MPI support

Users view and prospectives

A. Costantini[1], L. Pacifici[1], A. Laganà[2], S. Crocchianti[2]

[1] Dept. of Mathematics and Computer Science
[2] Dept. of Chemistry
University of Perugia

alex@dyn.unipg.it

Summary

- COMPCHEM VO
- MPI applications in COMPCHEM
- MPI state of the art
- Experiences using MPI
- Conclusions

COMPCHEM VO

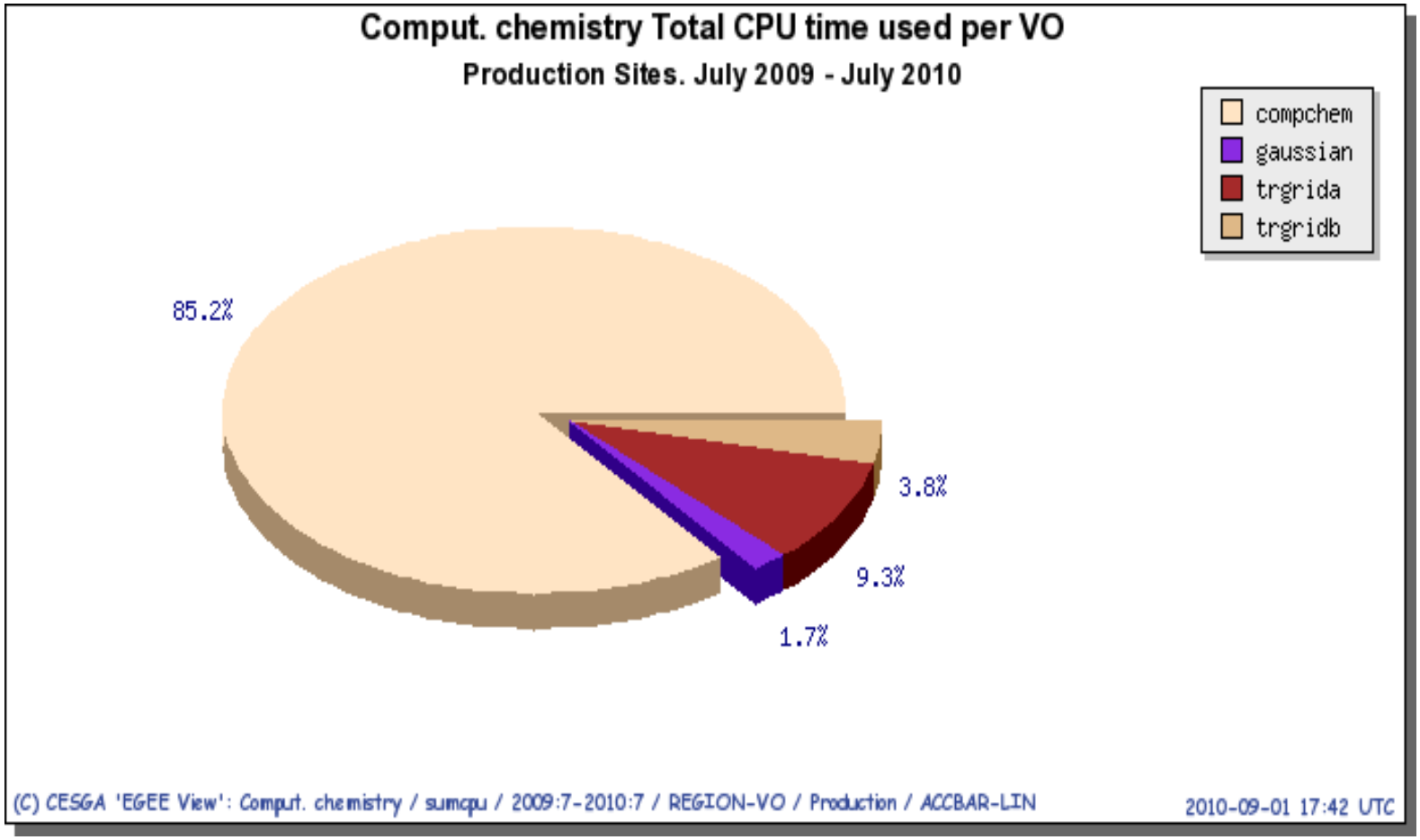
COMPCHEM VO (http://compchem.unipg.it)

- Represent the Molecular and Material Science community
- Deploy Computational Chemistry applications running on a segment of the production European Grid

- Activity started in EGEE project from the end of 2004
- 105 total users
- 10000 CPUs (~10% of the European Grid resources)

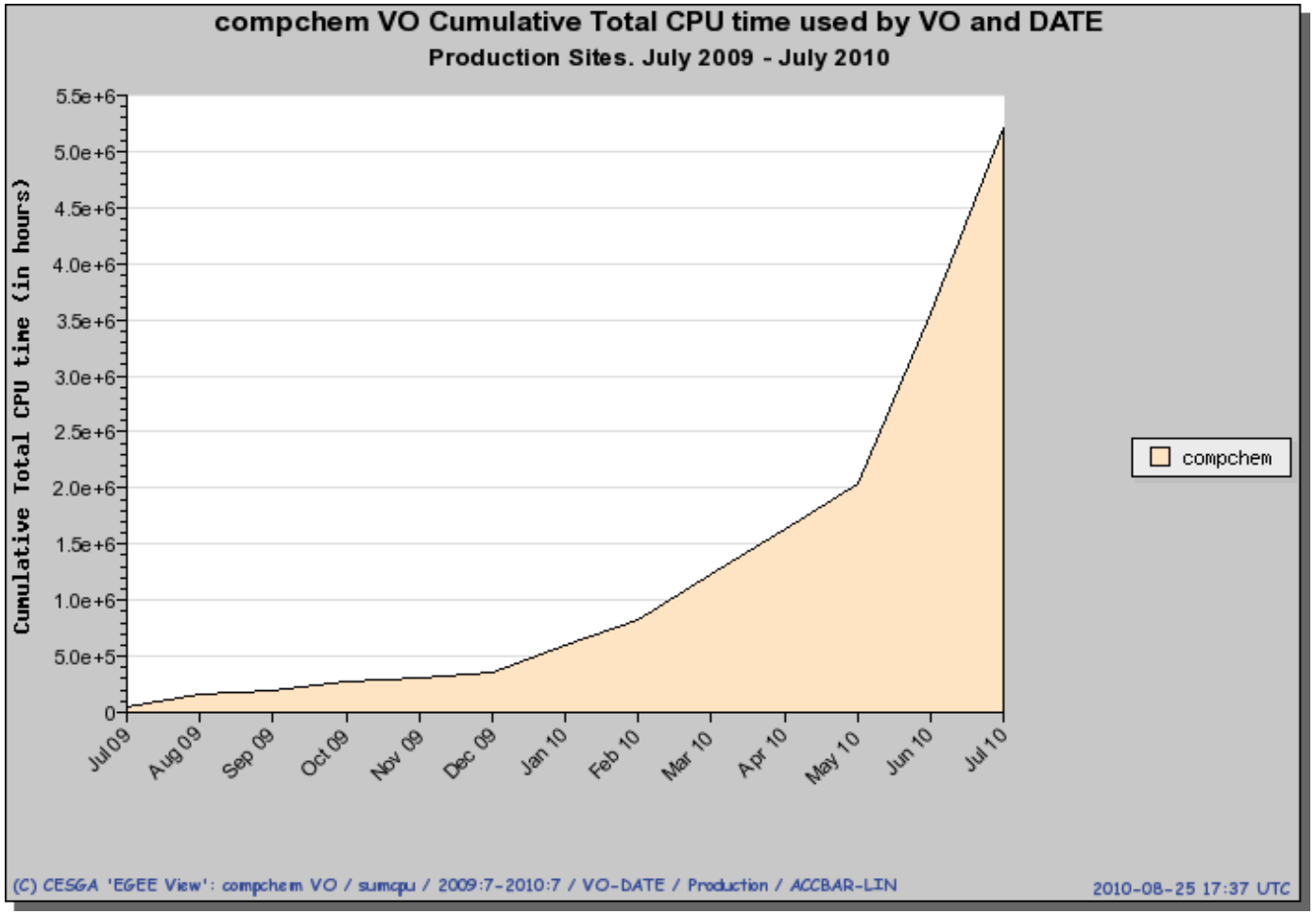
The Comp Chem Discipline

From the EGEE Accounting Portal at the *Centro de Supercomputación de Galicia*
http://www3.egee.cesga.es/gridsite/accounting/CESGA/egee_view.html



Statistics

From the EGEE Accounting Portal at the *Centro de Supercomputación de Galicia*
http://www3.egee.cesga.es/gridsite/accounting/CESGA/egee_view.html



Costantini et al. EGI-TF 2010

Applications

- 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.
- Interactive jobs: GEMS (Grid Enabled Molecular simulator)
- We are developing web-related Grid Services
  - to access the standard functionalities of the programs
  - to evaluate QoU and QoS

Parallel Applications

-Basic Linear algebra algorithms (low level complexity codes)

- Cannon algorithm
- Fox algorithm
- Strassen algorithm

- Medium complexity in house developed codes
  - RWAVEPR quantum time-dependent reactive dynamics
  - SC-IVR semiclassical-initial value representation

- High complexity general purpose computational codes
  - GAMESS-US high-level *ab initio* molecular quantum chemistry
  - DL_POLY molecular dynamics simulation of complex systems
  - NAMD molecular dynamics simulation of complex systems

Costantini et al. EGI-TF 2010

MPI: current status

- COMPCHEM VO is supported by 25 sites over Europe

- Up to date 16 of 25 sites on COMPCHEM VO support MPI applications (22/25 in 2009)

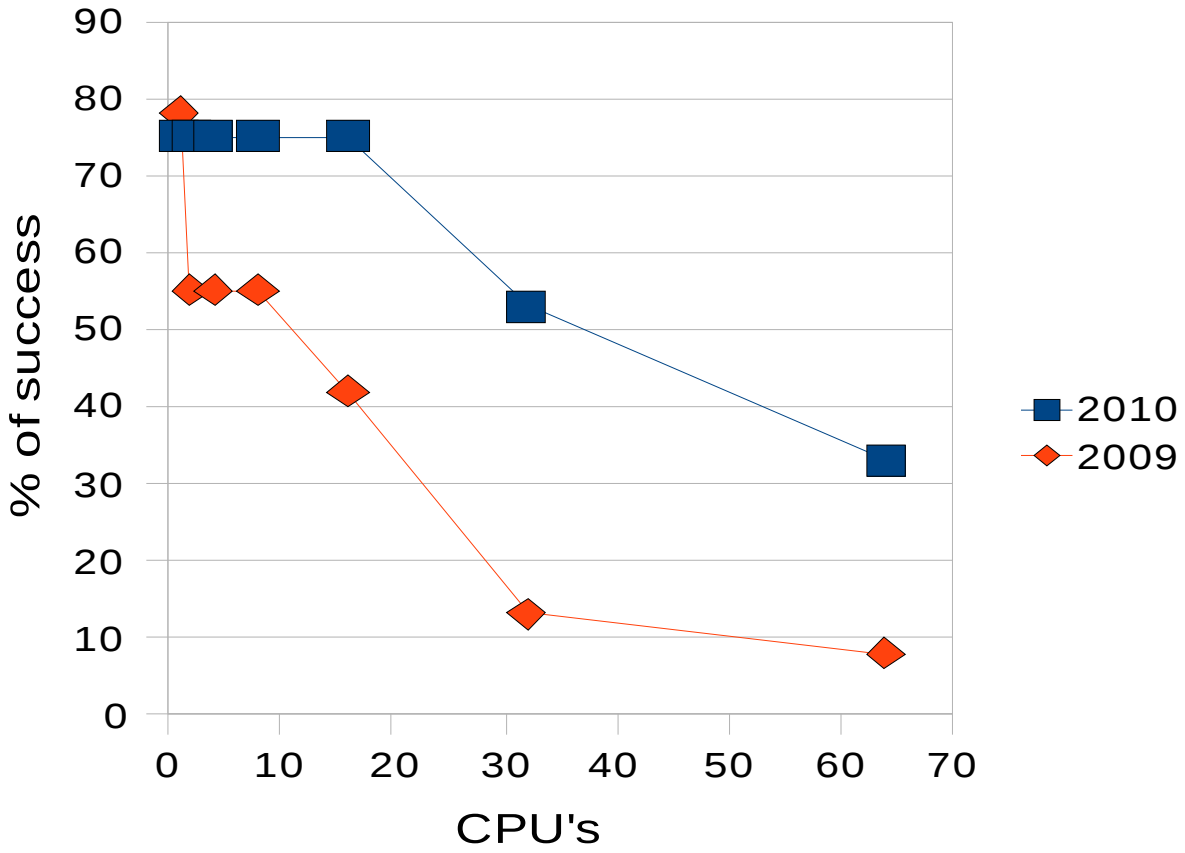
  - Requirements MPI-START && MPICH

DL_POLY as MPI test case

- 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)
  - Compiled using IFC, MKL, MPICH (static compiled on the UI)
- The calculation ran sequentially on one node and in parallel on 2, 4, 8, 16, 32, 64 nodes
- Related performances and statistics were evaluated

Costantini et al. EGI-TF 2010

Performances over the Grid



- SAM-MPI tests enabled
- Parallel applications run properly on 12 sites up to 16 CPUs

Up to 8 CPUs

Job status	%(2009)	%(2010)
Success	53	75
Not success	47	25

Not success	%(2009)	%(2010)
Abortion (CE)	52	0
Scheduler Error	39	100
MPI-START	9	0

- Job got an error while in the CondorG queue (Globus error 17)

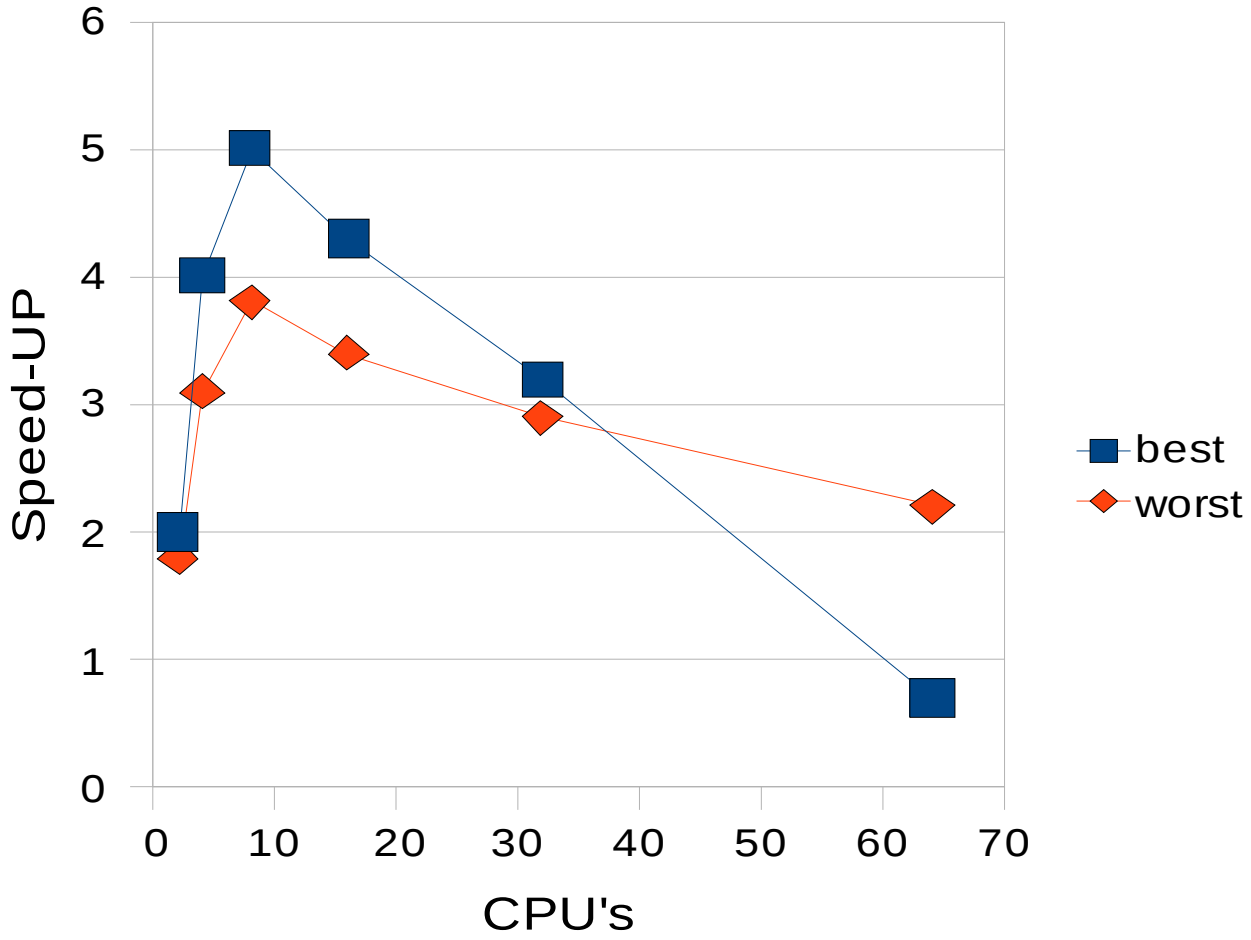
From 16 up to 64 CPU

Job status	%(2009)	%(2010)
Success	21	54
Not success	79	46

Not success	%(2009)	%(2010)
Abortion (CE)	73	0
Scheduler Error	23	93
Proxy expired	4	7

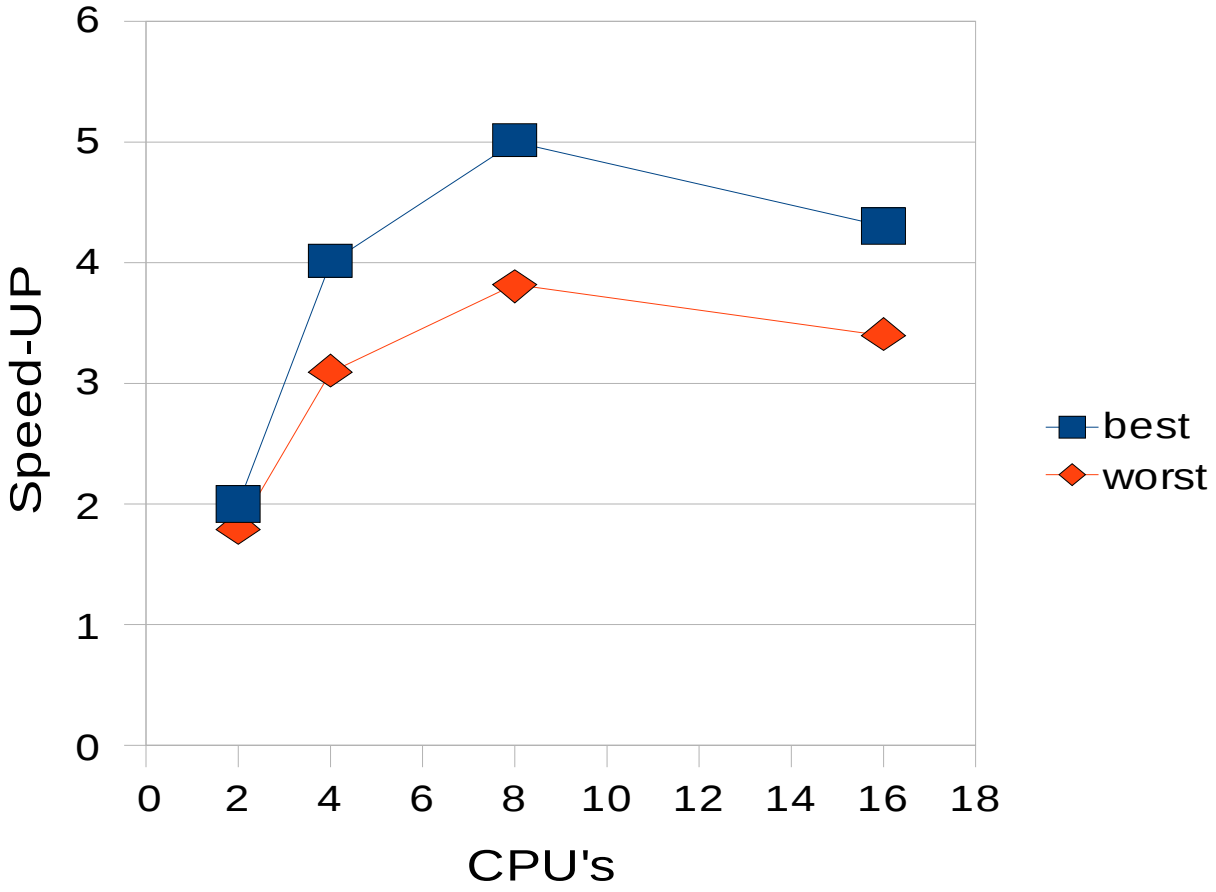
- Job got an error while in the CondorG queue
- Request expired

Performances



Costantini et al. EGI-TF 2010

Performances



- For good S-UP the CPUs must belong to the same node
- SMP tag should be enabled in the WMS used for production

Costantini et al. EGI-TF 2010

Conclusions

- SAM-MPI tests solved most of the abortion reasons
  - Understand abortion reasons
- Waiting time
  - CPUs in a cluster need to be free at the same time
  - Load of the Resource Broker
    - Delay on the submission procedure
- Best performances
  - improve the comm btw different WNs on the CE :(
  - enable SMP tag :)