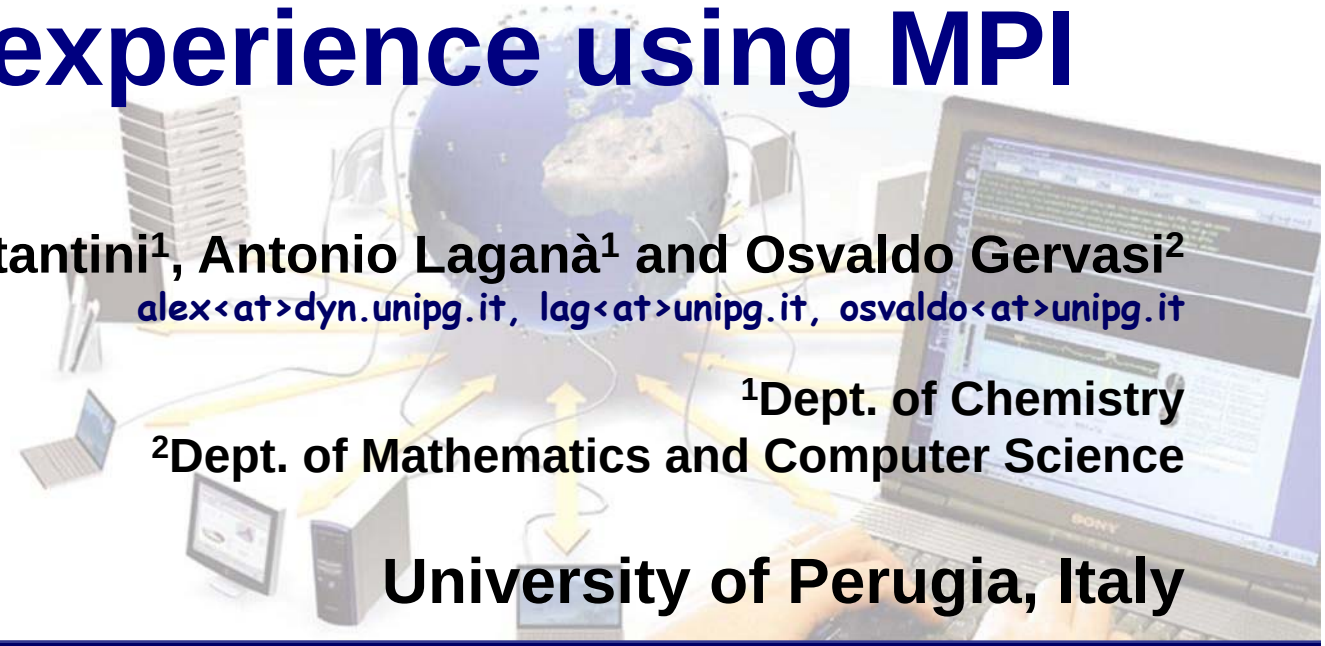
Enabling Grids for E-science in Europe
www.eu-egee.org

MPI Workshop
Bologna (I)
March 19th–20th 2008

www.unipg.it

CompChem VO: User experience using MPI



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Summary

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- Molecular Science community and EGEE project
- CompChem VO
- Characteristic of CompChem applications
- MPI state of the art
- Experiences using MPI
- Conclusions

The Molecular Science community and the EGEE project

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- The EGEE Grid environment allows us to carry out simulation of molecular systems increasing the quality and the quantity of properties investigated.
- The researcher is able to perform computational campaign:
  - Massive submission of sequential jobs running on different input datasets
  - Submission of parallel jobs
- Offers efficient data management facilities
  - Storage of large amount of data

CompChem VO

- CompChem VO is running on the EGEE production Grid from the end of 2004 to support Computational Chemistry applications (http://compchem.unipg.it)
- The VO has up to 30 active users
- Several EGEE sites are supporting the VO
  - the Italian EGEE sites, CESGA (Spain), IN2P3 (France), Trinity College of Dublin (Ireland), CYFRONET and POZNAN Supercomputing Center (Poland), Hellas Grid and GRNET (Greece), University of Cyprus (Cyprus).

CompChem and COST

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- Most of the CompChem users started the collaboration in the COST in Chemistry D23 Action, called *Metachem*
- COST is one of the longest-running project supporting co-operation among scientists and researchers across Europe with 35 member countries.
- In the COST in Chemistry program has been recently activated the Action D37, called *GridChem*
  - devoted to develop and deploy computational chemistry codes in the existing e-infrastructure

Main characteristics of CompChem applications

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- Both CPU-bound and data intensive jobs are present
  - Massive submission of sequential jobs running on different input datasets
- Parallel jobs: some programs have been structured to run in parallel.
  - Contribution of compchem to MPI international workshop, Dublin, Dec 11-12th, 2006.
- Interactive jobs: GEMS (Grid Enabled Molecular simulator)
- We are implementing Grid Services
  - to access the standard functionalities of the programs
  - to create visualization and Web3D interfaces in order to visualize the simulations coming from the calculations

http://compchem.unipg.it

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EGEE Home | Technical Pages Home | Calendar | Agenda | Glossary

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CompChem Virtual Organization

Information Society Technologies

CompChem Info Sheet | CompChem FAQ | Report a problem on CompChem to the EGEE Suppor Team (GGUS)

The CompChem Virtual Organization has been established in the EGEE Production Grid environment to support the Computational Chemistry applications. The collaboration has been defined in a **Memorandum of Understanding**. The text of the MoU is available here.

To be enabled to EGEE Grid you need a valid X.509 Certificate. If do not have it, you must request it to the Certification Authority that serves your Institution or your Country. If in trouble check the LCG User registration guide to find the most suitable Certification Authority for your needs.

To join CompChem VO, please connect with a web browser equipped with your personal X.509 certificate to the following URL: https://voms.cnaf.infn.it:8443/voms/compchem/webui/request/user/create.

A short description of the operations to be performed to start using CompChem VO is available here.

If you are an administrator of an EGEE Grid production site, please follow the following instructions to support the CompChem VO applications in your site.

The CompChem VO Manager

MPI current status

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- CompChem is supported by 24 hosts with more than 5000 cpus
- Up to date 14 of 24 hosts on CompChem VO support MPI applications
- But only 2 have support MPI-START
  - grid10.lal.in2p3.fr
  - gridgate.cs.tcd.ie

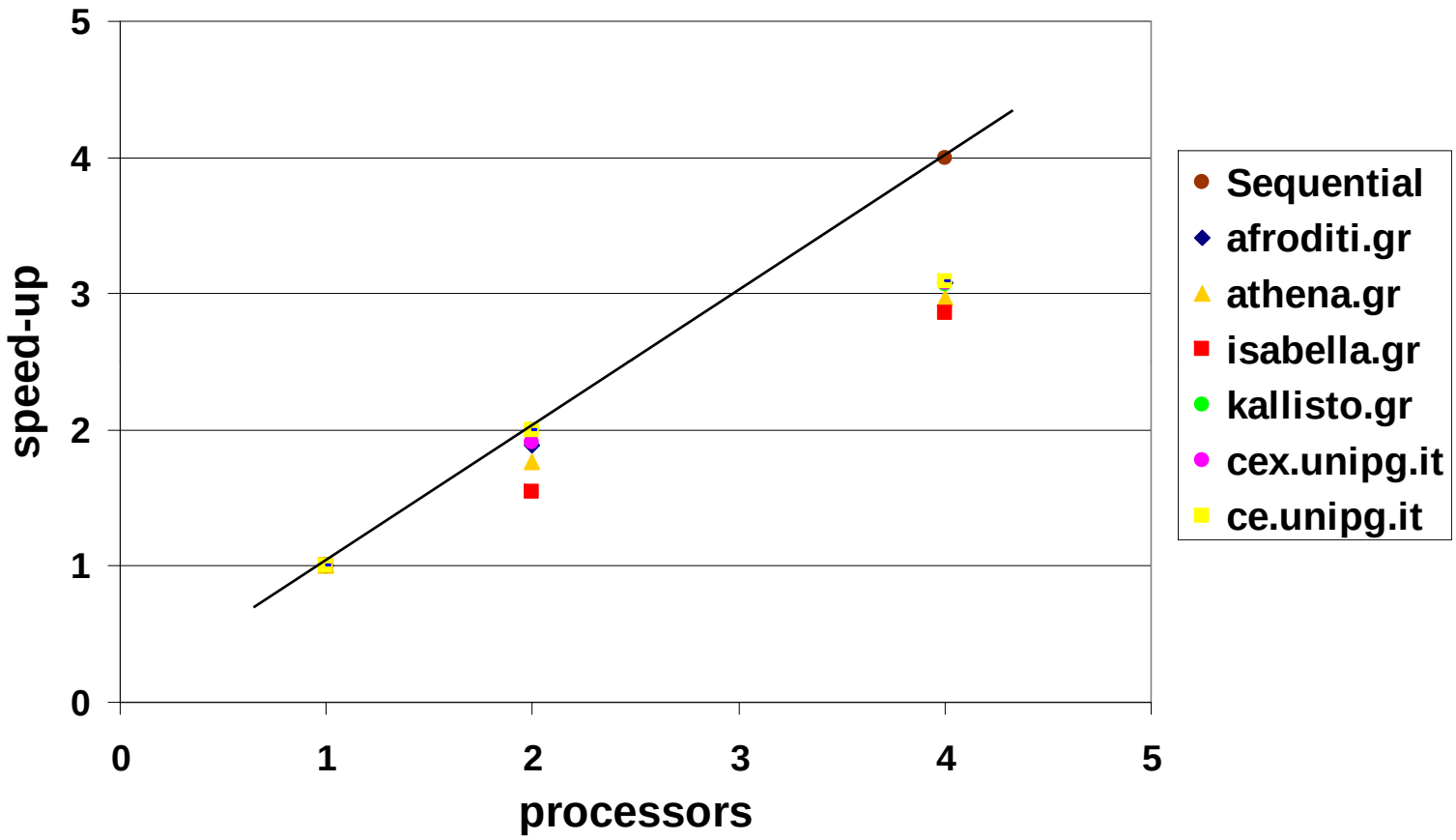
MPI: script and submission

- All the 14 hosts support the base MPI procedure
  - Prepare a script that include
    - Support for shared / not shared home
    - Compiling stage (facultative)
    - Running stage
  - Submission with jdl attribute
    - JobType = "MPICH";
    - NodeNumber = 2;

Performance of the platform

- Performance of the sites were obtained by running a DL_POLY test case
  - Developed by Daresbury Laboratory
  - Developed for MD calculations
  - Native parallel (SPMD schema, Replicated Data strategy)
- The calculation ran sequentially on one node and in parallel on 2 and 4 nodes
- Related speed up was evaluated

Speed-ups



- Parallel applications run properly only on 6 hosts
- Parallel performance of each cluster not necessary depend only from the time sharing regime adopted by them

Statistics

Job status	Number	%
Success	12	43
Not success	16	57

Not success reasons	Number	%
Communic. Error	8	50
mpirun Error	5	31
Scheduler Error	3	19

- Statistical analysis were calculated on 28 parallel jobs
- Only 43% of the jobs ran properly and 57% were not

Main problems using MPI

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- Compiling stage
  - Few users can compile the source code on the destination machine
    - Absence of libraries required by the application on the selected hosts
    - Some of the MPI compilers don't work correctly
      - Absence of f90 modules for mpif90 compiler using mpich-1.2.6-1.sl3.cl package

Main problems using MPI

- Compiling stage
  - Users need to compile their source code on UI machine and link it statically
    - •Production of an executable architecture dependent
    - •Increase of the dimension of the file uploaded via InputSandbox

Main problems using MPI

- Submission stage
  - Crossig-MPI not possible
  - Requested CPUs of a PC cluster need to be free at the same time
    - Waiting time too long for requests involving more than 4 CPUs
  - Load of the Resource Broker too high
    - Delay on the submission procedure

Main problems using MPI

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- Running stage
  - Problems afflicting some hosts
    - Communication problems (ssh intracluster)
    - MPI executable problems (mpirun)
    - Scheduler problems
  - Users need to select the working sites running preliminary jobs

Main problems using MPI

- Get-output stage
  - No problems with OutputSandbox if the total amount of files is less to 80 MB
  - In other cases the use of the SE is up to date encouraged

Conclusions

- Parallel applications don’t run properly in all the hosts supporting MPI libraries
- Users need to
  - compile statically their own code
  - select the hosts that work properly
- YAIM-mpi package prepared for gLite 3.1
  - YAIM-mpi package for gLite 3.0 ?
  - Open-MPI for intracluster MPI?