Gridification of PANAM, a phylogenetic pipeline for High Throughput Sequencing Analysis using the DIRAC framework

By Doan Trung Tung et al.

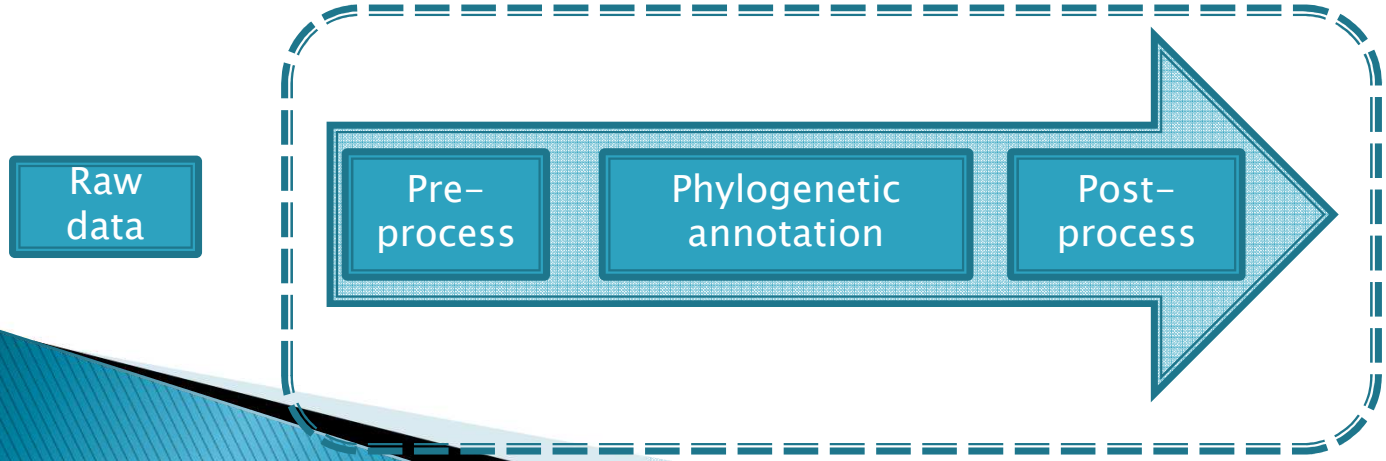
EGI Technical Forum 2013

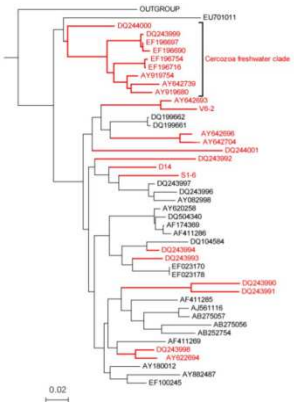
Plan

- What is PANAM, why grid?
- PANAM gridification with DIRAC
- Results
- Remarks for DIRAC
- Conclusion and perspectives

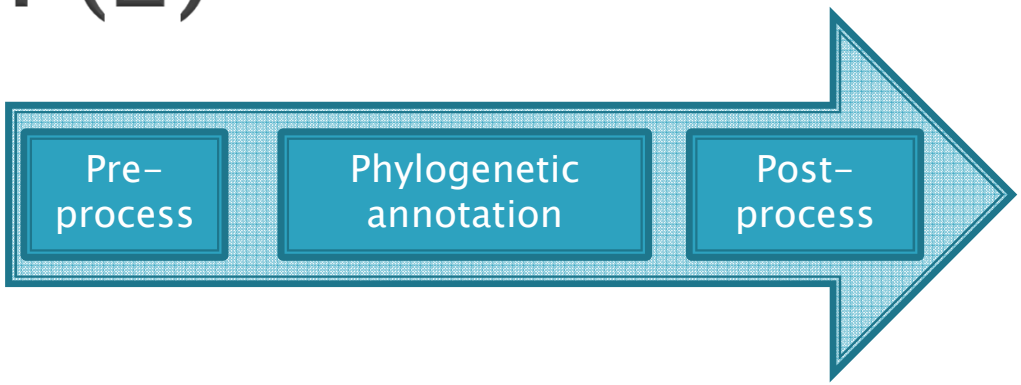
PANAM (Phylogenetic Annotation of Next generation Amplicons)

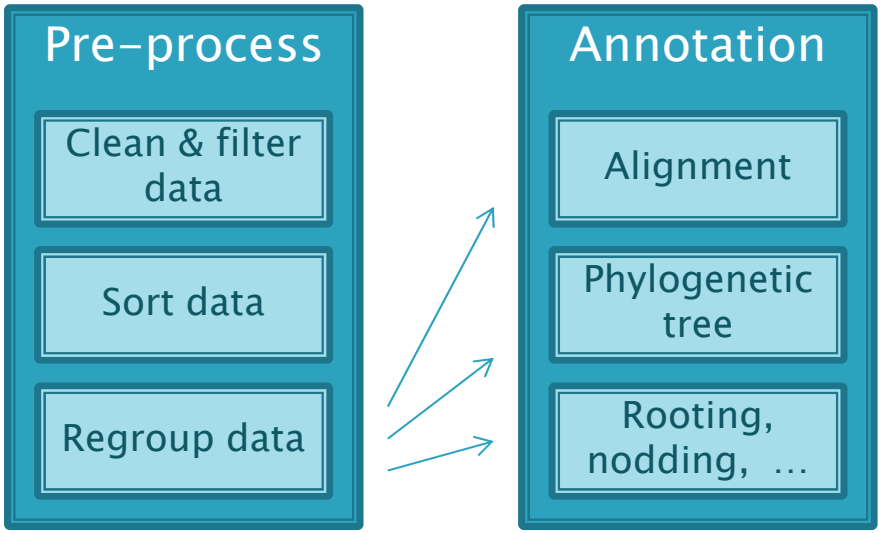
- High-throughput phylogenetic annotation approach
  - A strategy of analyzing NGS (Next Generation Sequencing) data to study the microbial diversity
  - A pipeline that automatically affiliates sequences from SSU rRNA amplicons and build phylogenetic trees of very large numbers of sequences.

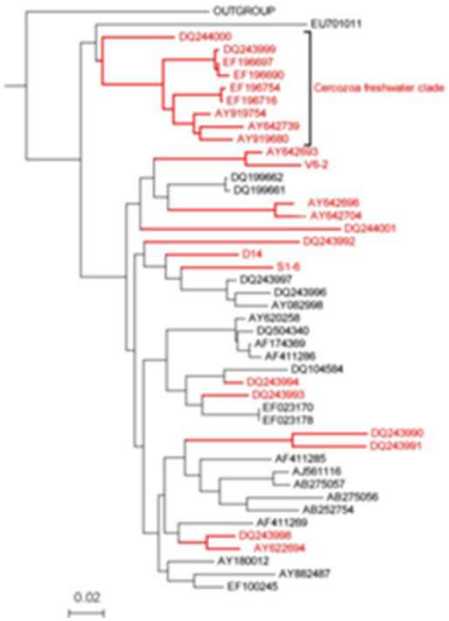




PANAM (2)

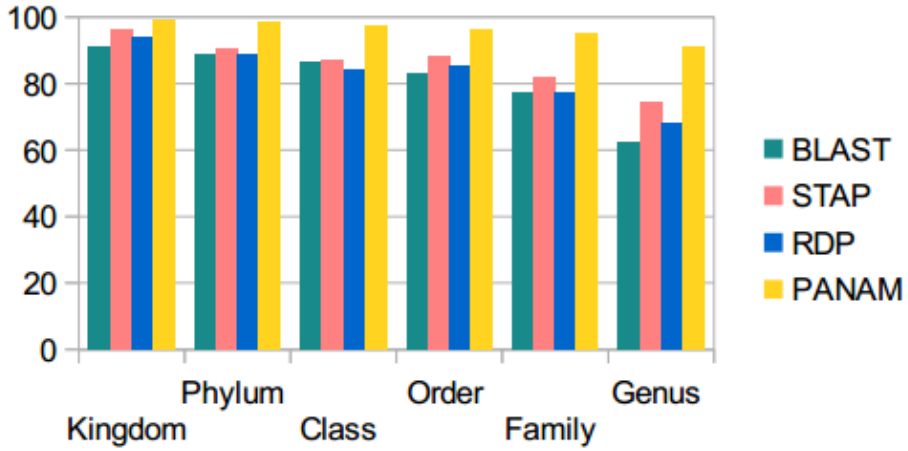

Pre-
process
Phylogenetic
annotation
Post-
process


Pre-process
Clean & filter data
Sort data
Regroup data
Annotation
Alignment
Phylogenetic tree
Rooting, nodding, …


OUTGROUP
Cercozoa freshwater clade
0.02

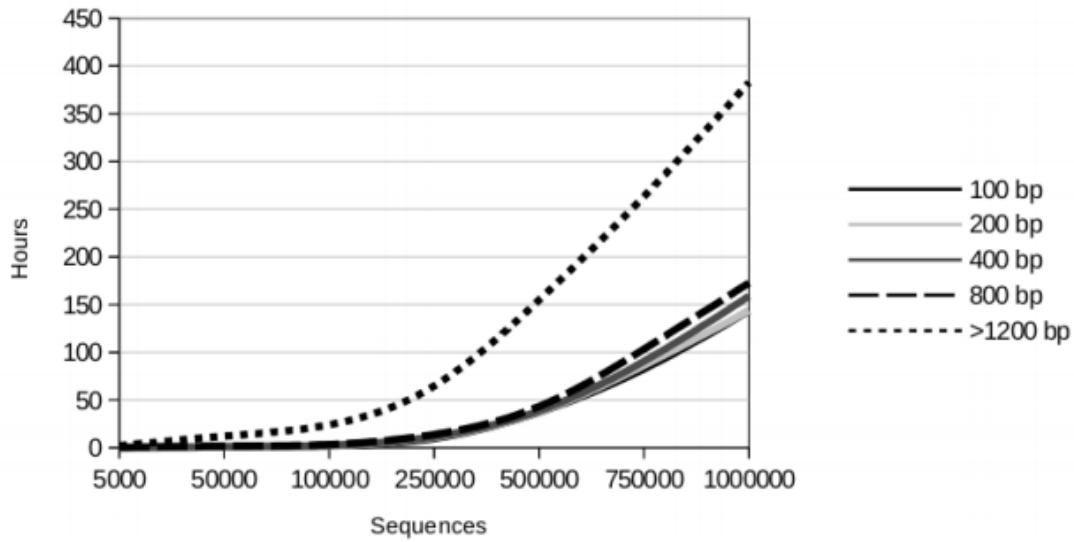
PANAM performance

- Specificity



Taib N, Mangot JF, Domaizon I, Bronner G, Debroas D. Phylogenetic affiliation of SSU rRNA genes generated by massively parallel sequencing: new insights into the freshwater protist diversity. PLoS One. 2013;8(3):e58950. doi:10.1371/journal.pone.0058950.

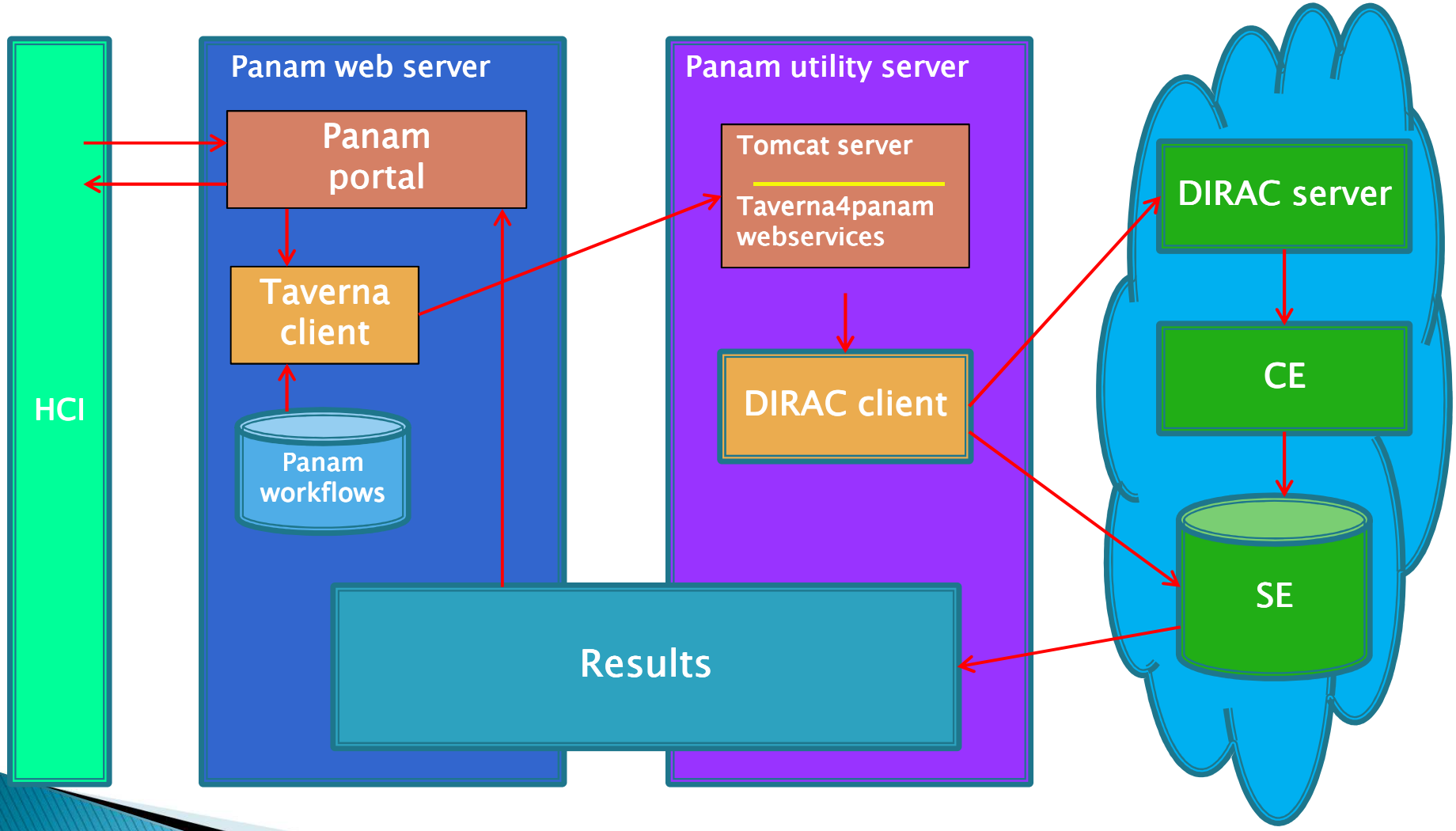
- Time



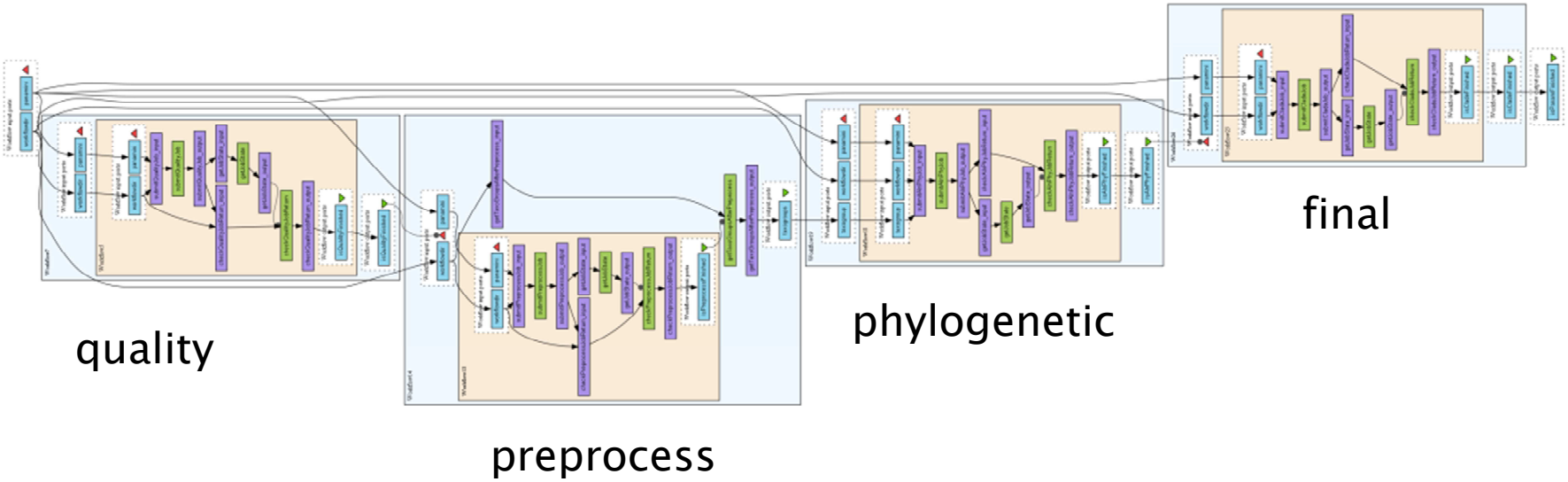
Gridification PANAM (1)

- DIRAC (Distributed Infrastructure with Remote Agent Control)
  - Grid platform for WMS and DMS
  - A service provided by French Grid Initiative
- Taverna
  - Created by Univ. of Manchester
  - Very common workflow engine, especially for bioinformatics
  - Support: webservices, command-line, desktop tool, etc.
- VO biomed
  - A large scale international and multi-disciplinary VO supporting Life Sciences communities
  - Supported by many different sites, delivering access to tens of thousands CPU cores to its users

Gridification PANAM (2)



PANAM workflow



Parallel jobs

Select All Select None

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6418155	Running	Job Initialization	Unknown	LCG.BEIJING.cn	alnphy-Test001...	2013-09-16 14:50	2013-09-16 14:50	2013-09-16 14:47	dttung
6418154	Running	Job Initialization	Unknown	LCG.UNINA.it	alnphy-Test001...	2013-09-16 14:47	2013-09-16 14:47	2013-09-16 14:47	dttung
6418153	Running	Application	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:57	2013-09-16 14:58	2013-09-16 14:47	dttung
6418152	Running	Job Initialization	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:48	2013-09-16 14:48	2013-09-16 14:47	dttung
6418151	Running	Application	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:59	2013-09-16 14:59	2013-09-16 14:47	dttung
6418149	Running	Job Initialization	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:48	2013-09-16 14:48	2013-09-16 14:47	dttung
6418148	Running	Job Initialization	Unknown	LCG.SARA.nl	alnphy-Test001...	2013-09-16 14:47	2013-09-16 14:47	2013-09-16 14:47	dttung
6418147	Running	Application	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:57	2013-09-16 14:57	2013-09-16 14:47	dttung
6418146	Running	Job Initialization	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:49	2013-09-16 14:49	2013-09-16 14:47	dttung
6418145	Running	Job Initialization	Unknown	LCG.WROC.pl	alnphy-Test001...	2013-09-16 14:47	2013-09-16 14:47	2013-09-16 14:47	dttung
6418144	Running	Job Initialization	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:48	2013-09-16 14:48	2013-09-16 14:47	dttung
6418143	Running	Application	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:59	2013-09-16 14:59	2013-09-16 14:47	dttung
6418142	Running	Job Initialization	Unknown	LCG.UPV.es	alnphy-Test001...	2013-09-16 14:54	2013-09-16 14:54	2013-09-16 14:47	dttung
6418141	Running	Job Initialization	Unknown	LCG.LAL.fr	alnphy-Test001...	2013-09-16 14:48	2013-09-16 14:48	2013-09-16 14:47	dttung
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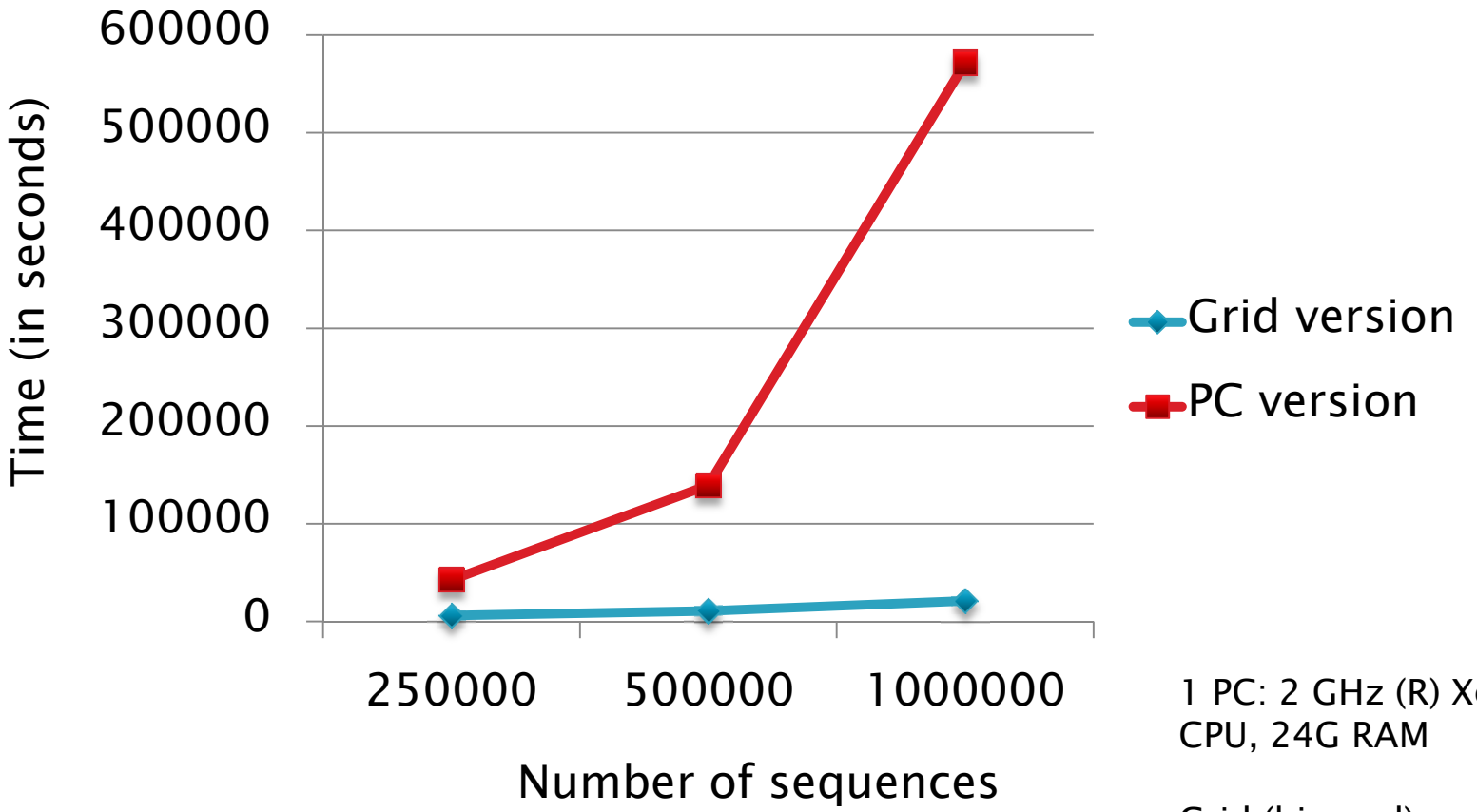
6418117	Done	Execution Com...	Unknown	LCG.CNAF.it	preprocess-Te...	2013-09-16 14:46	2013-09-16 14:46	2013-09-16 14:38	dttung
6418084	Done	Execution Com...	Unknown	LCG.CNAF.it	quality-Test001	2013-09-16 14:38	2013-09-16 14:38	2013-09-16 14:26	dttung

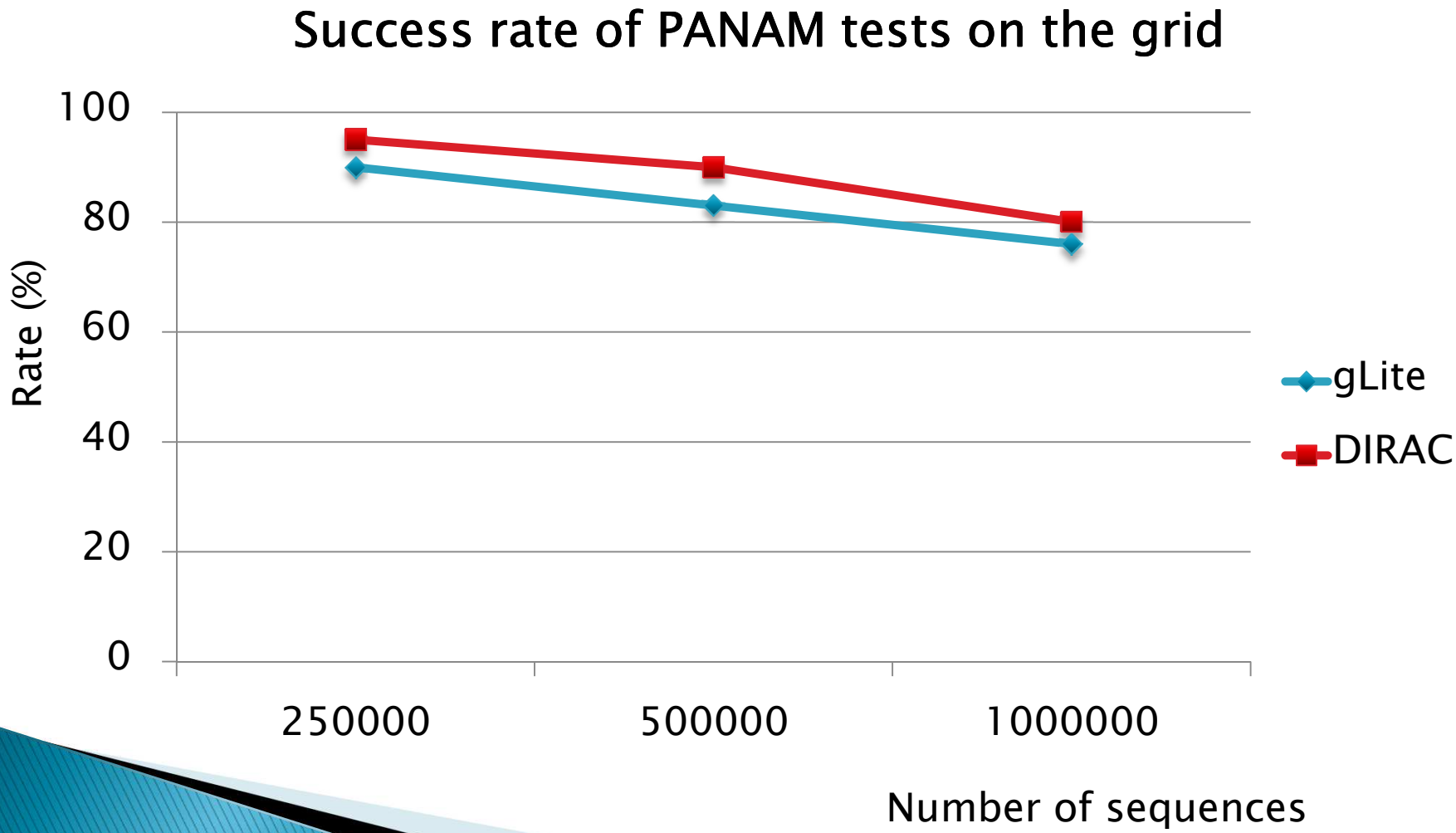
Performance comparison



1 PC: 2 GHz (R) Xeon (R) CPU, 24G RAM

Grid (biomed): number of nodes is based on number of sequences

Success rate



Known problems / inconveniences

- DIRAC
  - Jobs failed
  - Only python APIs
  - Outputs of CLI commands is sometime not friendly-readable
- Taverna
  - Cannot rerun a service based on output of other service
  - RAM consumed when running with large workflow

Perspective

- Integrate with ePANAM portal (http://panam-meb.univ-bpclermont.fr/index.php)
- Optimize the success rate
- Parallelize the 'quality' step to analyze data from other sequencing method (Miseq)