

GridWay Scalability and Interoperation for DRMAA codes

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1. The GridWay Metascheduler
2. The DRMAA standard and GridWay
3. GridWay Approach to Scalability and Interoperability
4. The CD-HIT Application

“The more man meditates upon good thoughts, the better will be his world and the world at large.”





1. The GridWay Metascheduler

What is GridWay?

GridWay is a Globus Toolkit component for meta-scheduling, creating a scheduler virtualization layer on top of Globus services (GRAM, MDS & GridFTP)

- For **project and infrastructure directors**
 - GridWay is an open-source community project, adhering to Globus philosophy and guidelines for collaborative development.
- For **system integrators**
 - GridWay is highly modular, allowing adaptation to different grid infrastructures, and supports several OGF standards.
- For **system managers**
 - GridWay gives a scheduling framework similar to that found on local LRM systems, supporting resource accounting and the definition of state-of-the-art scheduling policies.
- For **application developers**
 - GridWay implements the OGF standard DRMAA API (C, JAVA & more bindings), assuring compatibility of applications with LRM systems that implement the standard, such as SGE, Condor, Torque,...
- For **end users**
 - GridWay provides a LRM-like CLI for submitting, monitoring, synchronizing and controlling jobs, that could be described using the OGF standard JSDL.

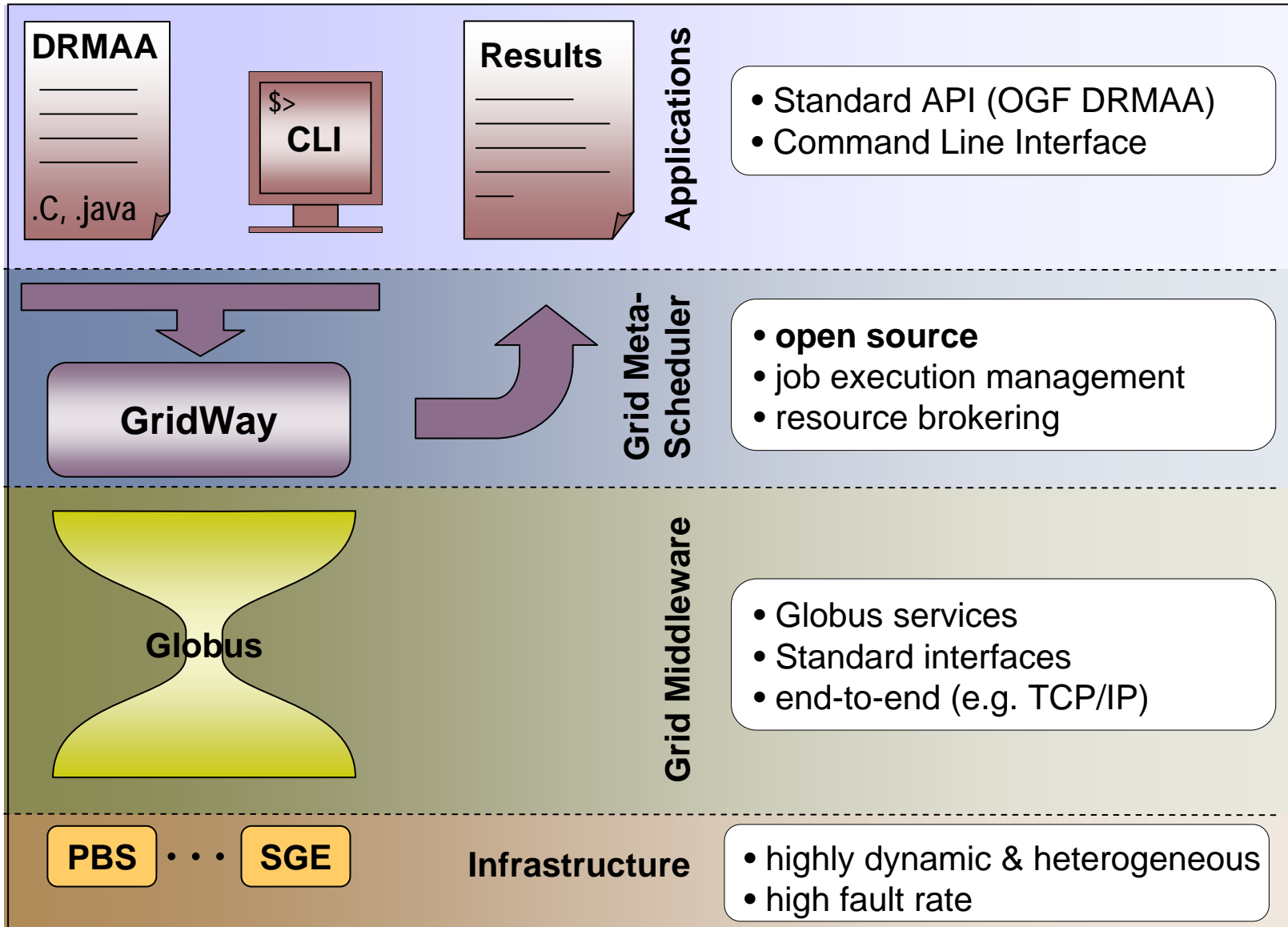


1. The GridWay Metascheduler

Global Architecture of a Computational Grid

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Application-Infrastructure decoupling

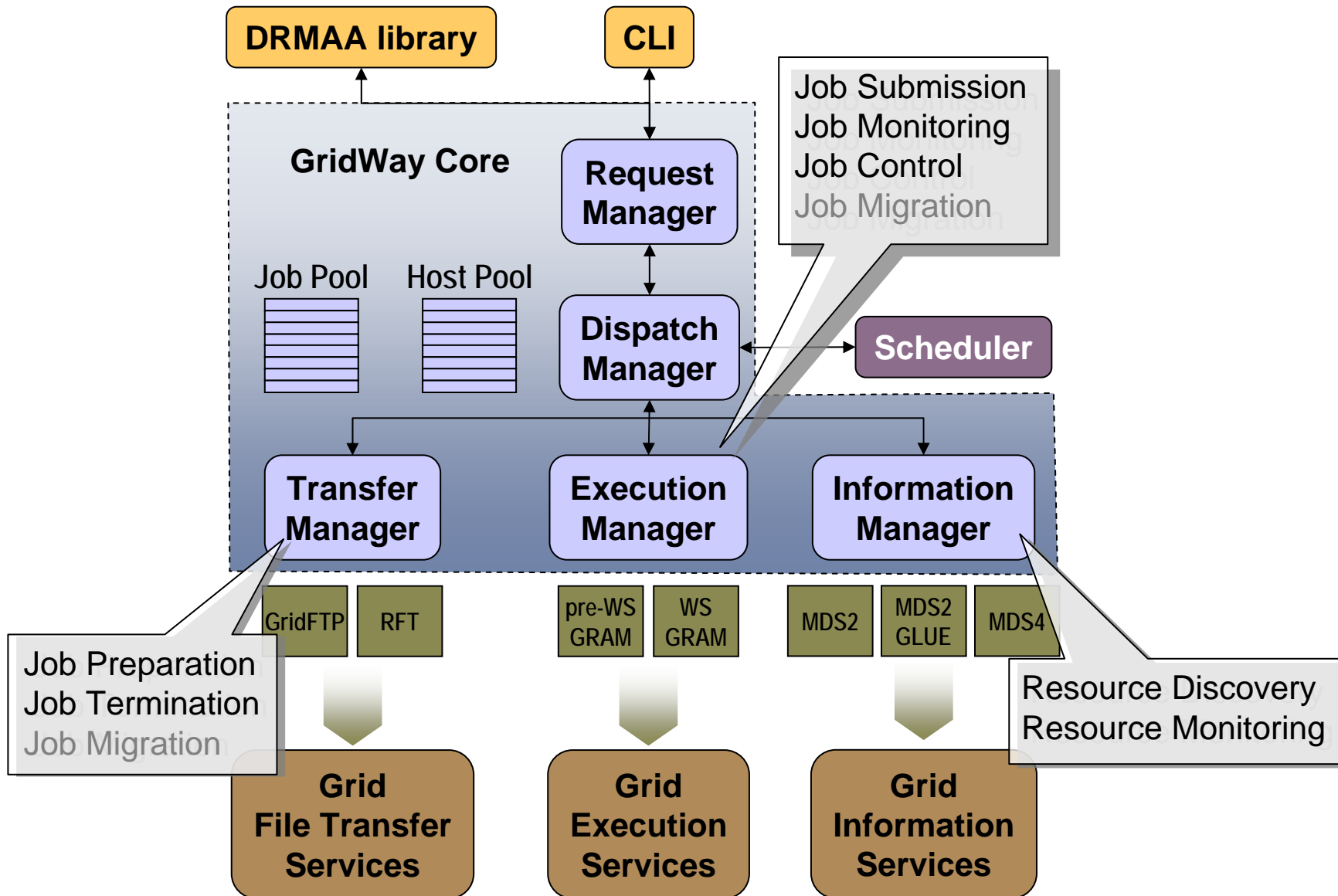




1. The GridWay Metascheduler

GridWay Internals

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2. The DRMAA standard and GridWay

What is DRMAA?

- Distributed Resource Management Application API
 - <http://www.drmaa.org/>
- Open Grid Forum Standard
- Homogeneous interface to different Distributed Resource Managers (DRM):
 - **SGE**
 - **Condor**
 - **PBS/Torque**
 - **GridWay**
 - **C**
 - **JAVA**
 - **Perl (GW 5.2+)**
 - **Ruby (GW 5.2+)**
 - **Python (GW 5.2+)**



2. The DRMAA standard and GridWay

C Binding

- The native binding
- All the others are wrappers around this
- Features a dynamic library to link DRMAA applications with
 - They will automatically run on a Grid offered by GridWay

```
drmaa_run_job  
    ( job_id,  
      DRMAA_JOBNAME_BUFFER-1 ,  
      jt ,  
      error ,  
      DRMAA_ERROR_STRING_BUFFER-1 ) ;
```



2. The DRMAA standard and GridWay

Java Binding

- Uses Java Native Interface (JNI)
 - performs calls to the C library to do the work
- Two versions of the DRMAA spec
 - 0.6
 - 1.0 - Not yet officially recommended by OGF

```
session.runJob(jt);
```




2. The DRMAA standard and GridWay

Ruby Binding

- SWIG : C/C++ wrapper generator for scripting languages and Java
- SWIG binding for Ruby developed by dsa-research.org

```
(result, job_id, error)=drmaa_run_job(jt)
```

2. The DRMAA standard and GridWay

Python Binding

- SWIG binding developed by 3rd party
 - Author: Enrico Sirola
 - License: GPL --> external download

```
(result, job_id, error)=drmaa_run_job(jt)
```

Perl Binding

- SWIG binding developed by 3rd party
 - Author: Tim Harsch
 - License: GPL --> external download

```
($result, $job_id, $error)=drmaa_run_job($jt);
```

3. GridWay Approach to Scalability and Interoperability

Definition (by OGF GIN-CG)

- **Interoperability:** The native ability of Grids and Grid technologies to interact directly via common open standards in the near future.
 - A rather long-term solution within production e-Science infrastructures.
 - GridWay provides support for established standards: DRMAA, JSDL, WSRF...
- **Interoperation:** What needs to be done to get production Grid and e-Science infrastructures to work together as a short-term solution. Two alternatives:
 - Adapters: "A device that allows one system to connect to and work with another".
 - Change the middleware/tools to insert the adapter
 - Gateways: adapters implemented as a service.
 - No need to change the middleware/tools

GridWay provides both adapters (Middleware Access Drivers, MADs) and a gateway (GridGateWay, WSRF GRAM service encapsulating GridWay),.

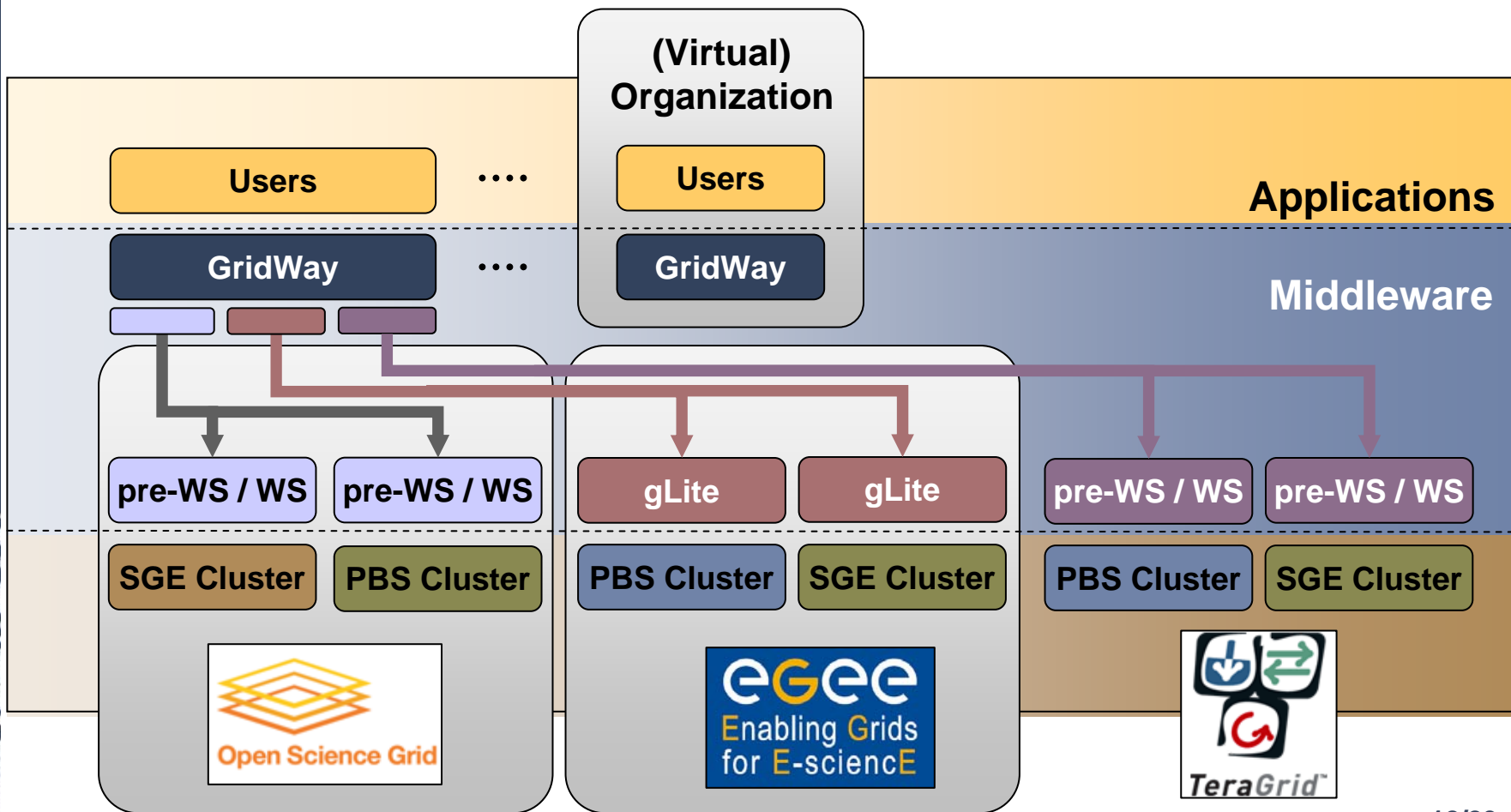
GridWay's light concept helps to maintain **Scalability**.

3. GridWay Approach to Scalability and Interoperability

How do we achieve interoperability

- By using adapters:

“A device that allows one system to connect to and work with another”



3. GridWay Approach to Scalability and Interoperability

EGEE

- The Enabling Grids for E-science European Commission funded project brings together scientists and engineers from more than 240 institutions in 45 countries world-wide to provide a seamless Grid infrastructure for e-Science that is available to scientists 24 hours-a-day.



- Interoperability Issues

- Execution Manager Driver for preWS
- Different data staging philosophy
 - Cannot stage to front node
 - Don't know Execution Node beforehand
 - SOLUTION : Wrapper
- Virtual Organization support



3. GridWay Approach to Scalability and Interoperability

Open Science Grid

- The Open Science Grid brings together a distributed, peta-scale computing and storage resources into a uniform shared cyberinfrastructure for large-scale scientific research. It is built and operated by a consortium of universities, national laboratories, scientific collaborations and software developers.

- Interoperability Issues

- MDS2 info doesn't provide queue information
 - static monitoring
- Globus container running in a non standard port
 - MAD modification





3. GridWay Approach to Scalability and Interoperability

TeraGrid

- TeraGrid is an open scientific discovery infrastructure combining leadership class resources at eleven partner sites to create an integrated, persistent computational resource

- Interoperability Issues

- Separated Staging Element and Working Node
 - Shared homes
 - Use of SE_HOSTNAME
 - Mix of static and dynamic data
- Support for raw rsl extensions
 - To bypass GRAM and get info to DRMS



4. The CD-HIT Application

Application Description

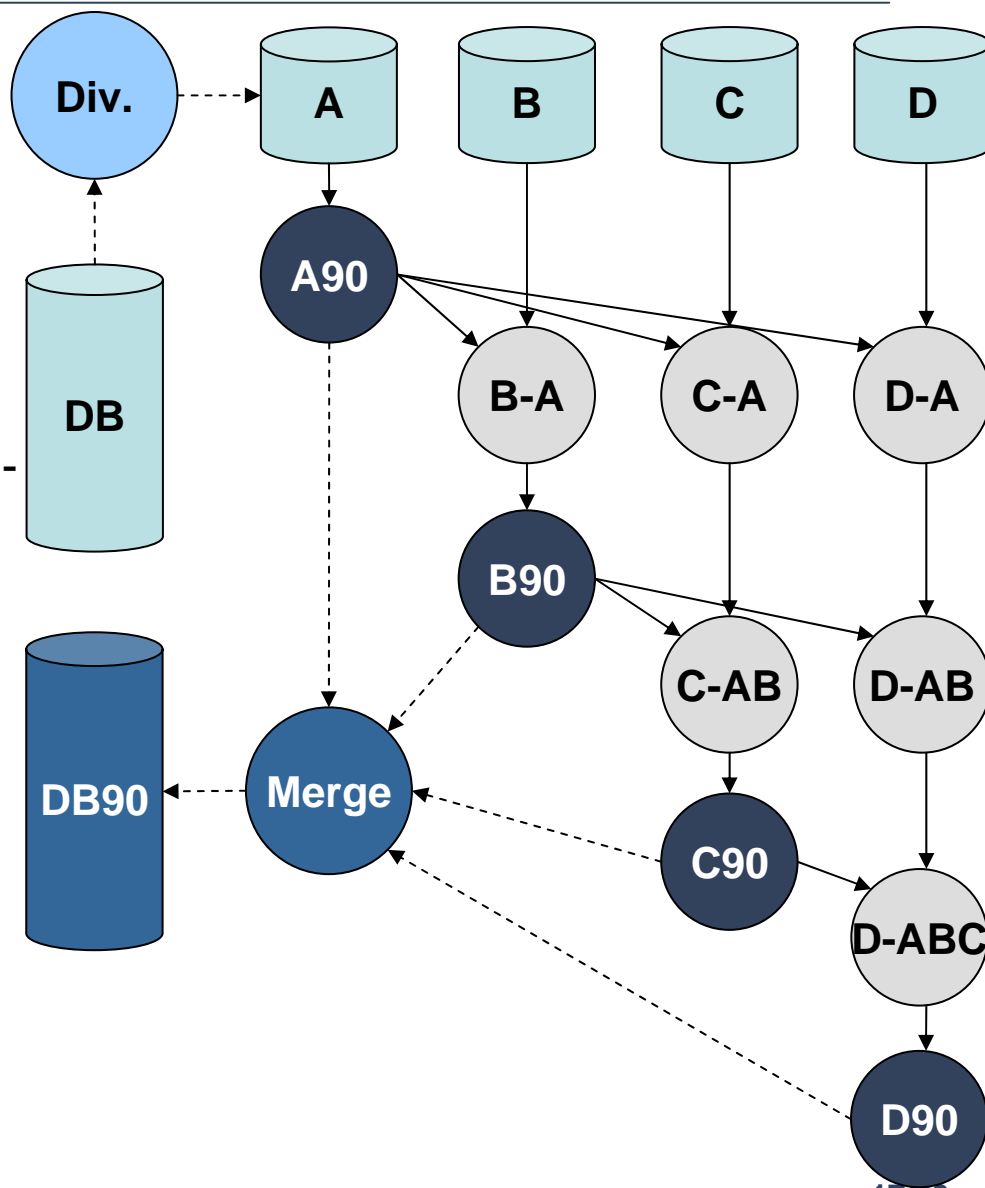
- “*Cluster Database at High Identity with Tolerance*”
- Protein (and also DNA) clustering
 - Compares protein DB entries
 - Eliminates redundancies
- Example: Used in UniProt for generating UniRef data sets
- Our case: Widely used in the Spanish National Oncology Research Center (CNIO)
 - Input DB: 504,876 proteins / 435MB
- Infeasible to be executed on single machine
 - **Memory requirements**
 - Total execution time
- UniProt is the world's most comprehensive catalog of information on proteins. CD-HIT program is used to generate the UniRef reference data sets, UniRef90 and UniRef50.
- CD-HIT is also used at the PDB to treat redundant sequences



4. The CD-HIT Application

CD-HIT Parallel

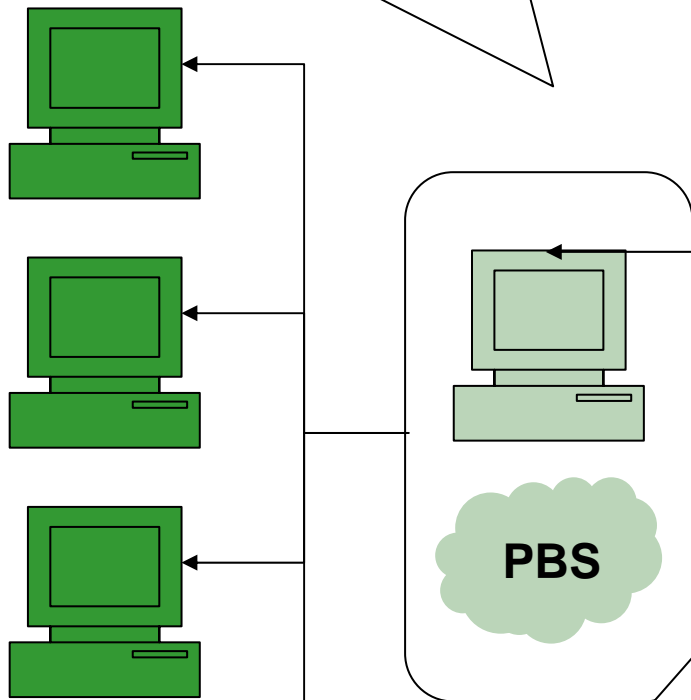
- Execute cd-hit in **parallel mode**
- **Idea:** divide the input database to compare each division in parallel
 - Divide the input db
 - Repeat
 - Cluster the first division (cd-hit)
 - Compare others against this one (cd-hit-2d)
 - Merge results
- Speed-up the process and deal with **larger databases**
- **Computational characteristics**
 - Variable degree of parallelism
 - Grain must be adjusted



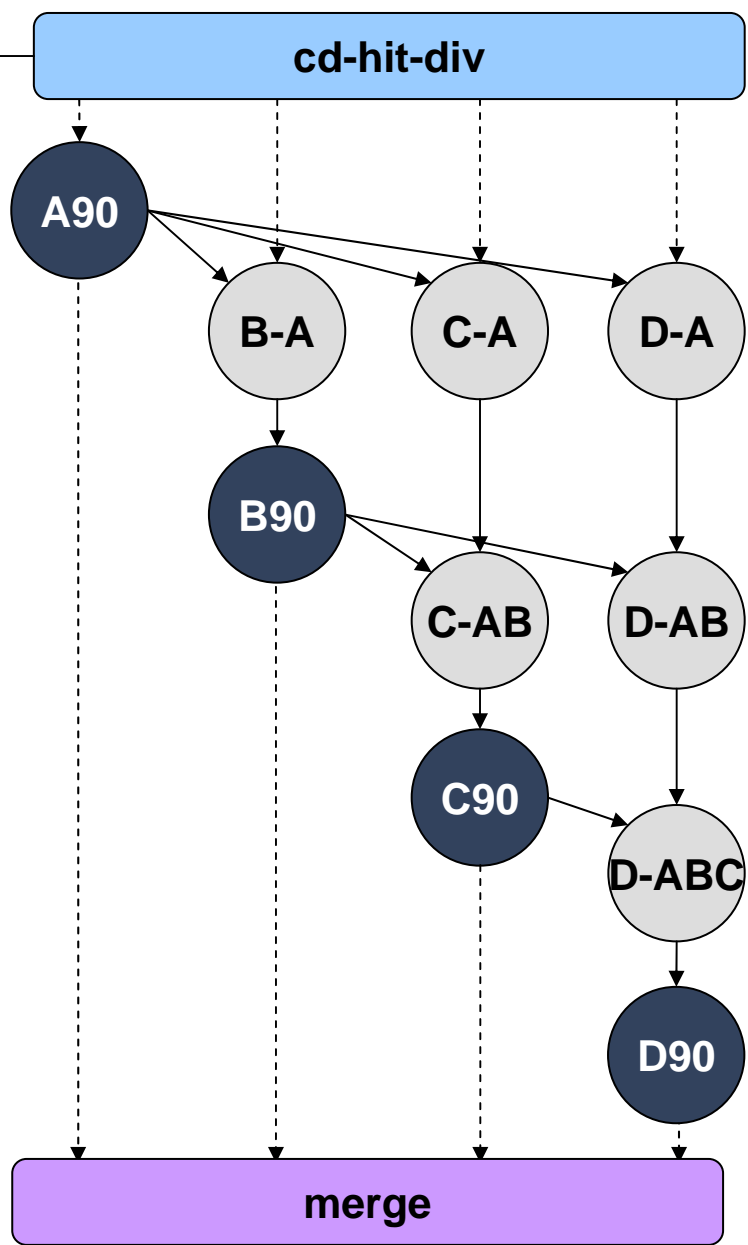


4. The CD-HIT Application

Database division/merging is performed in the front-end



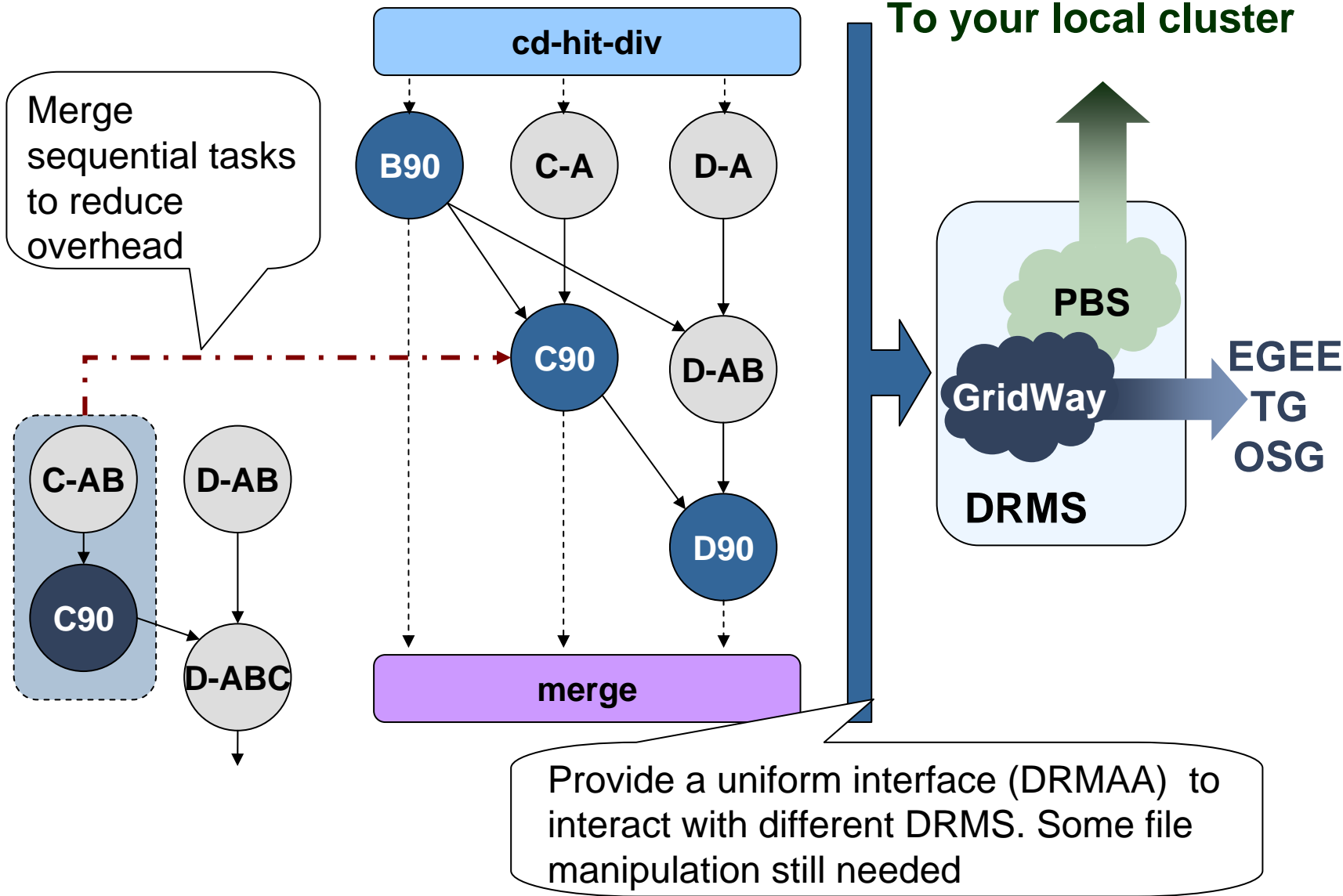
- Several structures to invoke the underlying DRMS
- PBS, SGE and ssh





4. The CD-HIT Application

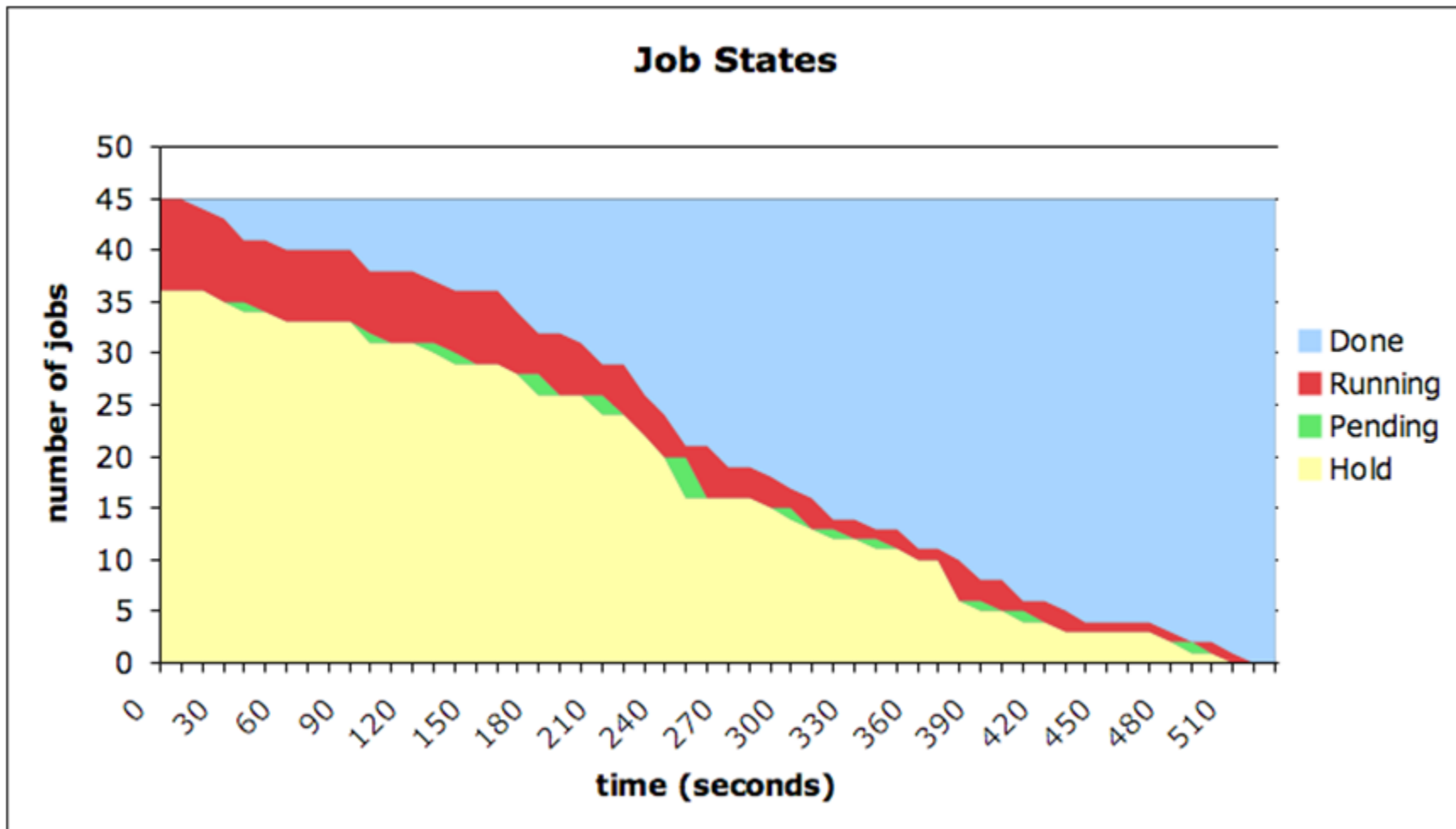
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4. The CD-HIT Application

Running with 10 divisions

- Using previous set-up on TG, EGEE, OSG and UCM local cluster



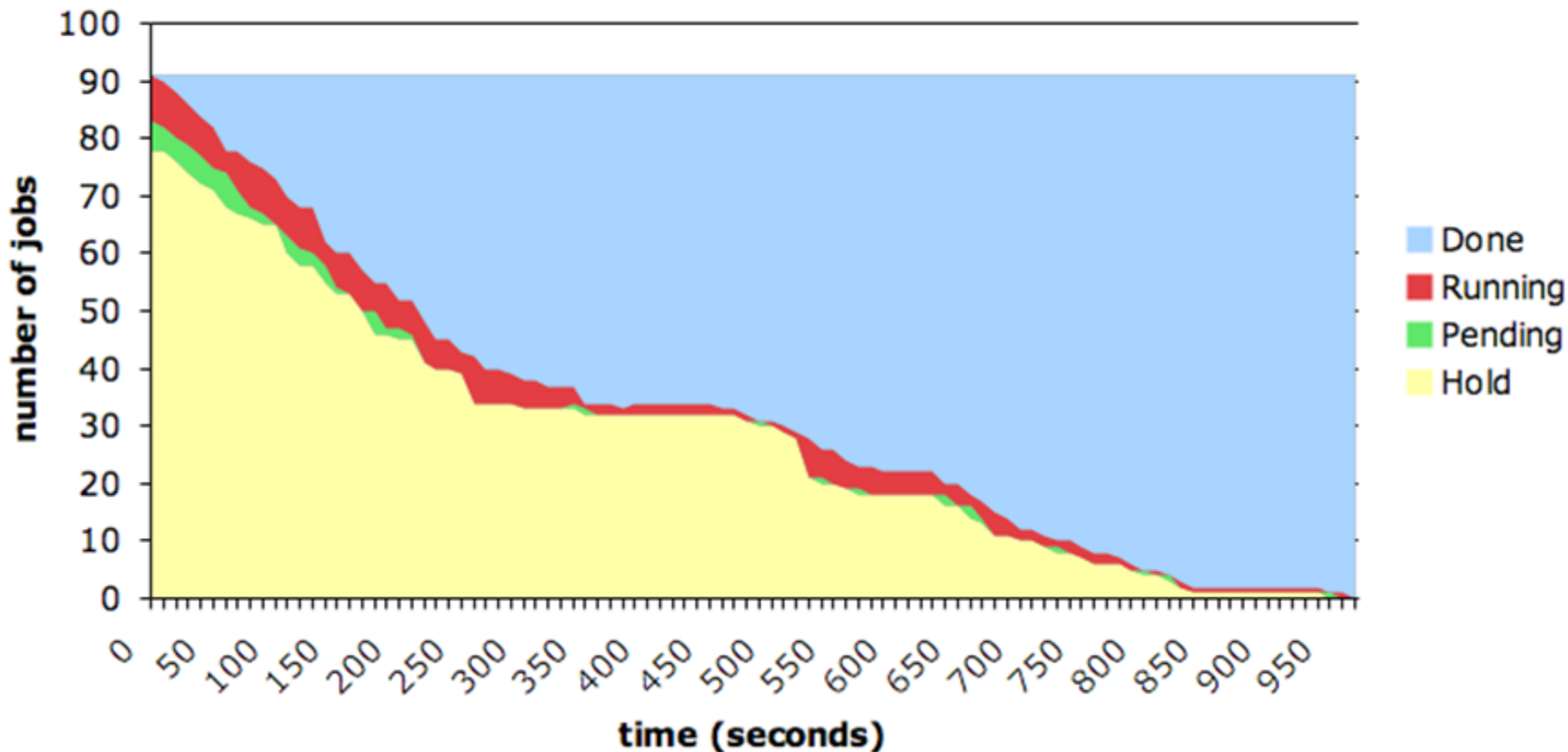


4. The CD-HIT Application

Job States - Running with 14 divisions

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Job States



Who's behind the GridWay Metascheduler?

- Ignacio M. Ilorente (Leader)
- Rubén S. Montero
- Eduardo Huedo
- José Herrera
- José Luis Vázquez-Poletti
- Javier Fontán
- Tino Vázquez



Want to participate?

Visit <http://www.gridway.org/> now!



Questions?

**Thank you
for your attention!**

謝謝