

EGEE NA4
All Hands Meeting
Life Science Cluster

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Participation of ASGC to NA4 Lief Science Cluster

- Development of generic Virtual Screening Services: 12 PM
 - Make virtual screening a stand-alone services to the EGEE,
 - Integrated GUI client SW, supporting the portal services from job submission, job status checking, simulation and histogram analysis, etc.
 - Collaborate to extend the Virtual Screening services to be a Common Application Platform for drug discovery across variant underlying middleware systems (by making use of Ganga, AMGA and DIANE, etc)
- Integration of workflow management services into gLite and the Common Application Platform: 12 PM



Virtual Screening Service with GAP

A standalone GUI Application

• One-click job submission

Virtual Screening Service

File Edit Tools Help

Target Ligand Docking Parameter

Initial Factor Parameter for "analysis" command GA&LGA Parameter Local Search Parameters

Translation step / A :
Quaternion step/deg :
Torsion step/deg :
Translation reduction factor :
Quaternion reduction factor :
Torsion reduction factor / p :

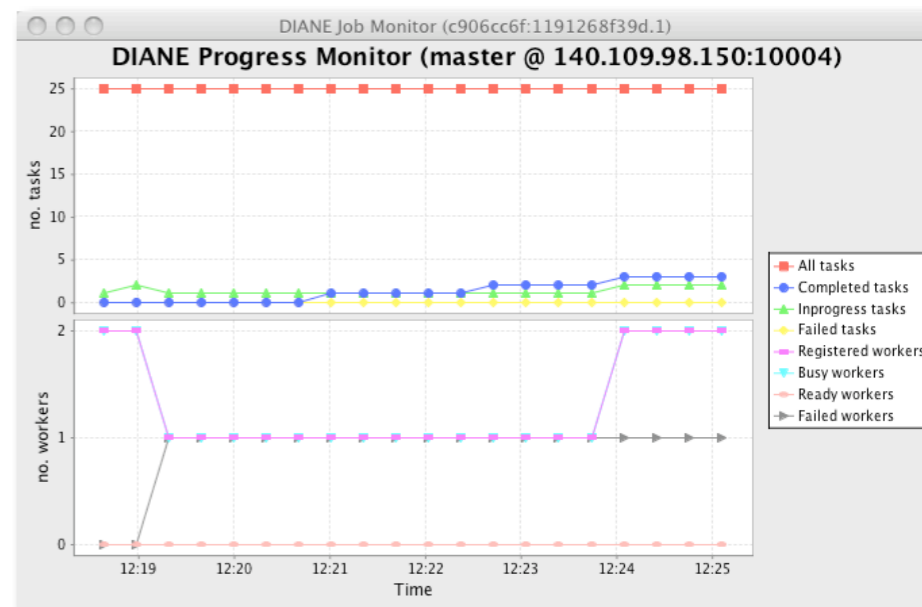
Submitting "Hi, I am Job."
1. Generating Ligand List ... ✓
2. Generating Docking Parameter File ... ✓
3. Setting Job Parameters ... ✓
4. Job Submission ... ✓

100%
OK Close after 8 seconds.

Restore to default

Job Description : Hi, I am Job. Resource Domain : * Worker Number : 10 **Submit**

Submit the docking job to the Grid with just one click



• Visualize your job status

• View the best conformation of a simulation

Job History

Job Description	Job Group ID	Command	Submitted Time	Success Rate	Status
Hi, I am Job.	1207194678172	DianeVirtualScreeningProc	2008-04-03 12:14:56	100%	DONE
Small job submission	1207149478850	DianeVirtualScreeningProc	2008-04-02 23:18:08	100%	DONE
test docking.1	1207110549492	DianeVirtualScreeningProc	2008-04-02 12:32:15	100%	DONE
Running job progress testing.3	1207017000992	DianeVirtualScreeningProc	2008-04-01 10:30:45	100%	DONE
Running job progress testing.2	1207017000988	DianeVirtualScreeningProc	2008-04-01 10:30:23	100%	DONE
Running job progress testing.	1207017000984	DianeVirtualScreeningProc	2008-04-01 10:30:09	100%	DONE
More job without lns	1207016351346	DianeVirtualScreeningProc	2008-04-01 10:20:14	100%	DONE

Hi, I am Job.

Target Ligand

DC2_TOSIAN	cdi_000A-0111
DC2_TOSIAN	cdi_000A-0506
DC2_TOSIAN	cdi_000A-0800
DC2_TOSIAN	cdi_000A-0829
DC2_TOSIAN	cdi_000A-0742
DC2_TOSIAN	cdi_000A-0601
DC2_TOSIAN	cdi_000A-0606
DC2_TOSIAN	cdi_000A-0823
DC2_TOSIAN	cdi_000A-0650
DC2_TOSIAN	cdi_000A-0815

Show Best Complex
Show Best Conformation
Show Energy Histogram

Energy Threshold -6

Best Complexes Best Conformations Histograms

• Generate the histogram with a given energy threshold

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DC2_TOSIAN	cdi_000A-0742
DC2_TOSIAN	cdi_000A-0601
DC2_TOSIAN	cdi_000A-0606
DC2_TOSIAN	cdi_000A-0823
DC2_TOSIAN	cdi_000A-0650
DC2_TOSIAN	cdi_000A-0815

Show Best Complex
Show Best Conformation
Show Energy Histogram

Energy Threshold -8

Best Complexes Best Conformations Histograms

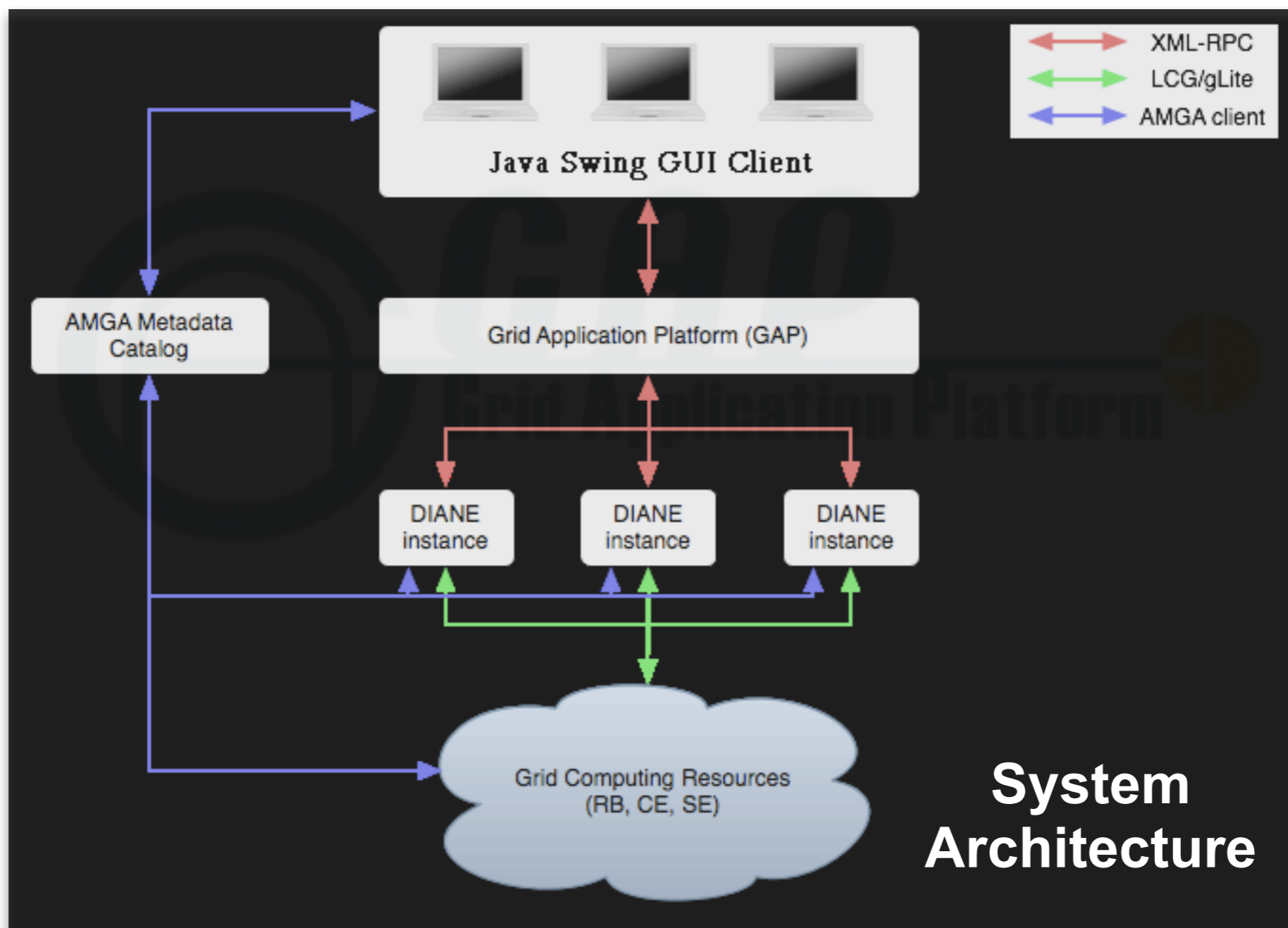
Histogram on 25 screens: DC2_TOSIAN

Histogram on 21 screens: DC2_TOSIAN



Virtual Screening Service with GAP

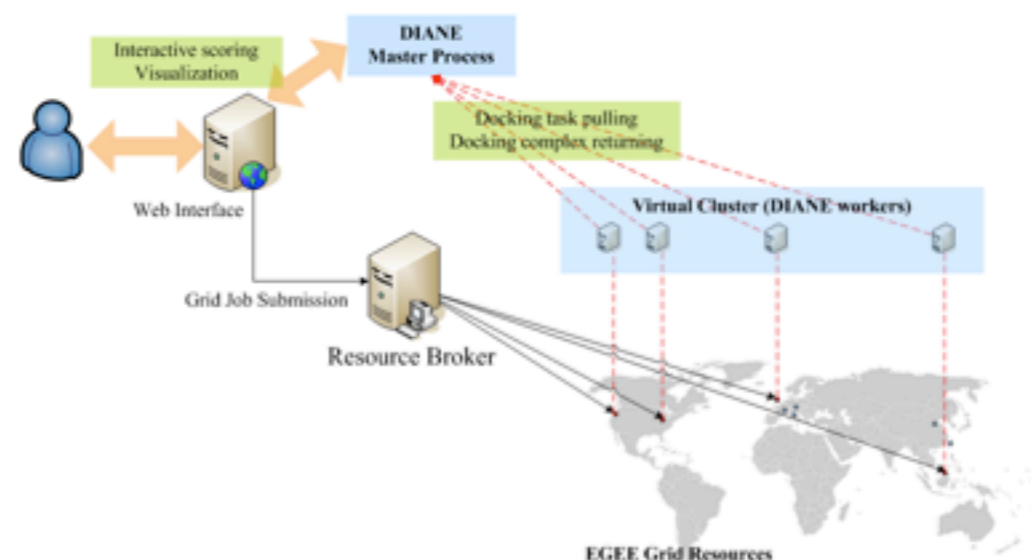
- Stand-alone GUI application for virtual screening service with GAP.



WISDOM



DIANE/GANGA



	WISDOM	DIANE
Total number of completed dockings	2 * 10 ⁶	308,585
Estimated duration on 1 CPU	88.3 years	16.7 years
Duration of the experience	6 weeks	4 weeks
Cumulative number of the Grid jobs	54,000	2580
Max. number of concurrent CPUs	2,000	240
Crunching rate	912	203
Approximated distribution efficiency	46%	84%
Approximated throughput	2 sec/docking	10 sec./ docking

> 100 CPU years in 6 weeks on the EGEE grid

300,000 compounds => 2000 focus library => 123 potential hits => more analysis in wet lab.

in-silico docking on the grid

SDDB re-ranking

in-vitro test