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Computational Chemistry Requirements and experiences with use of MPI in EGEE

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Summary

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

COMPCHEM VO

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- **COMPCHEM VO** (http://compchem.unipg.it)
  - runs in the EGEE production Grid from the end of 2004
  - 80 active users
  - 8000 CPUs (~8% of the EGEE resources)
  - Several EGEE sites are supporting the VO
    - 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).

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.
- 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

MPI current status

- COMPCHEM VO is supported by 35 sites over Europe

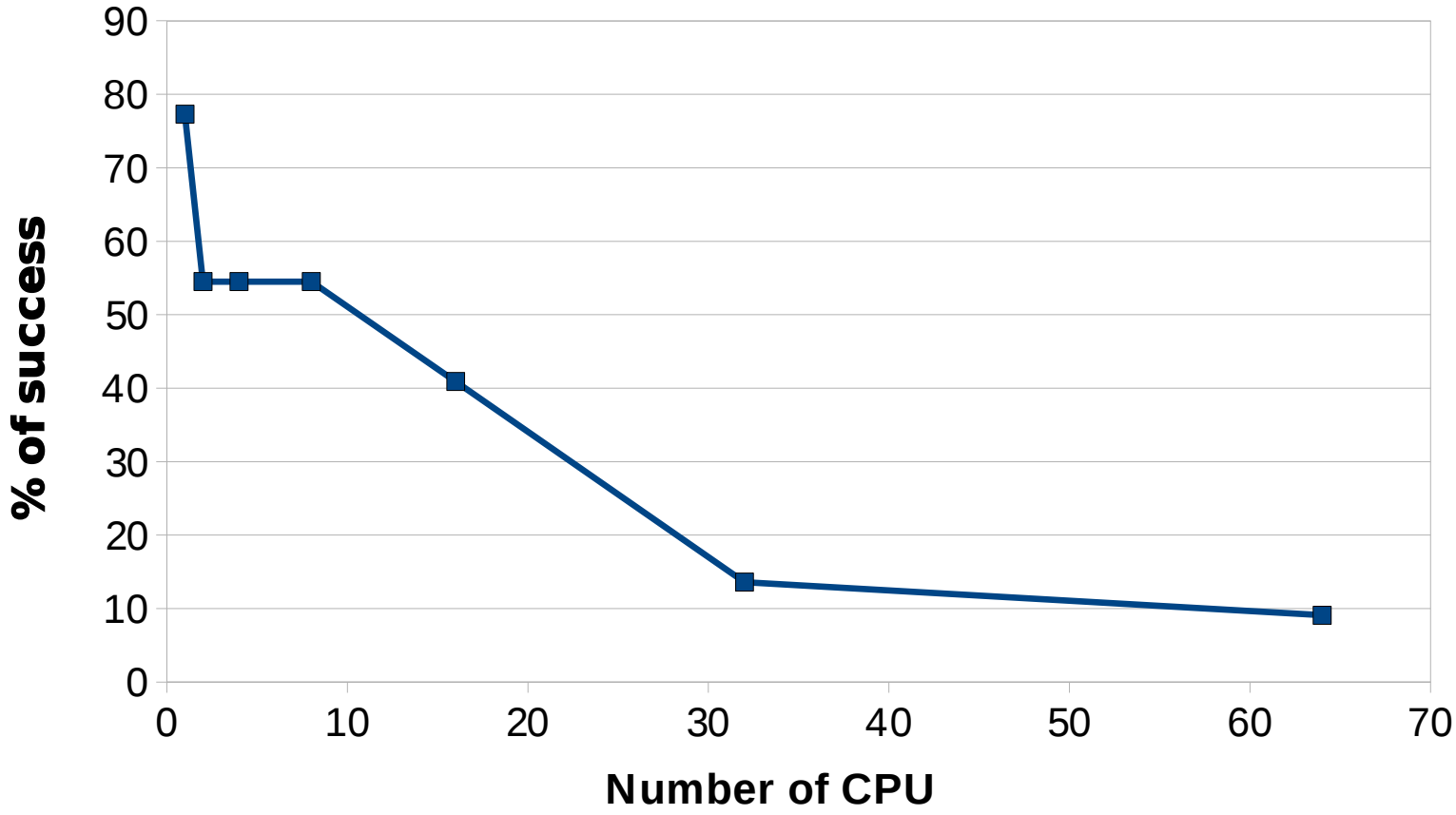
- Up to date 22 of 35 sites on COMPCHEM VO support MPI applications

  - 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 MPICH1
- The calculation ran sequentially on one node and in parallel on 2, 4, 8, 16, 32, 64 nodes
- Related performances and statistics were evaluated

Performances over the Grid



- Parallel applications run properly on 12 sites up to 8 CPUs
- High level of abortion using above 16 CPUs

Statistics
using up to 8 processors

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Job status	Number	%
Success	35	53
Not success	31	47

Not success reasons	Number	%
Abortion	16	52
Scheduler Error	12	39
MPI-START	3	9

- Statistical analysis were calculated on 66 parallel jobs
- Only 53% of the jobs ran properly and 47% were not

Statistics
using 16 up to 64 processors

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Job status	Number	%
Success	14	21
Not success	52	79

Not success reasons	Number	%
Abortion	38	73
Scheduler Error	12	23
Proxy expired	2	4

- Statistical analysis were calculated on 66 parallel jobs
- Only 21% of the jobs ran properly and 79% were not

Not success jobs: possible reasons

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- MPI-START

  . Problems related to sites supporting MPI_SHARED_HOME

- Problems with sites using lsf scheduler

  . Exit != 0

  mpiexec: Error: PBS_JOBID not set in environment.

  Problem fixed in the next release of YAIM-MPI package

- Bad JDL declaration variable

  . Using JobType = "Normal";

The NodeNumber variable is by-passed

Direct consequence: each site supporting MPI-START is suitable for the job submission even if the number of CPUs of the farm is lower than requested

High level of abortion

Main problems using MPI

- Requested CPUs in a cluster need to be free at the same time

- Waiting time too long for Requirements involving more than 8 CPUs (5H - 20H)

- Load of the Resource Broker too high

    - Delay on the submission procedure

- Users need to select the working sites running preliminary jobs

Conclusions

- Parallel applications don’t run properly in all the sites supporting MPI-START in COMPCHEM VO
- Users must to
  - Select the sites that work properly
  - Limit the use of CPUs to perform parallel calculations
- YAIM-mpi package for gLite 3.1 needs to be improved and tested