Interactive European Grid

MPI Applications in the Interactive European Grid

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EGEE 07, Budapest 1rst-5th October

Computational Chemistry: GROMACS

GROMACS has been installed in the i2g testbed

- Together with the fftw3 libraries
- Generally accesible applications software directory
  VO_ICOMPCHEM_SW_DIR.
- We have used **Open MPI** as MPI implementation and **GNU compilers**.

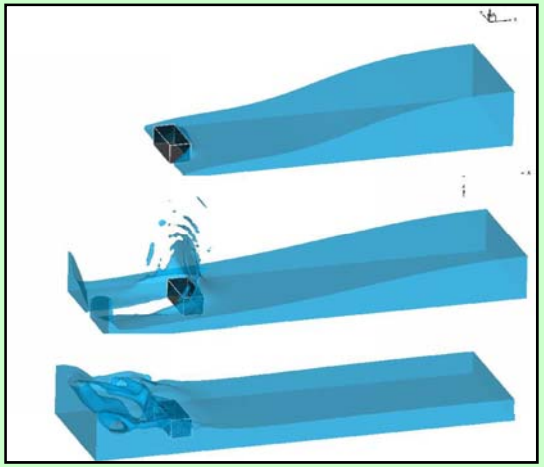
```
-----------------------------------------------
JobType = "Parallel";
SubJobType = "OpenMPI";
NodeNumber = 4;
VirtualOrganisation = "icompchem";
Executable = "mdrun";
Arguments ="-v -s full -e full-o full -c after_full -g flog -N 4";
StdOutput = "std.out"; StdError = "std.err";
InputSandbox = {"speptide.top","after_pr.gro","full.mdp","gromacs_hooks.sh"};
OutputSandbox = {"std.out","std.err"};
Environment =
{"I2G_MPI_PRE_RUN_HOOK=./gromacs_hooks.sh","I2G_MPI_POST_RUN_
HOOK=./gromacs_hooks.sh"};
-----------------------------------------------
```

Computational Chemistry: GROMACS

```
export OUTPUT_ARCHIVE=output.tar.gz
export OUTPUT_HOST=se.i2g.cesga.es
export OUTPUT_SE=lfn:/grid/icompchem/test
export OUTPUT_VO=icompchem

pre_run_hook ()
{
### Here comes the pre-mpirun actions of gromacs export
PATH=$PATH:/$VO_ICOMPCHEM_SW_DIR/gromacs-3.3/bin
grompp -v -f full -o full -c after_pr -p speptide -np 4
}

post_run_hook ()
{
echo "post_run_hook called"
echo "pack the data and bring it to an Storage Element"
tar cvzf $OUTPUT_ARCHIVE *
lcg-cr --vo $OUTPUT_VO -d $OUTPUT_HOST -l
$OUTPUT_SE/$OUTPUT_ARCHIVE file://$PWD/$OUTPUT_ARCHIVE

return 0 }
```

Some MPI Applications tested:

Telluride



Simulations of Dam breaking using TELLURIDE

Portability Analysis

- **Regarding Intel Fortran compilers ifc (F90)**
- **Libraries associated**
- **Open-MPI itself**

The Group of Research in Oceanography and Coasts of the University of Cantabria is using this code for landscape design of harbours in the North coast of Spain.

http://www.gioc.unican.es

Telluride is a MPI software used to simulate many problems in the areas of solidification, fluid flow, heat transfer, phase transformations and mechanical deformation

http://www.lanl.gov/telluride

Some MPI Applications tested: Telluride

JDL job script

```
Executable        = “truchas”;
Arguments         =  “broken_dam.inp”;
JobType           =  “openmpi”;
NodeNumber        =  8;
StdOutput         = “std.out”;
StdError          = “std.err”;
InputSandBox      = {“my_scripts.sh”,”gioc”,”broken_dam.inp”};
OutputSandBox = {“std.out”, “std.err”};
Environment       = {“I2G_MPI_PRE_RUN_HOOK=./my_scrips.sh”,
”I2G_POST_RUN_HOOK=./my_scripts.sh”};
```

Lattice QCD

- **Lattice quantum chromodynamics** (Lattice QCD) is a theory of quarks and gluons formulated on a space time lattice.That is, is a discretized version of QCD

- Analytic solutions in QCD are hard or impossible due to the nature of the forces involved

- Most importantly, lattice QCD provides the framework for investigation of non-perturbative phenomena such as confinement and quark-gluon plasma formation, which are intractable by means of analytic theories.

- Lattice QCD has already made contact with experiments at various fields with good results: calculations of quark masses and decya constants

Lattice QCD

- **DD-HMC algorithm for two-flavour lattice QCD**

http://luscher.web.cern.ch/luscher/DD-HMC/index.html

- Numerical simulations of lattice QCD are still limited to light-quark masses significantly larger than their physical values.
- The use of efficient simulation techniques can make an important difference in this competitive field, and there has consequently been a continuous effort to improve the simulation algorithms.
- The DD-HMC algorithm combines domain decomposition ideas with the Hybrid-Monte-Carlo algorithm.

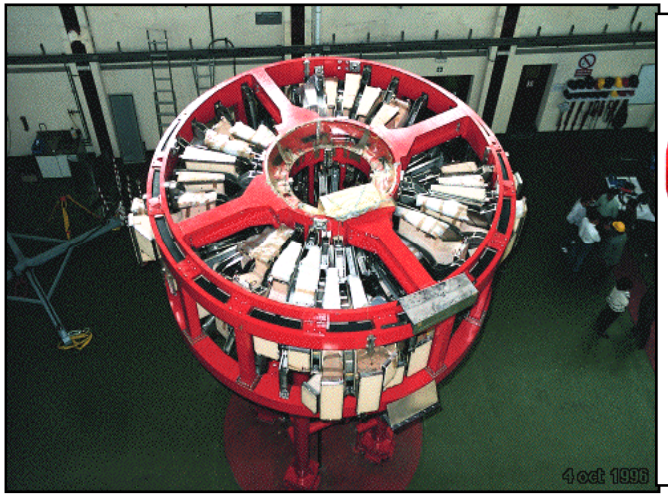
• Low latency intra-networks required

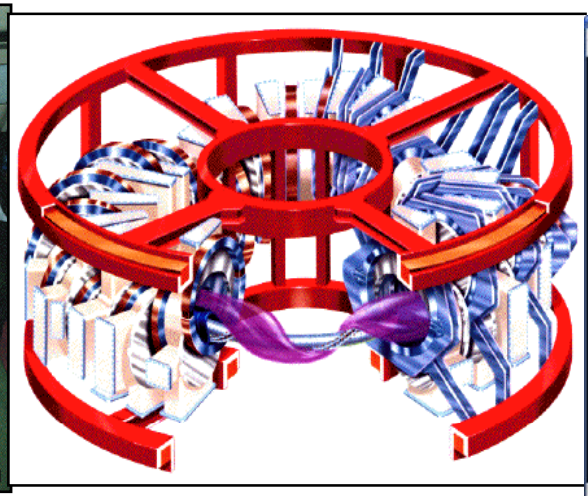
(~ 10 microsecond: Infiniband or Myrinet)

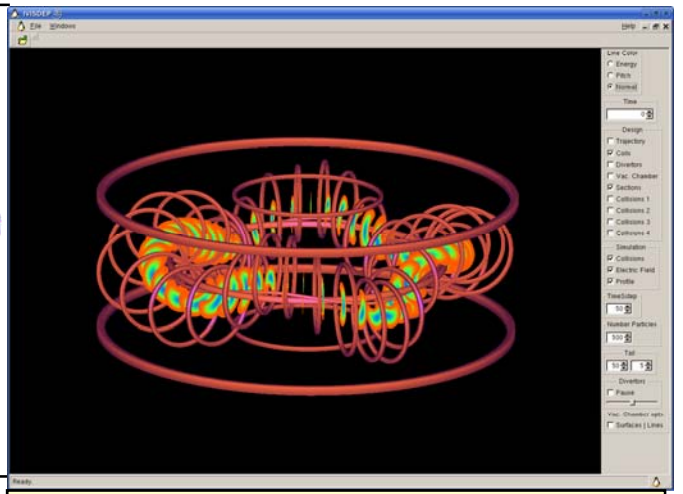
• Competitive simulations run for several weeks, or months, on cluster of 32 – 64 processors

MPI in farm mode:

Particle trajectories in Fusion devices







Stellerator TJ-II (Madrid)

- Magnetic Confinement
- Investigate Plasma prop.
- National infrastructure
- Research CIEMAT

Schema of the TJ-II design

Visualization using Computational tools (OpenGL, Fox toolkit)

Computing Visualization of TJ-II

Computational details

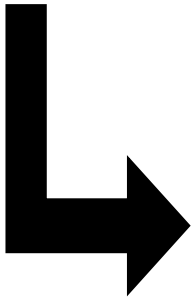
- The plasma is analyzed as a many body system consisting of N particles
- The application visualizes the behaviour of plasma inside a Fusion device
- Applicability
  - **Stellerator Design (vacuum chamber damages, coil designs, etc...)**

- Inputs
  - Geometry of the vacuum chamber
  - Magnetic field in the environment
  - Initial number, position, direction, velocity of particles
  - Possibility of collisions between particles
  - Density of particles inside the device

- Solves a set of Stochastic Differential Equations with Runge-Kutta method
- Outputs
  - Trajectories of the particles
  - Average of relevant magnitudes: densities, temperatures...

Porting the application to int.eu.grid

- Spread the calculation over hundreds of Worker Nodes on the Grid to increase the number of particles simulated using **MPI**
- Introduce remote **Visualization tools**
- **Interactive Steering**
- Design of a **Grid collaborative environment** for fusion device designing



N particles distributed among P processes: MPI

Particle trajectories are displayed graphically

Interactive simulation steering

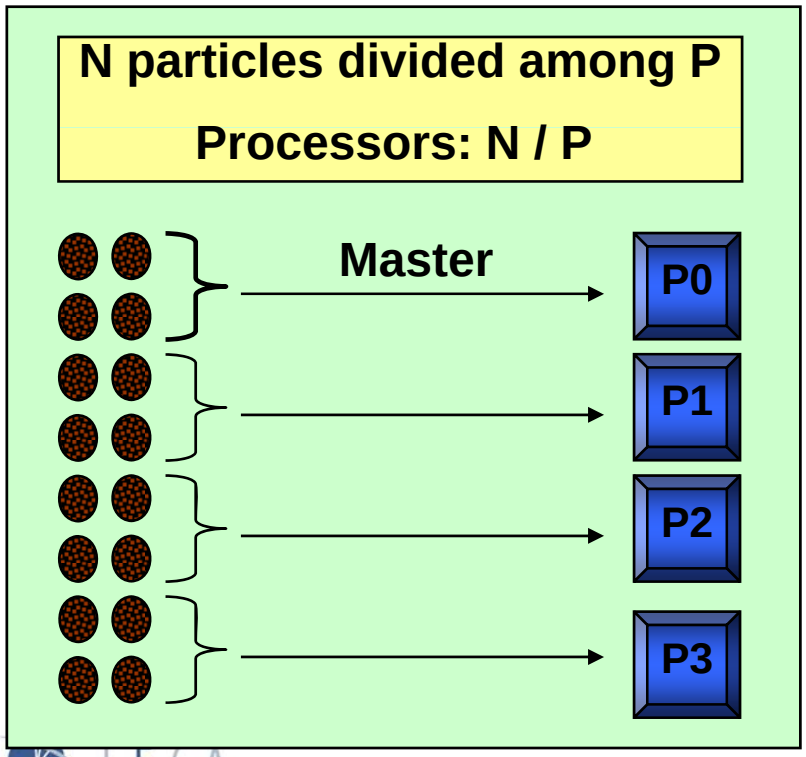
Application startup

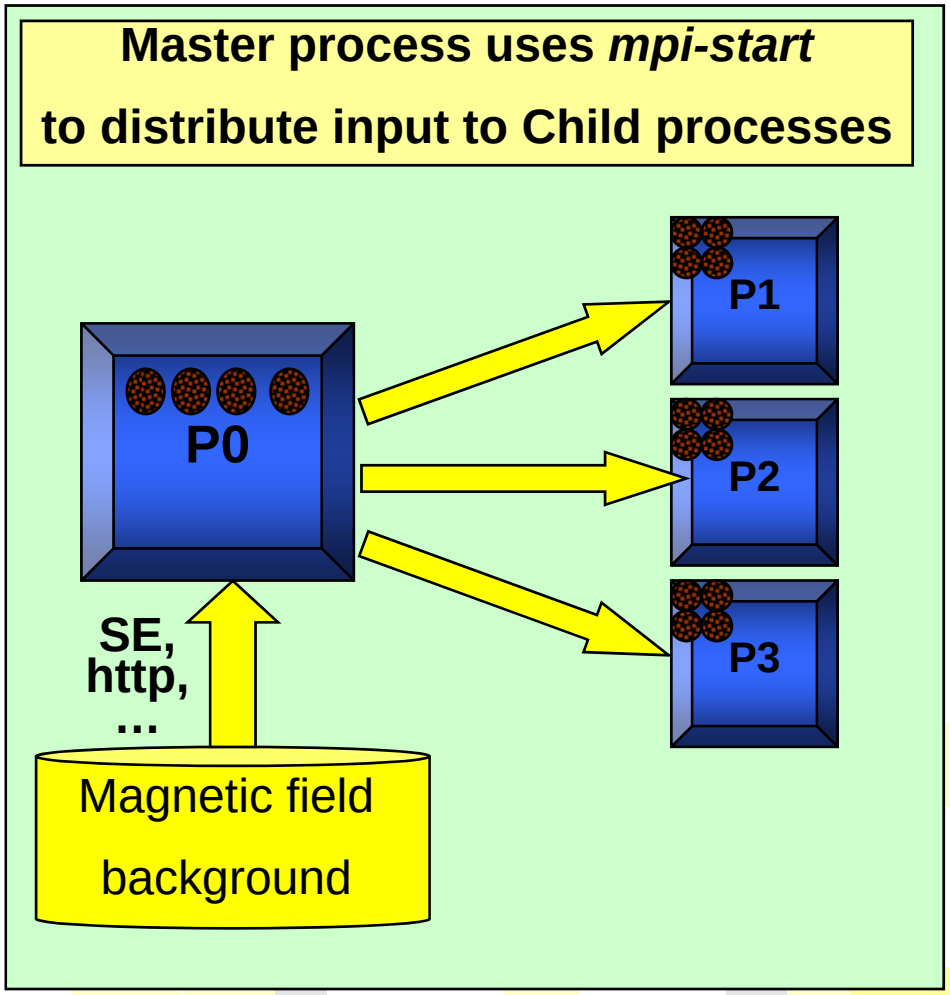
Input:

Number of particles,

Simulation properties (file),

Magnetic field background





Support to Environmental Applications

IMS Model Suite (IISAS)

Modelling dispersion of pollutants in the atmosphere

- Study the movement of individual independent particles.
- The term *particle* denotes any air pollutant or substance (or multiple substances) in the volume of air under consideration
- The particles travel with the wind and the particle trajectory and particle composition reflects natural phenomena such as turbulent diffusion, dry deposition, wet deposition caused by the rain and radioactive decay

- **Work done**
  - Grid enabled batch sequential and MPI versions
  - Migrating Desktop (MD) plugin
  - Integrated MPI version on Migrating Desktop