Scaling DRMAA codes to the Grid: A Demonstration on EGEE, TG and OSG

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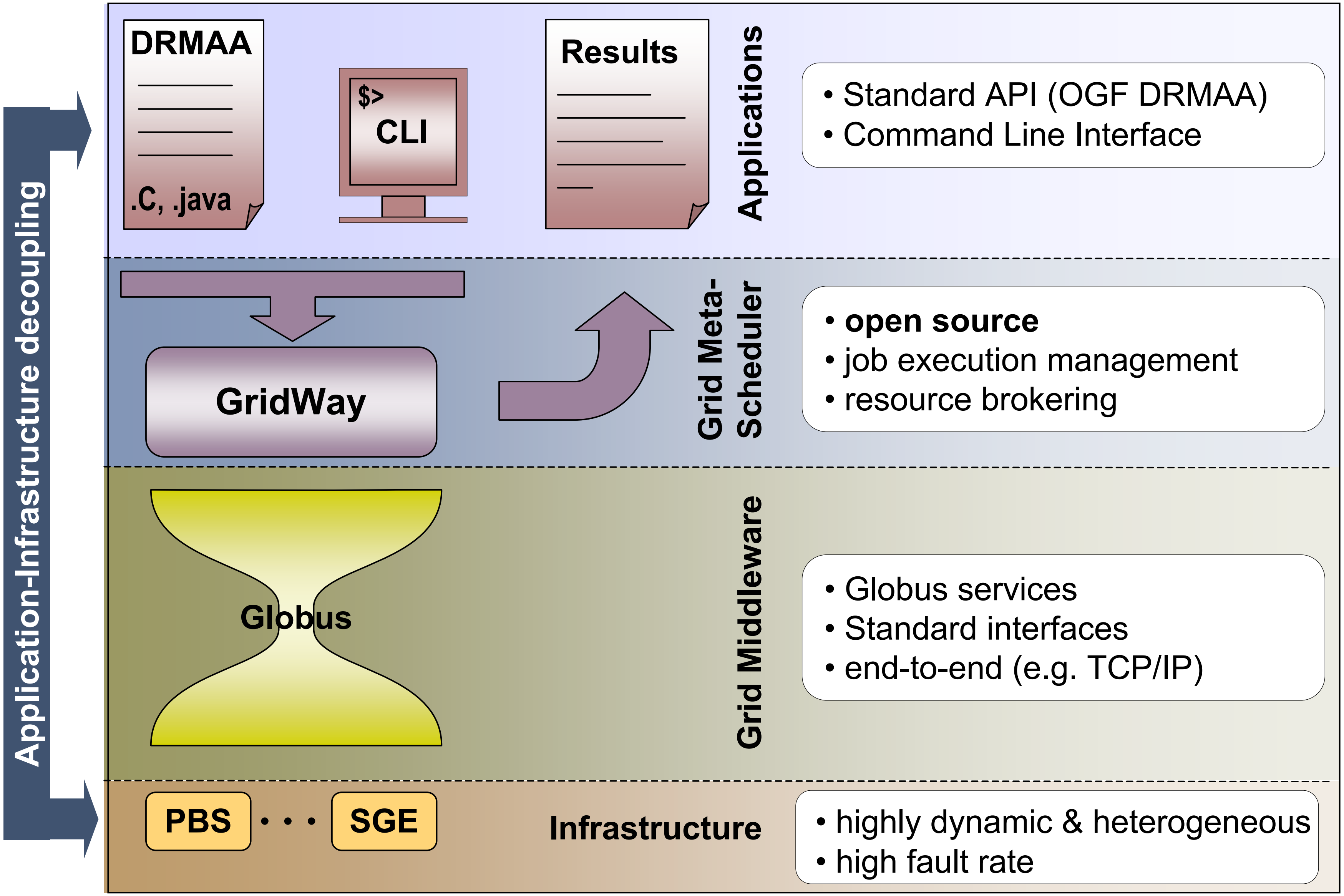
What is GridWay?

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.

Global Architecture of a Computational Grid



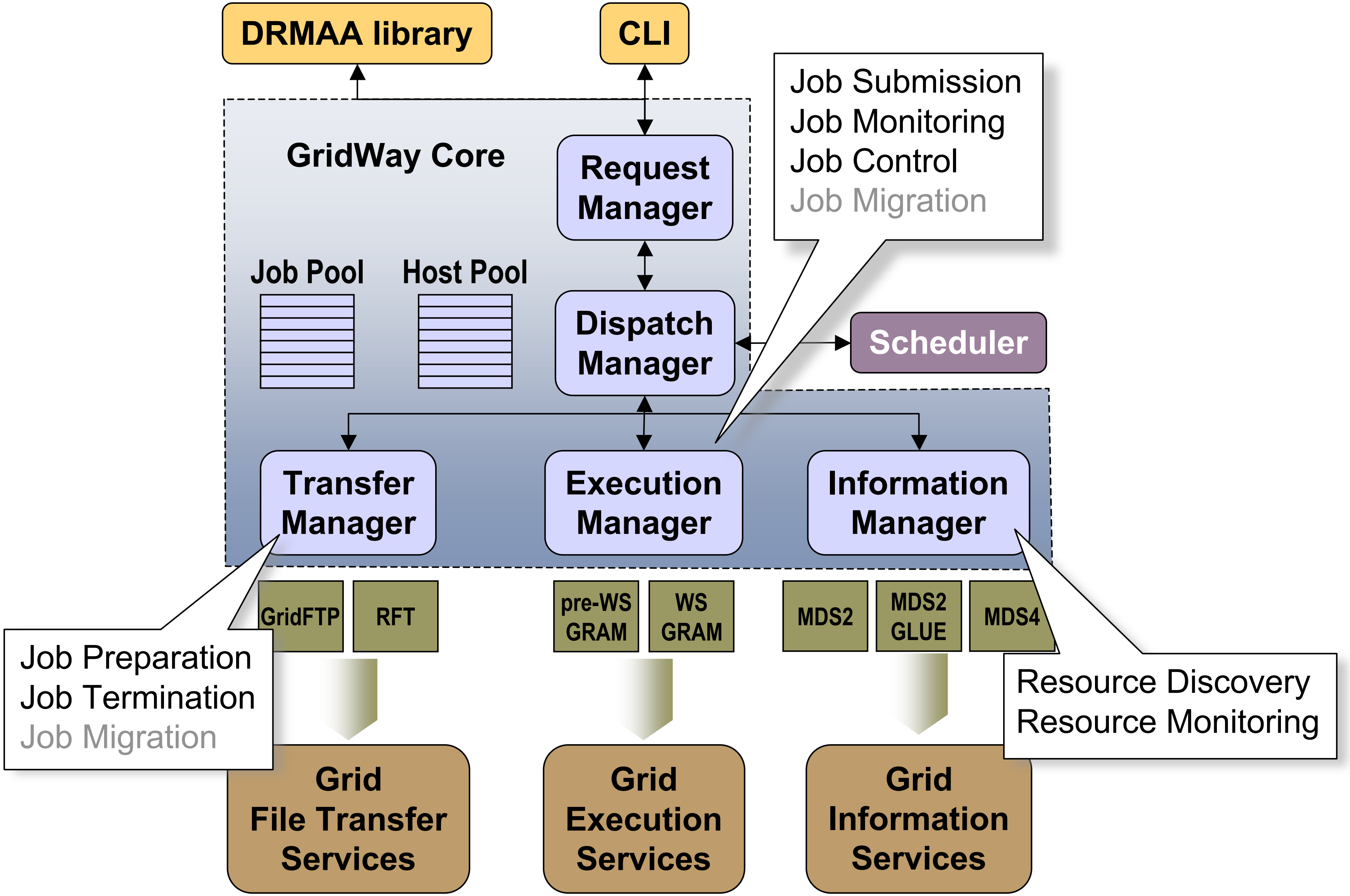
- Standard API (OGF DRMAA)
- Command Line Interface

- **open source**
- job execution management
- resource brokering

- Globus services
- Standard interfaces
- end-to-end (e.g. TCP/IP)

- highly dynamic & heterogeneous
- high fault rate

GridWay Internals



Job Submission
Job Monitoring
Job Control
Job Migration

Job Preparation
Job Termination
Job Migration

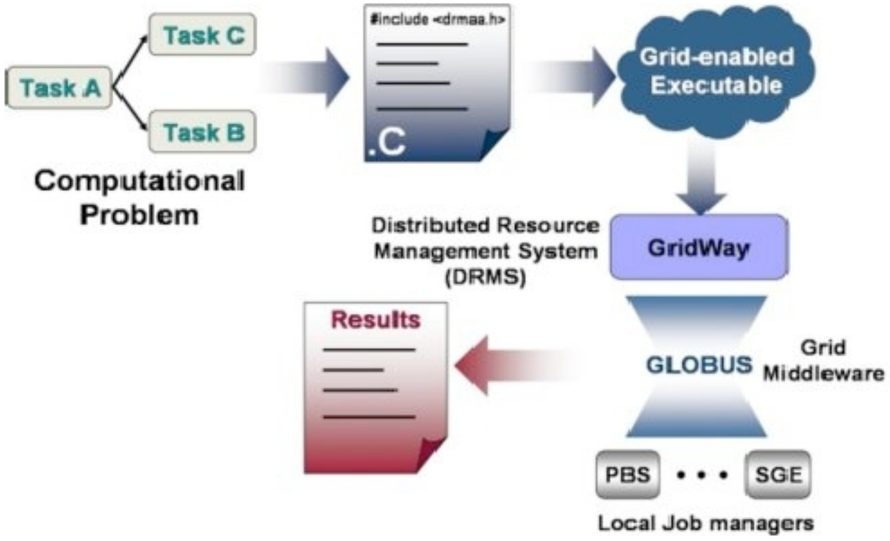
Resource Discovery
Resource Monitoring

What is DRMAA?

- Distributed Resource Management Application API
  - http://www.drmaa.org/
- Open Grid Forum Standard

OpenGridForum
OPEN FORUM | OPEN STANDARDS

- 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)
```

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);
```

Definition (by OGF GIN-CG)

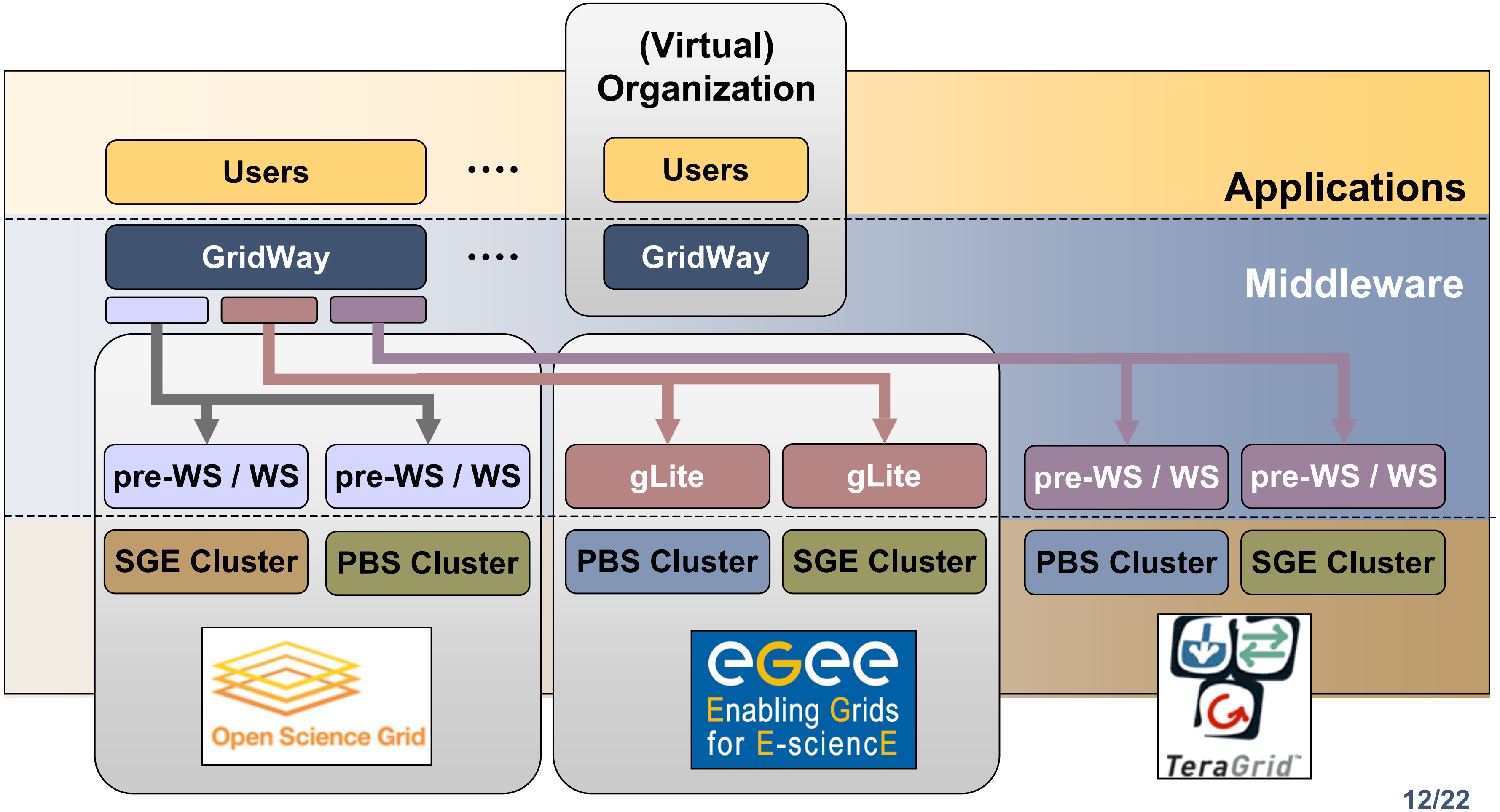
- **Interoperability**: The native ability of Grids and Grid technologies to interact directly via common open standards in the near future.
  - A rather long-term solution within production e-Science infrastructures.
  - GridWay provides support for established standards: DRMAA, JSDL, WSRF…
- **Interoperation**: 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".
    - o Change the middleware/tools to insert the adapter
  - Gateways: adapters implemented as a service.
    - o No need to change the middleware/tools

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

How do we achieve interoperability

- By using adapters:

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



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

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

Open Science Grid

3. GridWay Approach to Interoperability

TeraGrid

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

- <u>Interoperability Issues</u>
  - 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

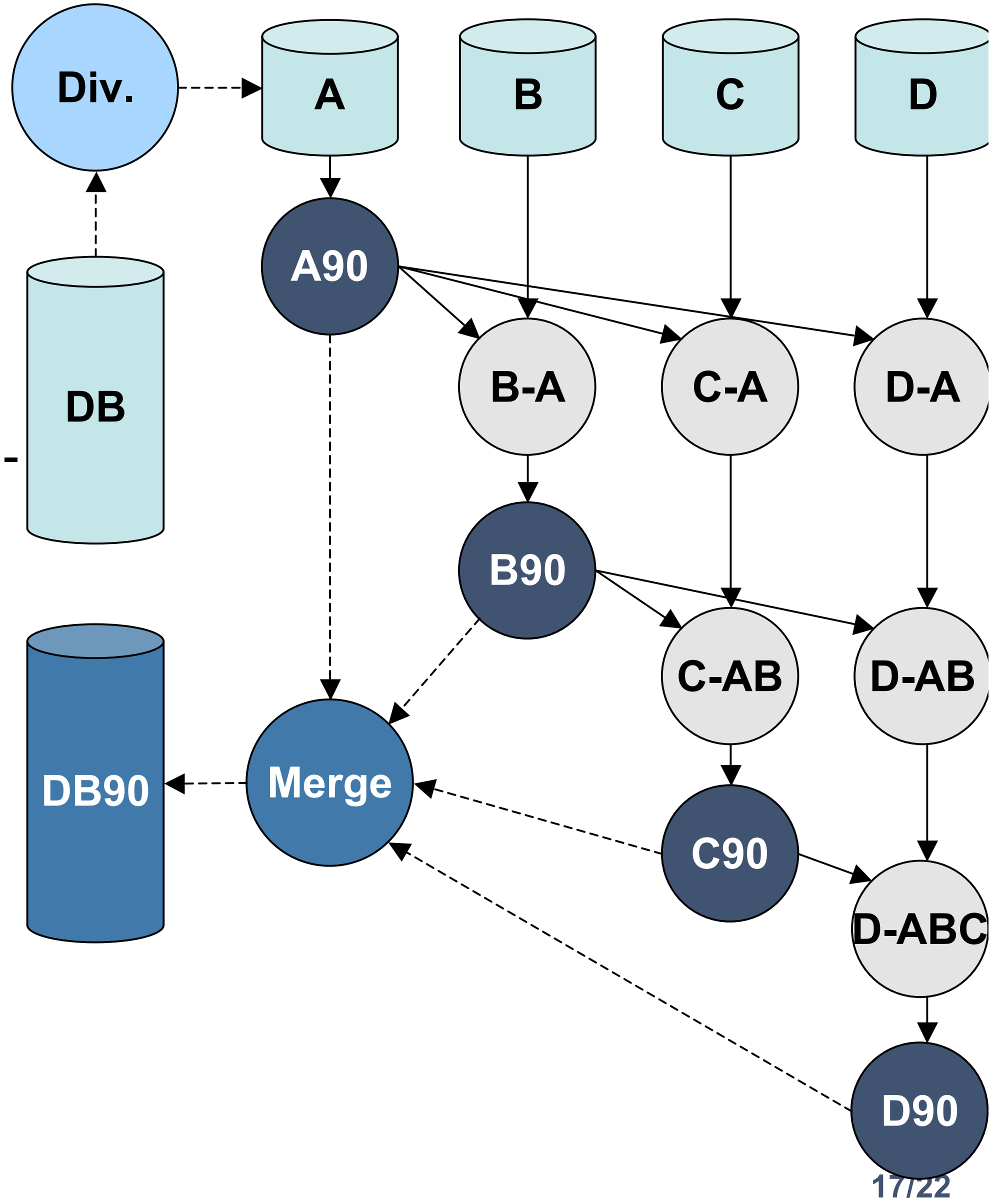
4. The CD-HIT Application

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

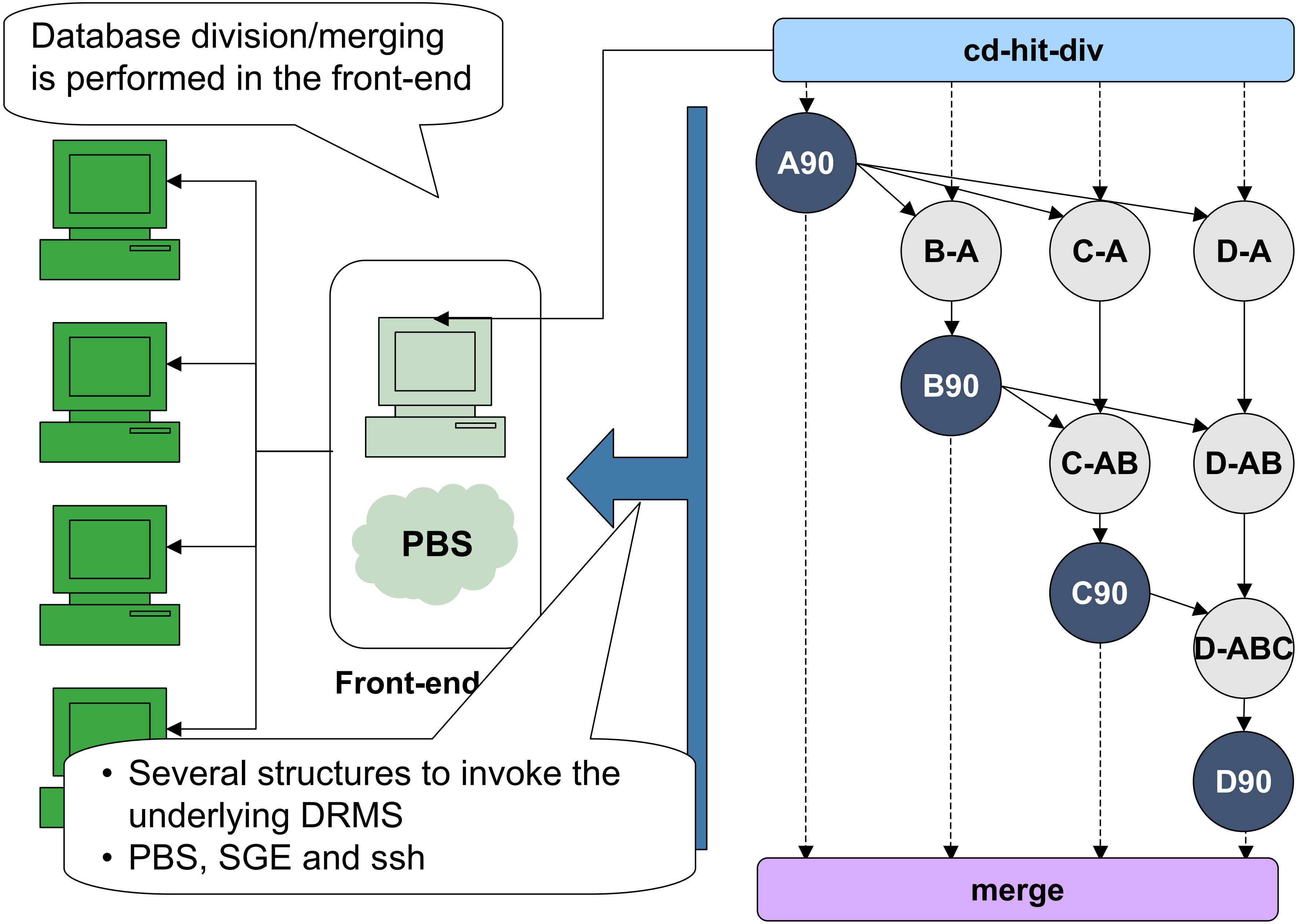
CD-HIT Parallel

- 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



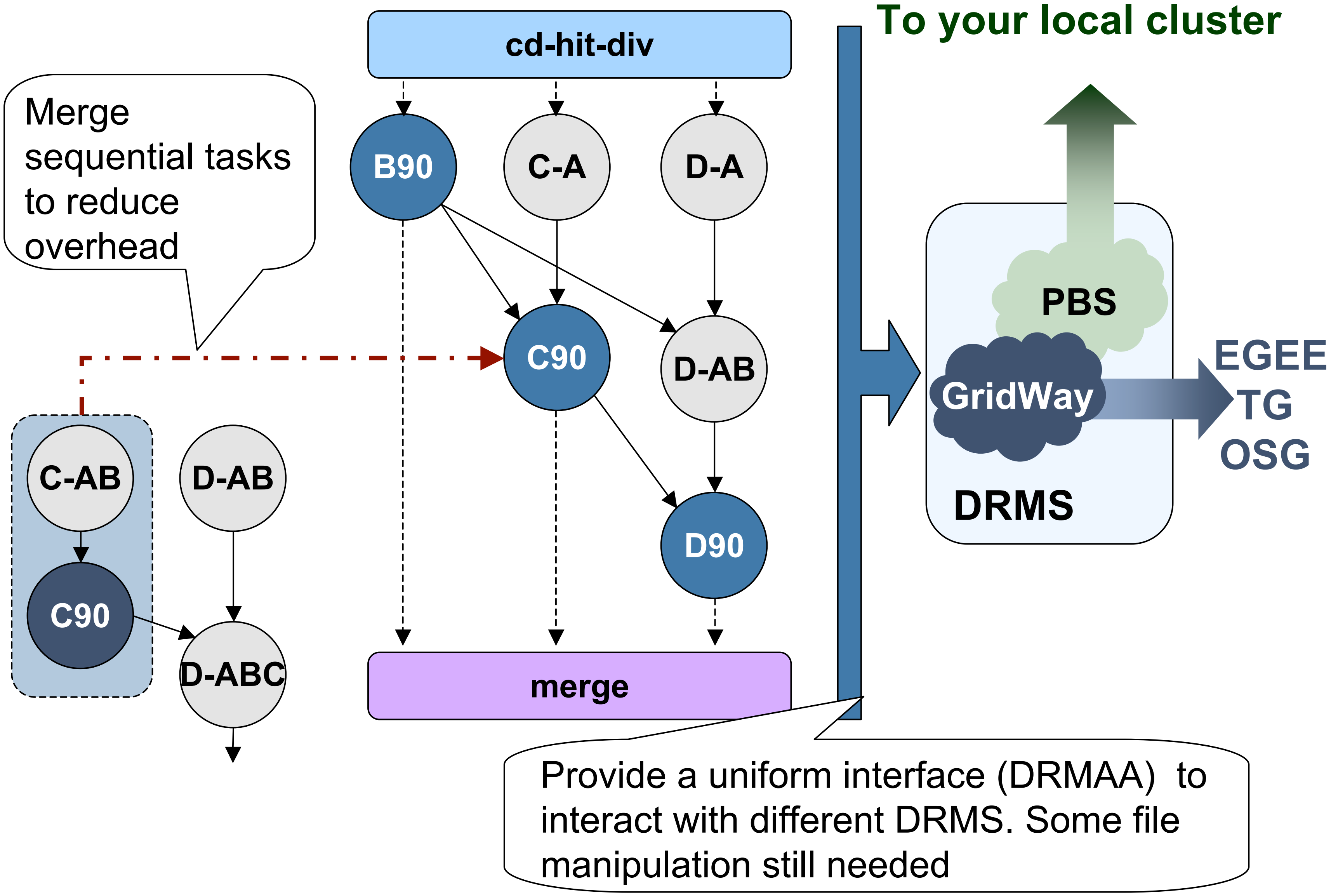
4. The CD-HIT Application

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



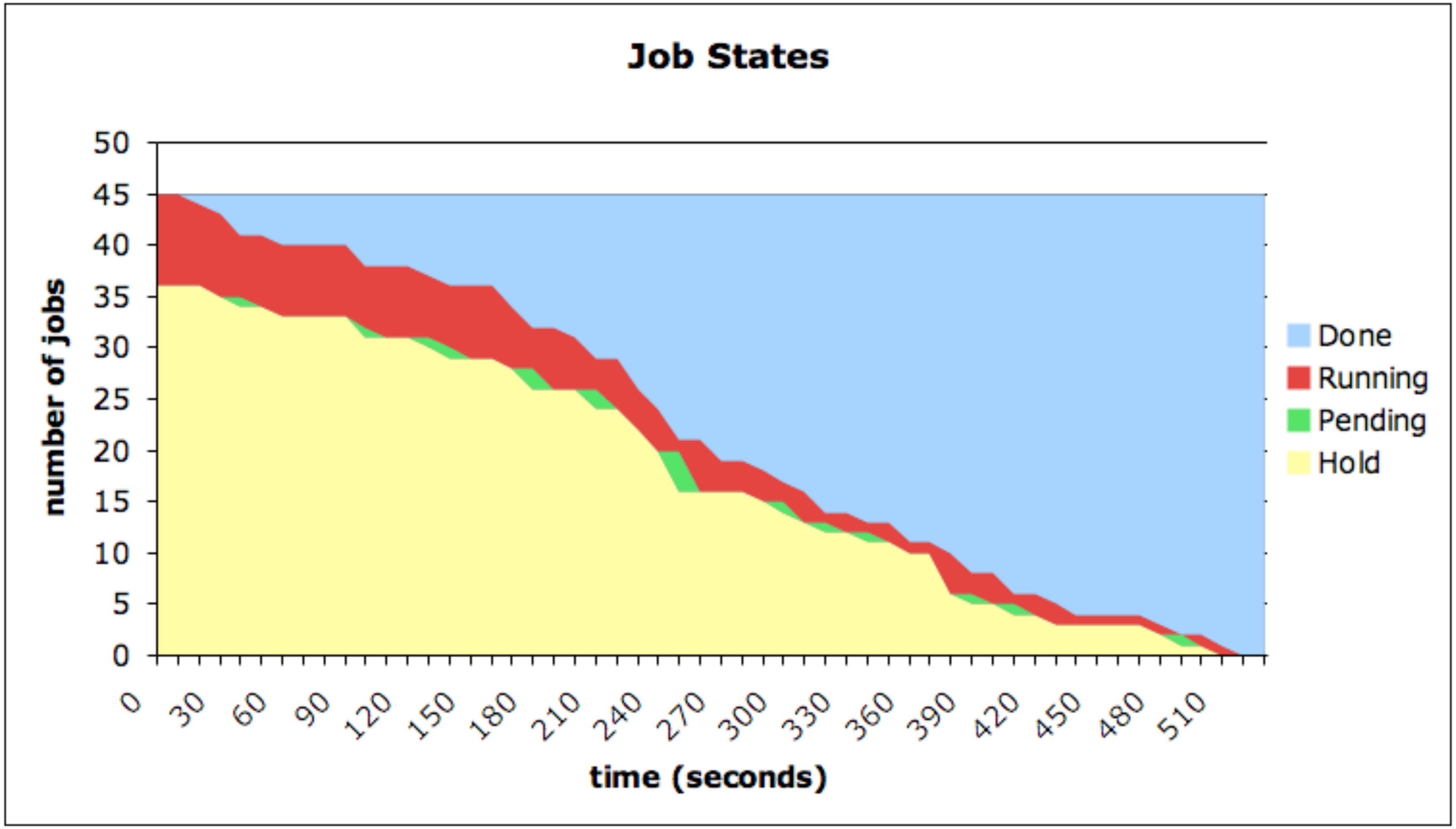
Merge sequential tasks to reduce overhead

Provide a uniform interface (DRMAA) to interact with different DRMS. Some file manipulation still needed

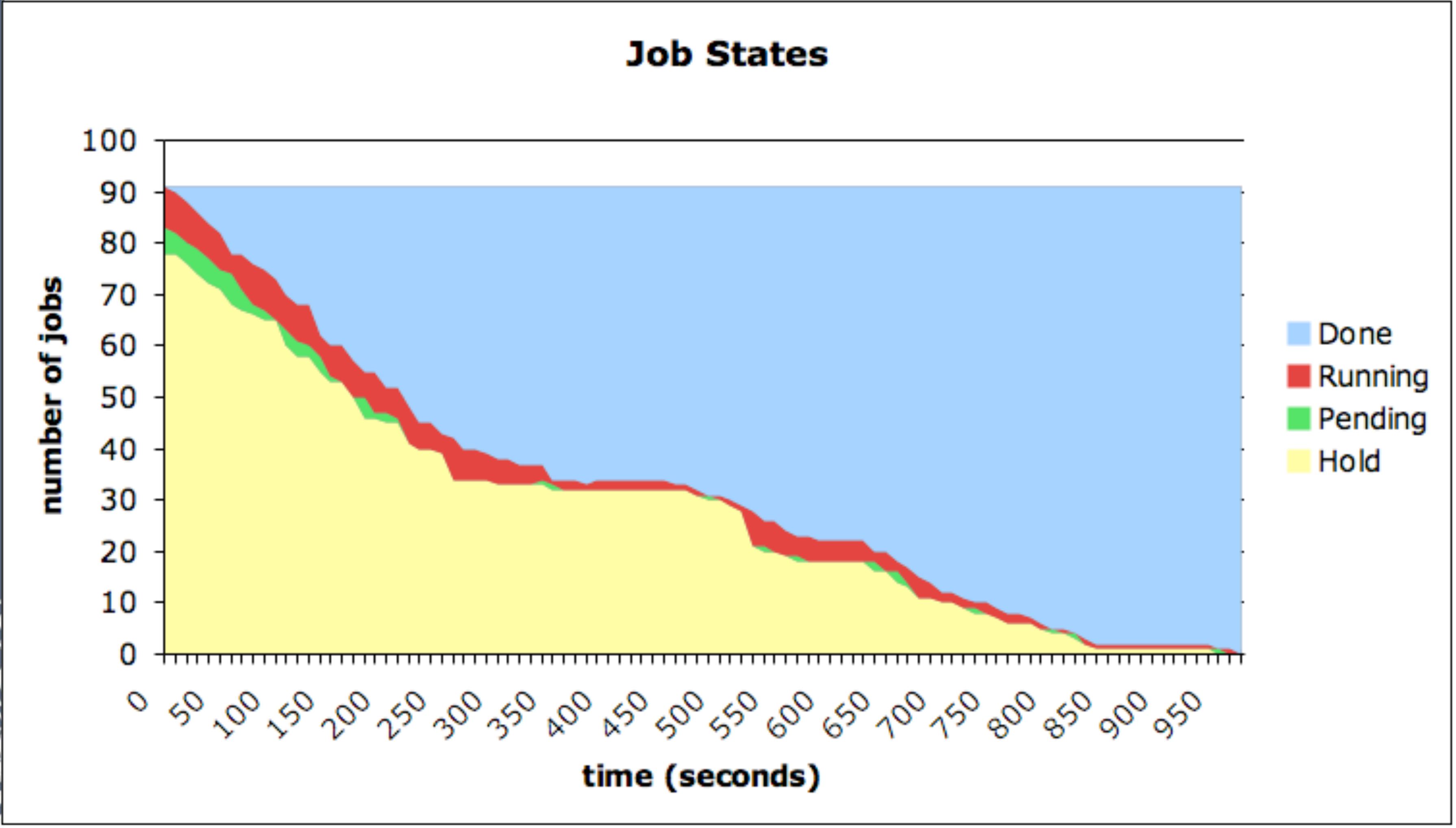
4. The CD-HIT Application

Running with 10 divisions

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



Job States - Running with 14 divisions



QUESTIONS?

**Thank you
for your attention!**