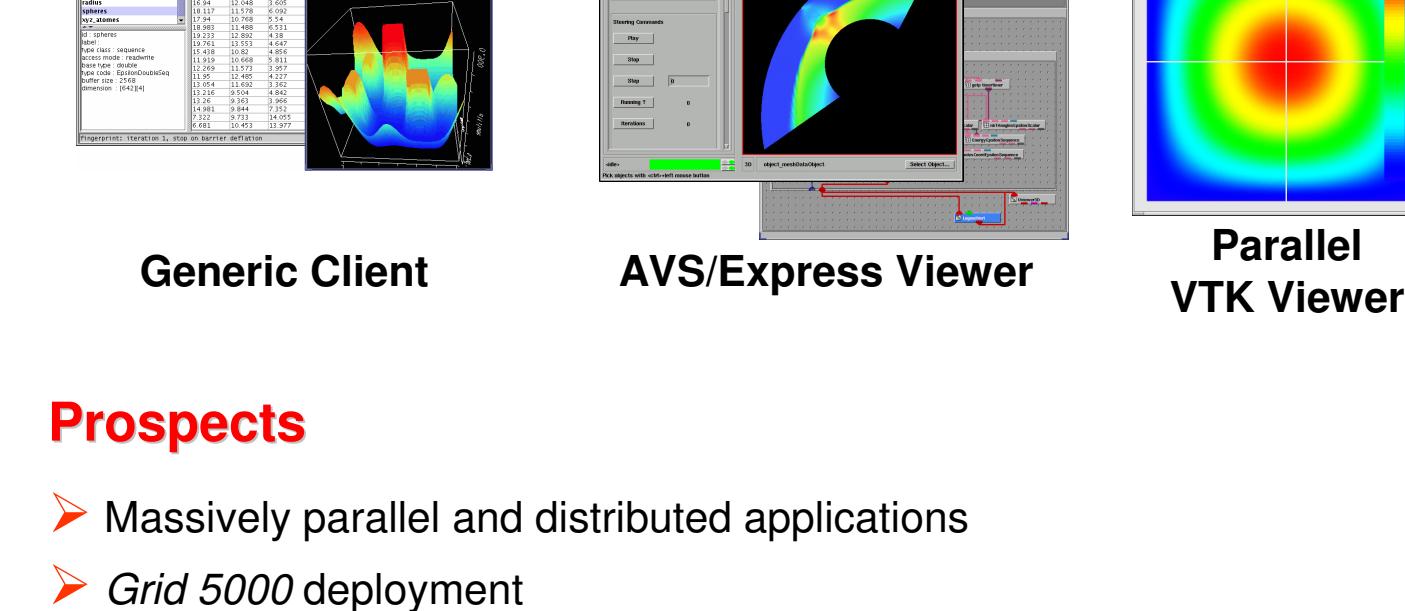
Instrumented source-code

```
struct Particle { double x, y, z, vx, vy, vz, ax, ay, az, mass, charge; };
Particle particles[MAX_PARTICLES];
MPI_Init(&argc, &argv);
...
init_particles(particles, my_offset, particles_number)
RedSYM::Points * points = new RedSYM::Points("particles", nb_pool_size);
points->setNumberOfPoints(particle_number, MAX_PARTICLES);
points->addCoordinate((particles->my_offset, sizedOffsetParticle), 0);
EPSN::SteerableSimulation::Interface * epsn_ifc = new EPSN::SteerableSimulation::Interface;
epsn_ifc->init("args");
if(my_rank == 0)
    epsn_ifc->initProxyAndNode("particles", "particles.xml", 0, pool_size);
else
    epsn_ifc->initNode("particles", my_rank, pool_size);
epsn_ifc->addDataObject(points); epsn_ifc->ready();
epsn_ifc->apply("main"); epsn_ifc->apply("main");
for (count = 0; count < N_OF_ITERATIONS; count++) {
    epsn_ifc->start("main");
    exchange_particles(particles, my_offset, particles_number)
    epsn_ifc->update("acceleration");
    compute_acceleration(particles, my_offset, particles_number)
    epsn_ifc->apply("acceleration");
    epsn_ifc->start("main");
    move_particles(particles, my_offset, particles_number)
}
epsn_ifc->end("main"); epsn_ifc->killORB();
MPI_Finalize();
```

XML Description

```
<simulation id="particles">
<data>
<points id="particles" dimension="3" />
<data>
<loop id="main" "false" >
<loop id="main" "synchronous"="no" >
<task id="acceleration" "synchronous"="no" >
<task id="move" "synchronous"="no" >
<data-context ref="particles" context="modified" />
<task>
<loop>
</loop>
</simulation>
```

Steerable Simulation



Prospects

- Massively parallel and distributed applications
- Grid 5000 deployment
- Evolution to parallel CORBA objects: Paco++ (PARIS project)
- Definition of high-level interaction objects and association with 3D widgets
- Virtual reality environment: haptic sensors, tiled display wall

Partners

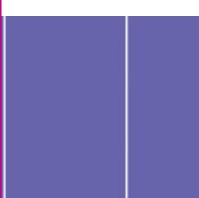
INRIA-Futurs Institut National de Recherche En Informatique et Automatique — **ScAlApplix** Project

LaBRI Laboratoire Bordelais de Recherche Informatique

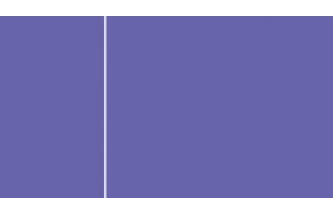
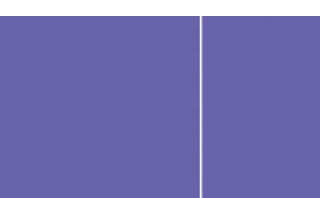
IECB Institut Européen de Chimie et Biologie

SRSMC Structure et Réactivité des Systèmes Moléculaires Complexes

CNRS/SMEL Station Méditerranéenne de l'Environnement Littoral



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