



A lightweight job execution control framework

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DIANE tool

- Help smaller scientific communities using distributed (Grid) resources more efficiently
 - reduce the application execution time
 - reduce the manual work overhead by providing fully automatic execution and failure management,
 - efficiently integrate local and Grid resources
- R&D project started in 2000
 - **<http://cern.ch/diane>**
 - now part of EGEE Respect suite
 - part of Grid Application Support Services at CERN
 - together with Ganga (Job Management Interface)
 - **<http://cern.ch/ganga>**

Grid Application Support @ CERN

- Infrastructure for smaller communities/generic applications
 - a set of configured master hosts hosted at CERN
 - Grid resources: GEAR VO
 - tools: DIANE + Ganga
- Applications

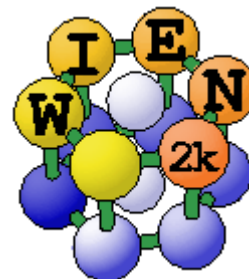
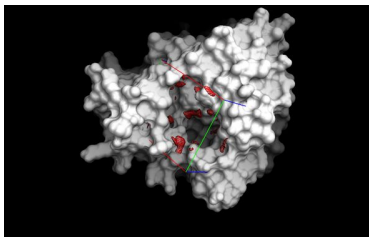
Geant 4



HARP

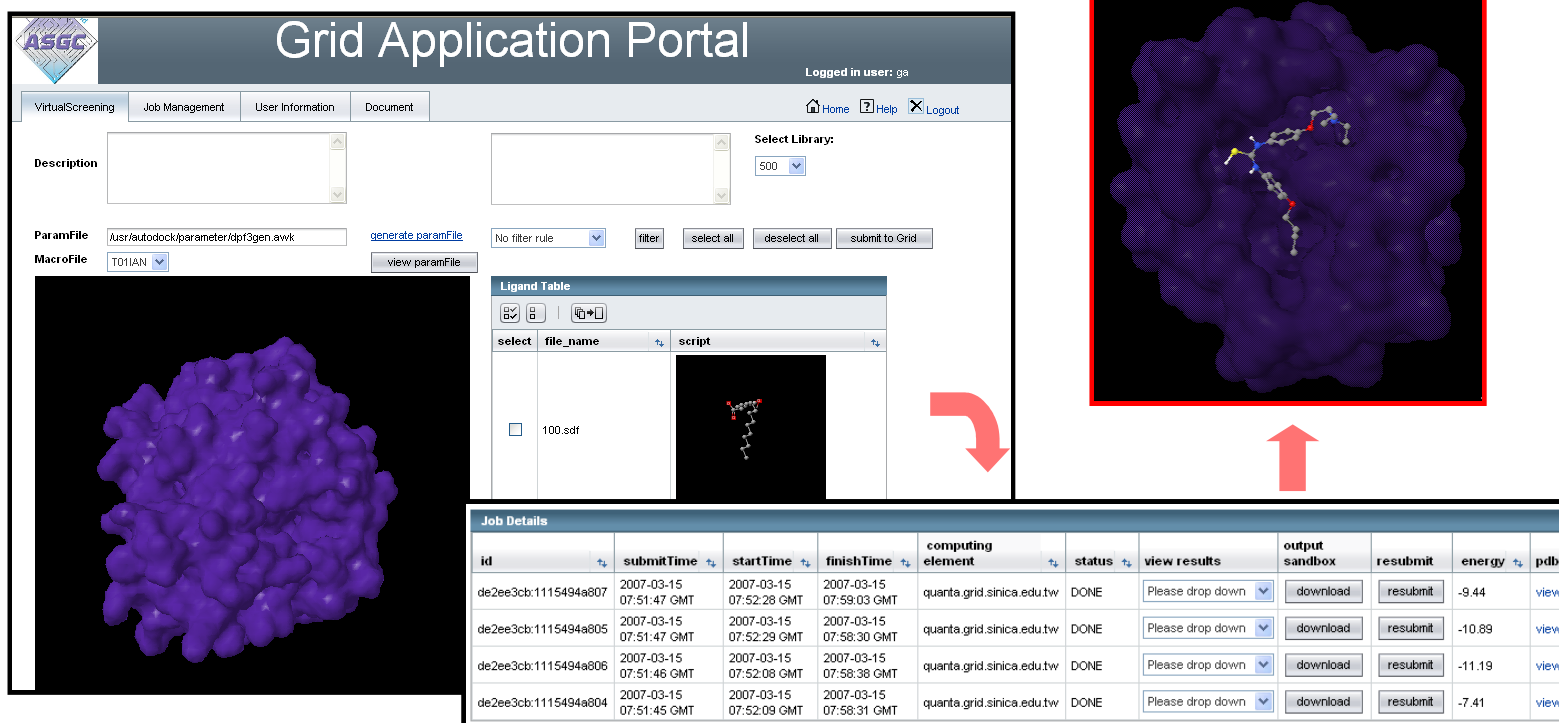


Garfield



Web-portal for biologists

- ASGC portal for virtual screening (docking)
 - AvianFlu Drug Search et al. (H.C.Lee 2006)
 - web-interface created by biologists
 - in the backend: DIANE and Ganga to handle Grid jobs



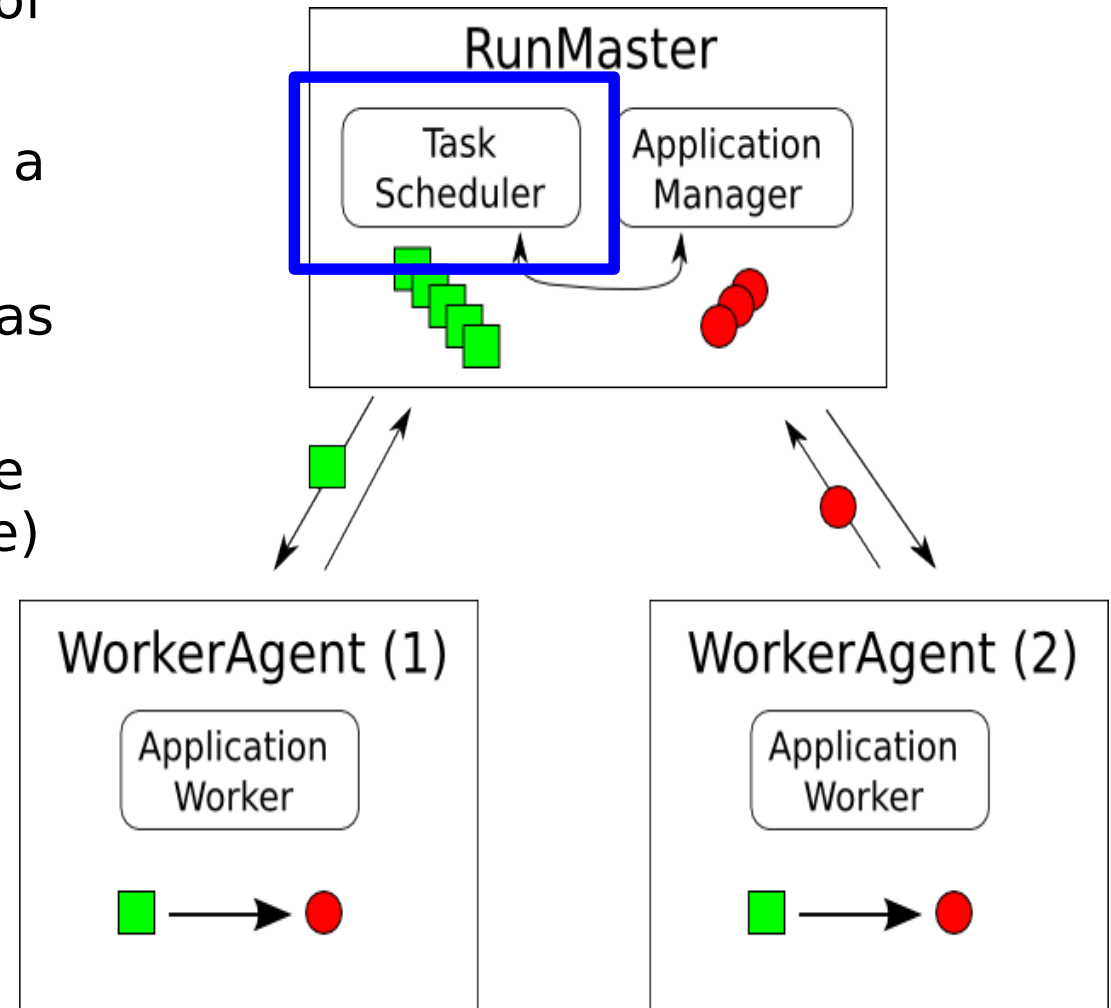
The screenshot displays the 'Grid Application Portal' interface. At the top, it shows the ASGC logo and the title 'Grid Application Portal'. The user is logged in as 'ga'. The interface includes a navigation menu with 'VirtualScreening', 'Job Management', 'User Information', and 'Document'. Below this, there are input fields for 'Description', 'ParamFile', and 'MacroFile'. A 'Ligand Table' is visible, containing a table with columns for 'select', 'file_name', and 'script'. A 'Job Details' table is also present, showing a list of jobs with their respective IDs, submission times, start and finish times, computing elements, status, and energy values. A 3D molecular model of a protein-ligand complex is shown on the right side of the interface.

select	file_name	script
<input type="checkbox"/>	100.sdf	

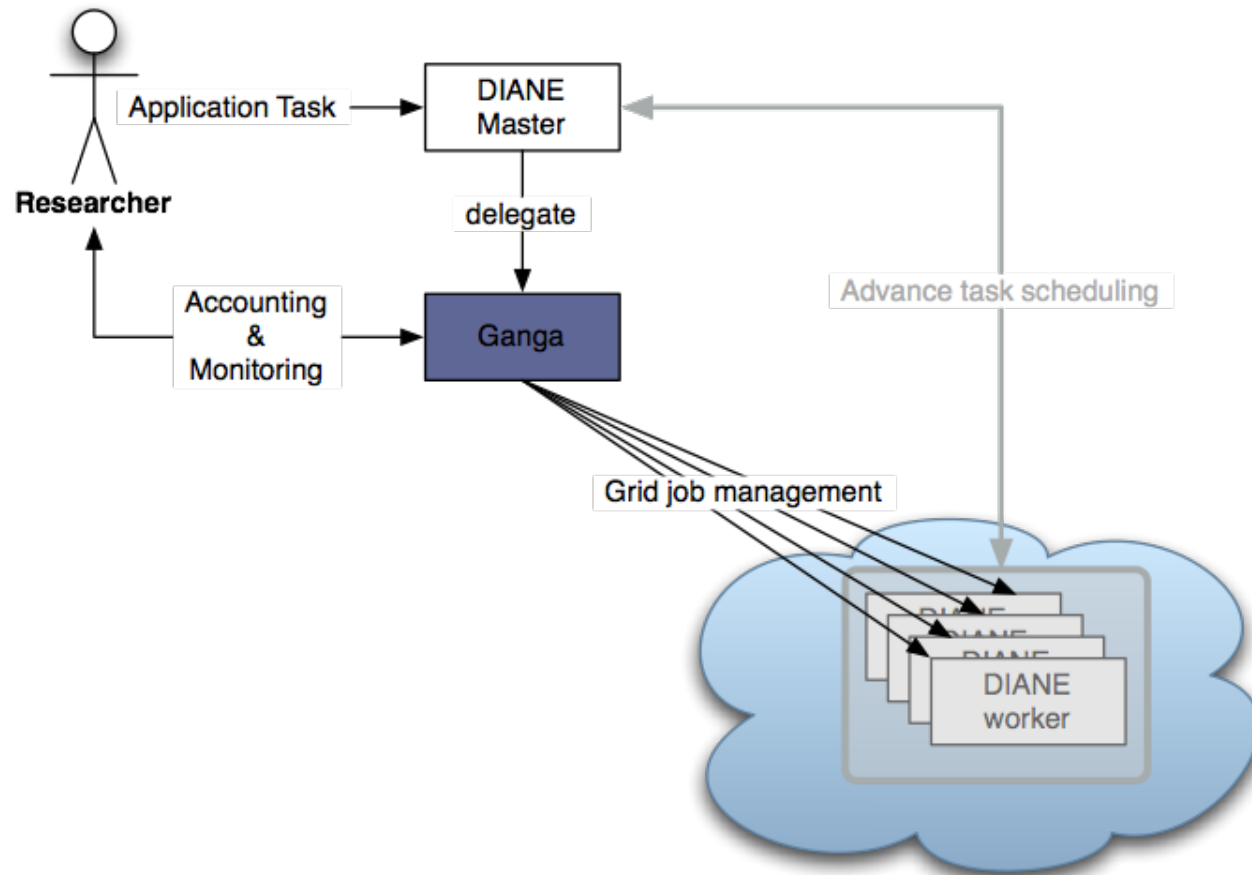
id	submitTime	startTime	finishTime	computing element	status	view results	output sandbox	resubmit	energy	pdb
de2ee3cb:1115494a807	2007-03-15 07:51:47 GMT	2007-03-15 07:52:28 GMT	2007-03-15 07:59:03 GMT	quanta.grid.sinica.edu.tw	DONE	Please drop down	download	resubmit	-9.44	view
de2ee3cb:1115494a805	2007-03-15 07:51:47 GMT	2007-03-15 07:52:29 GMT	2007-03-15 07:58:30 GMT	quanta.grid.sinica.edu.tw	DONE	Please drop down	download	resubmit	-10.89	view
de2ee3cb:1115494a806	2007-03-15 07:51:46 GMT	2007-03-15 07:52:08 GMT	2007-03-15 07:58:38 GMT	quanta.grid.sinica.edu.tw	DONE	Please drop down	download	resubmit	-11.19	view
de2ee3cb:1115494a804	2007-03-15 07:51:45 GMT	2007-03-15 07:52:09 GMT	2007-03-15 07:58:31 GMT	quanta.grid.sinica.edu.tw	DONE	Please drop down	download	resubmit	-7.41	view

Simple computation model

- Master/Worker processing of tasks
 - RunMaster executes on a local host
 - WorkerAgents execute as Grid jobs
- TaskScheduler is a software component (python module) which may be arbitrarily customized or replaced
- application “wrappers” (plugins):
 - ApplicationWorker
 - ApplicationManager



Architecture



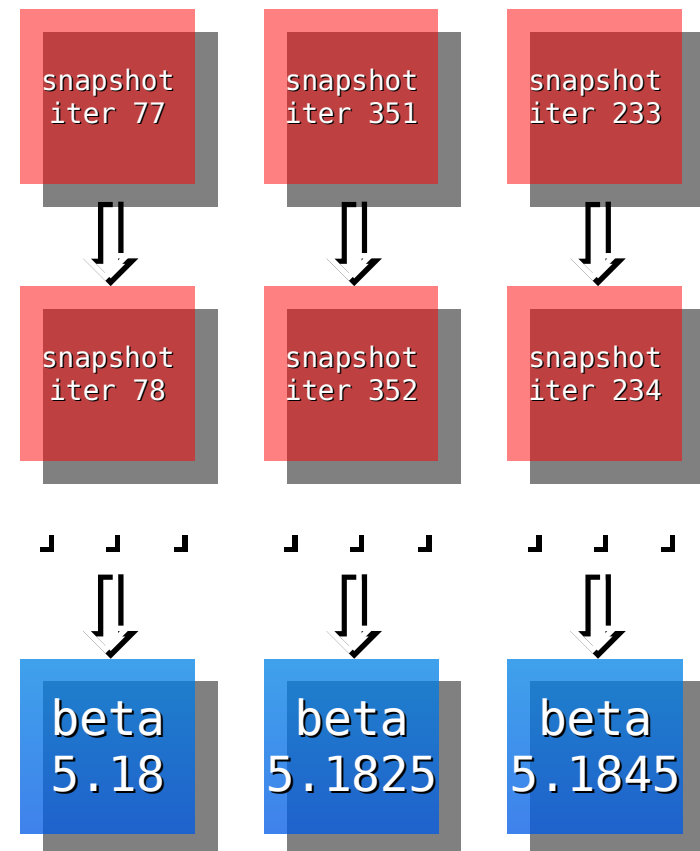
Example: Lattice QCD @ Grid

- Study the behaviour of the critical point of quark-gluon plasma
 - The scientific results obtained by the LQCD project were published in a paper P. de Forcrand et al.: "The chiral critical point of $N_f = 3$ QCD at finite density to the order $(\mu/T)^4$ " and are available at <http://arxiv.org/pdf/0808.1096>
- Monte-Carlo simulation of discrete space-time lattice
 - need a lot of CPU
 - relatively small data (\sim Gbs)



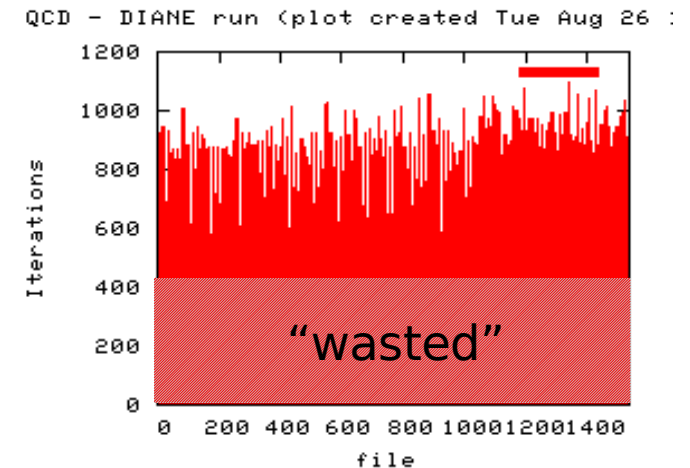
Structure of LQCD application

- Monte-Carlo simulation of discrete space-time lattice
 - snapshots of the lattice state are evolved iteratively
 - snapshot file is 10MB large
 - single iteration takes around 1.5 hours on a WN
 - task = one iteration
- 16 beta values x N random seeds = 400-1500 snapshots

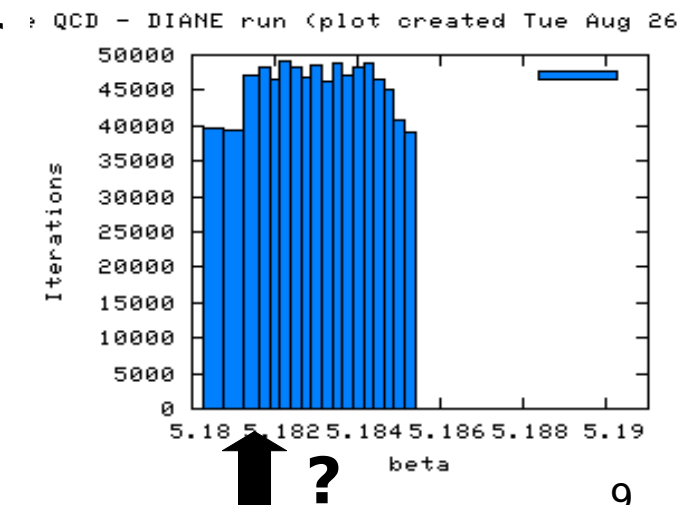
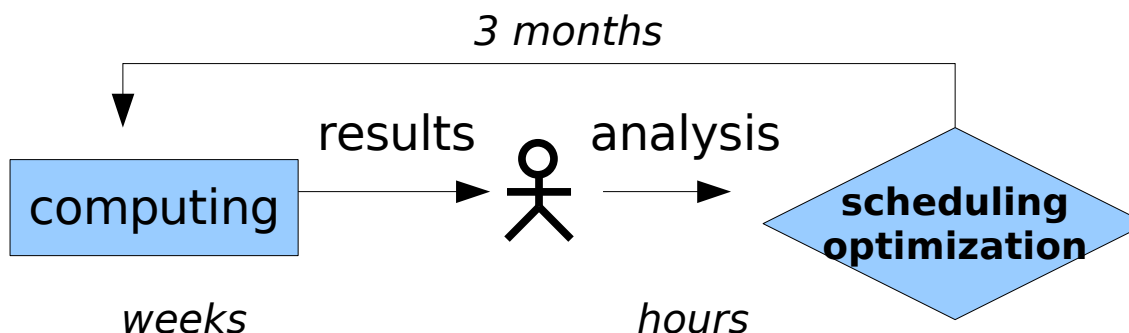


Scheduling of snapshots

- constant overhead
 - each snapshot must diverge from the original state in order to be significant
-> 300-500 iterations are “wasted”
i.e. 20-30 CPU days
- how to best schedule the iterations?
 - make convergence of snapshots equally slow for all beta values
 - or prefer some beta values if more important scientifically?

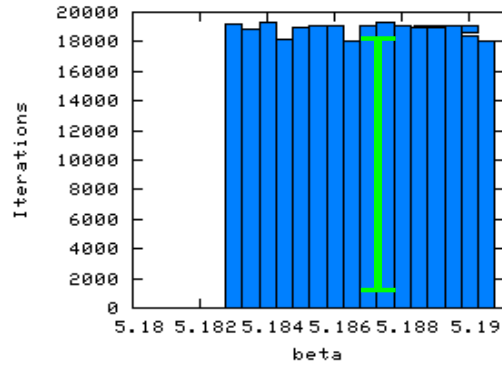
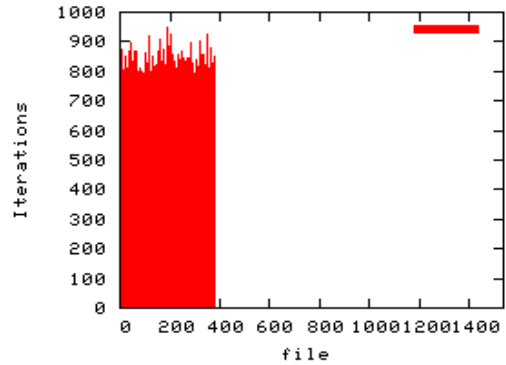


- long-term optimizations with the user



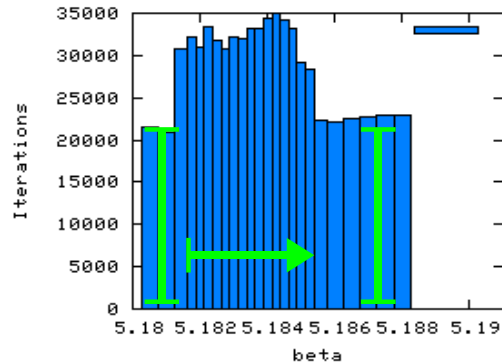
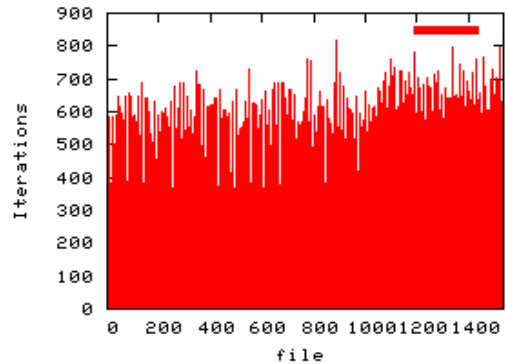
Scheduling of snapshots

QCD - DIANE run (plot created Tue Aug 26) QCD - DIANE run (plot created Tue Aug 26



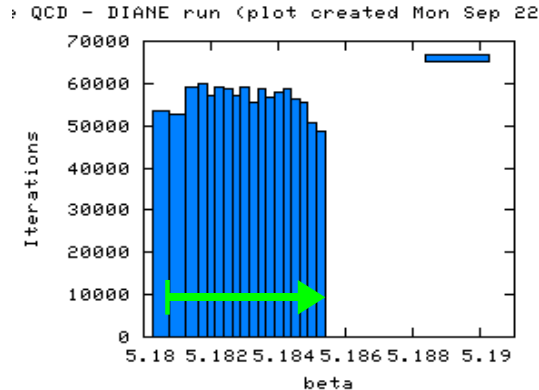
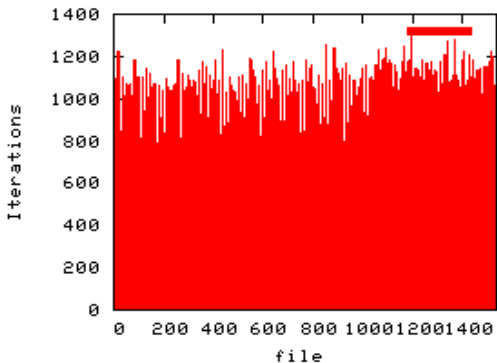
(1) 400 snapshots, 16 betas all equal

QCD - DIANE run (plot created Fri Aug 1) QCD - DIANE run (plot created Fri Aug 1



(2) 1500 snapshots, 16 betas priority window left-to-right equal outside of the window

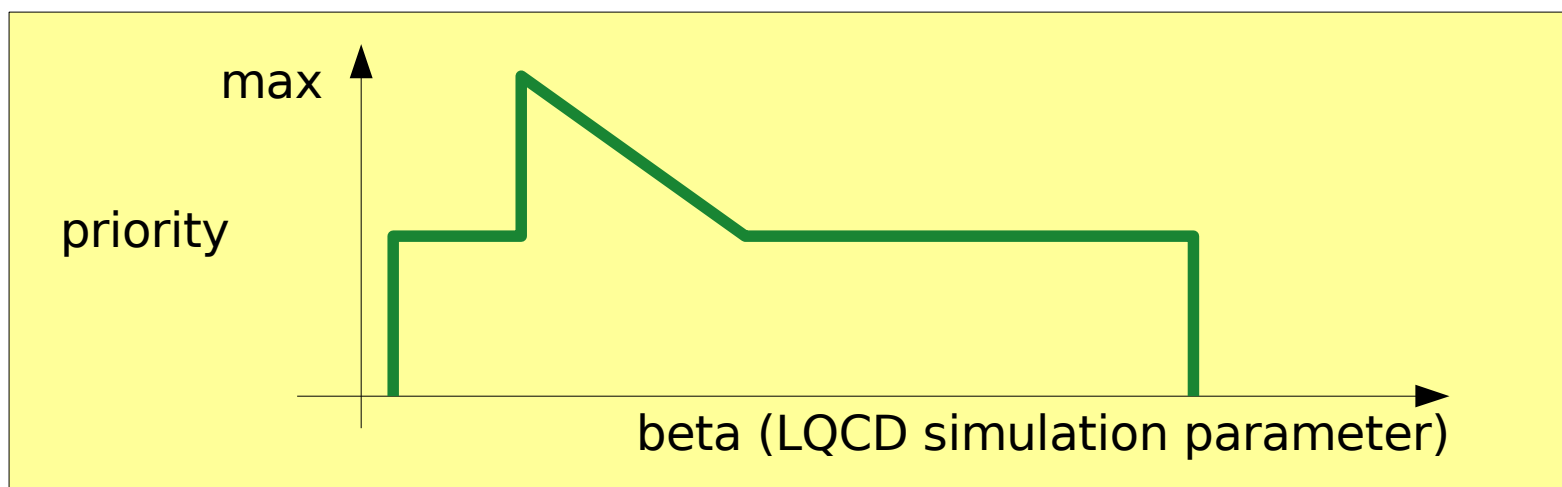
QCD - DIANE run (plot created Mon Sep 22 :



(3) 1000 snapshots, 10 betas priority left-to-right

Task Scheduler plugin

- LQCD Task Scheduler plugin
 - simple python class (around 100 lines)



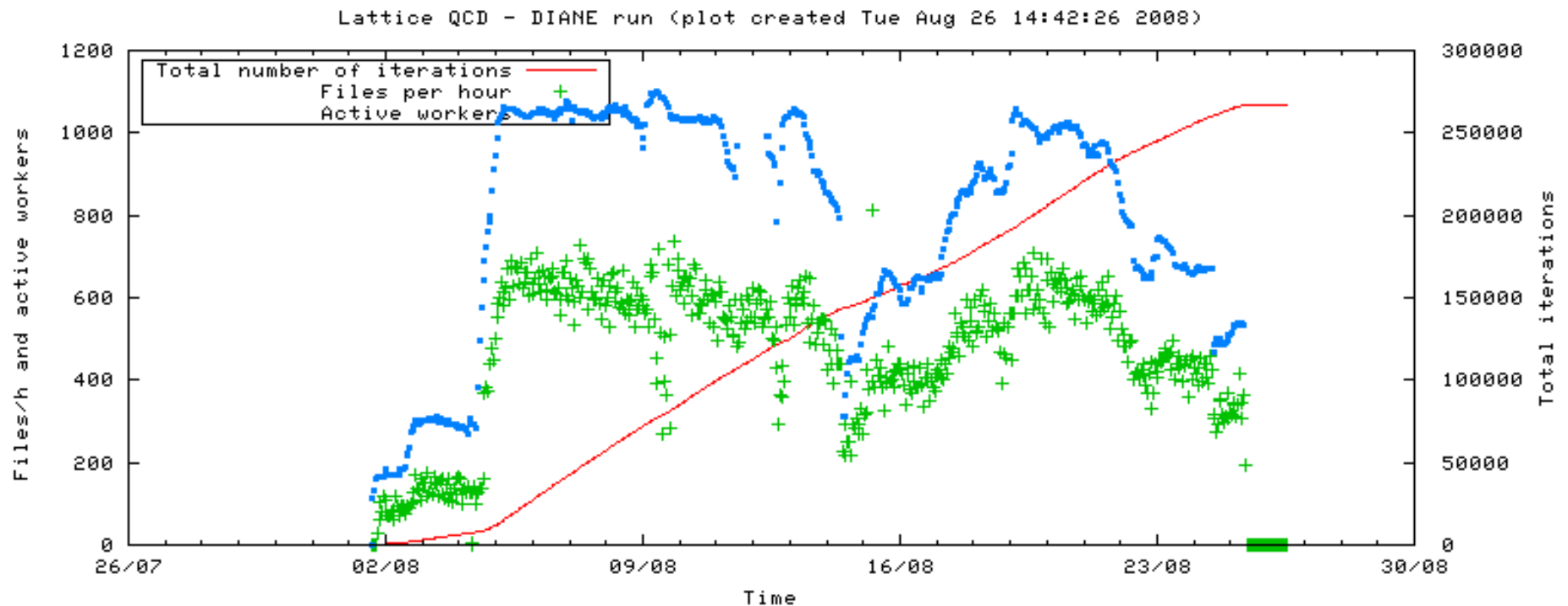
- standard DIANE scheduler
 - available out-of-the box
 - useful for most trivially parallel applications
 - simple scheduling policies
 - similar to gLite WMS: retry counts, etc.

LQCD execution history

- ongoing since May 2008
 - several phases (application and system upgrades, power-cuts, etc...)
 - long periods of uninterrupted computing
- little manual maintenance overhead
 - automatic task scheduling done by the master
 - automatic submission of pilot agents by an AgentFactory

LQCD throughput

- ~2 million CPU hours / 3 months
 - i.e. **231 CPU years**
- ~4.3 TB of data transferred
- **1000 simultaneous workers**



Summary

- DIANE main features
 - efficient application scheduling via python plugins
 - fully automatic job execution at large scale
 - 100% reliability from the user perspective
- Related events at EGEE 08:
 - ***(5) Grid-enabled Virtual Screening Service based on Grid Application Platform***
 - ***(24) Porting THIS on the EGEE Grid***
 - ***(42) Ganga and DIANE: powerful job management and resource***
- **<http://cern.ch/diane>**



backups

Other aspects

- One aspect was addressed: scheduling
- however DIANE may be used to control very short jobs too. Sometimes it may not be possible to statically optimize (cluster) short jobs (ITU) and then the only option is to use a “pull” scheduler.
- connection-oriented vs connectionless mode. possible to quasi-interactively control the worker nodes (cutting out the Grid scheduling overhead).
- a master may also serve as a synchronization point: e.g. one task requires output of other tasks (workflows) or task execution should be synchronized on some condition. such capabilities may be achieved by plugins.