GenWrapper: A Generic Wrapper for Running Legacy Applications on Desktop Grids

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Joint EGEE and EDGeS Summer School on Grid Application Support

29 June 2009 - 07 July 2009

Budapest, Hungary

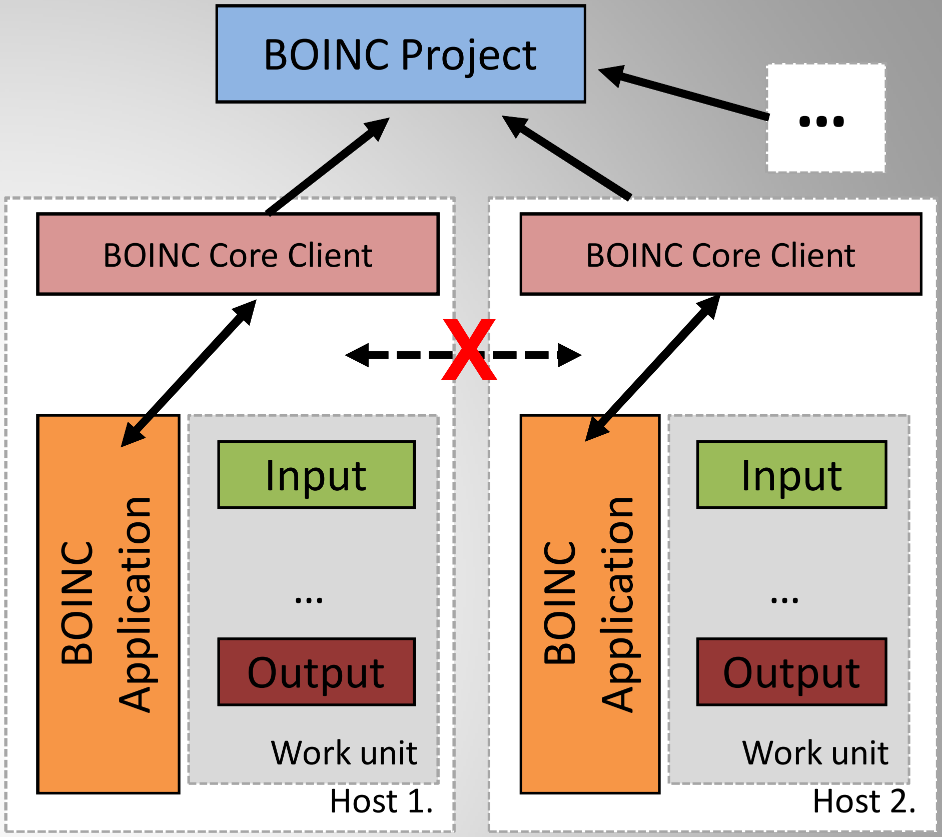
Outline

- **Volunteer Computing and Desktop Grid Computing**
- **BOINC –** Berkeley Open Infrastructure for Network Computing
  - native applications
  - the BOINC Wrapper
- **GenWrapper**
  - Motivation
  - Details
- **Applications and Projects utilizing GenWrapper**
- **Conclusion**

Volunteer Computing and Desktop Grid Computing

- **Volunteer Computing usually refers to aggregates formed by non-dedicated (volunteer) desktop nodes**
  - *public resource computing, public-based desktop grids, public desktop grids*
  - volatile nature of connected resources
  - the resource donating entity (“**donor**”) needs to trust the entity (“**project**”) gathering the resources
- **Desktop Grid Computing is using private resources available at institutions and companies**
  - *institutional desktop grids, enterprise desktop grids, local desktop grids*
  - adminsitrators have total control over the resources
  - donors may not be aware of donating (idle) CPU time
  - dedicated resources, different security requirements

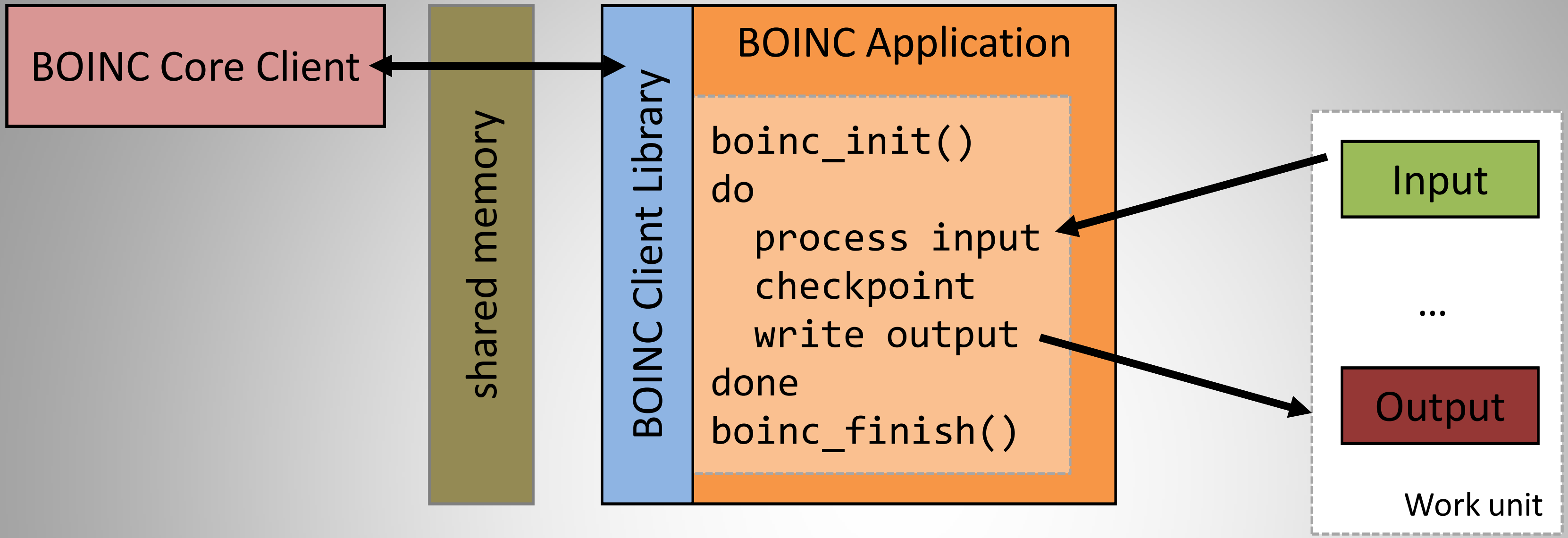
BOINC



- **donors install the BOINC Core Client and attach to a Project**
  - the client downloads an Application and sets of input data ("*Work units*")
  - the Application processes the input data
  - the client uploads the output ("*Completed result*")

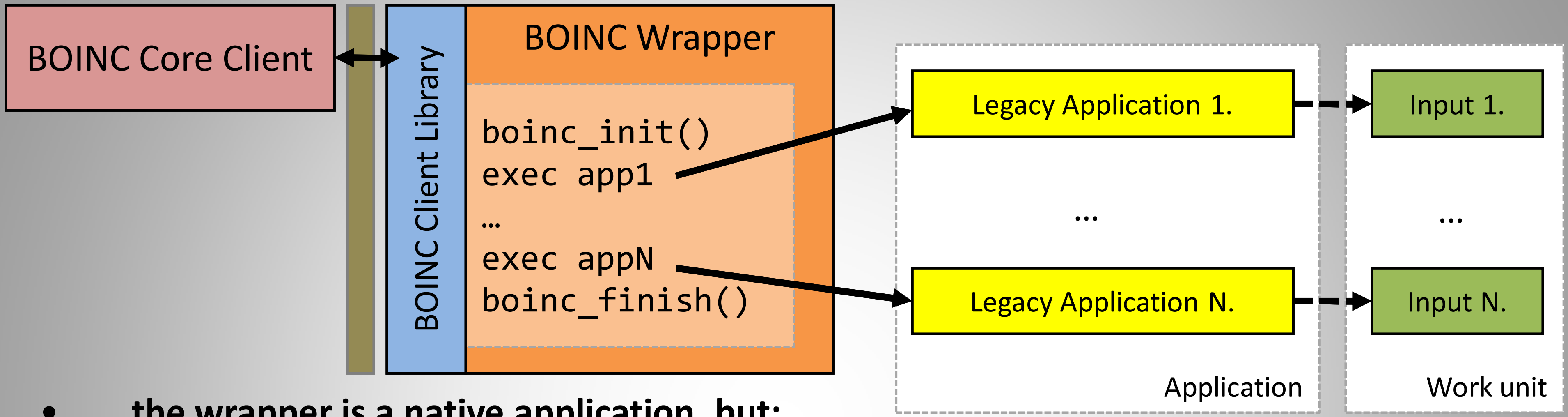
- **BOINC is suited for Master-Worker style applications**
  - no communication is possible between the "work units"

The native BOINC application



- **any application needs special preparation**
  - needs to be recompiled and linked with the BOINC library
  - has to call `boinc_init()` at the beginning and `boinc_finish()` before exit
    - the Core Client and the Application uses shared memory for communication
  - for each file to be opened needs to be resolved via `boinc_resolve()`
    - there is a separate working directory (“slot”) and storage dir (“project”)

The BOINC Wrapper



- **the wrapper is a native application, but:**
  - handles communication with the Core Client (suspends, resumes, starts and kills the application; reports fraction and CPU time used)
- **can be used to port Legacy Applications**
  - no need to change the original code
  - legacy applications are run as sub-processes
- **each application may have input, output files, environment and command line**
- **checkpoints after each finished application (task)**
- **uses an XML style configuration file for task description**

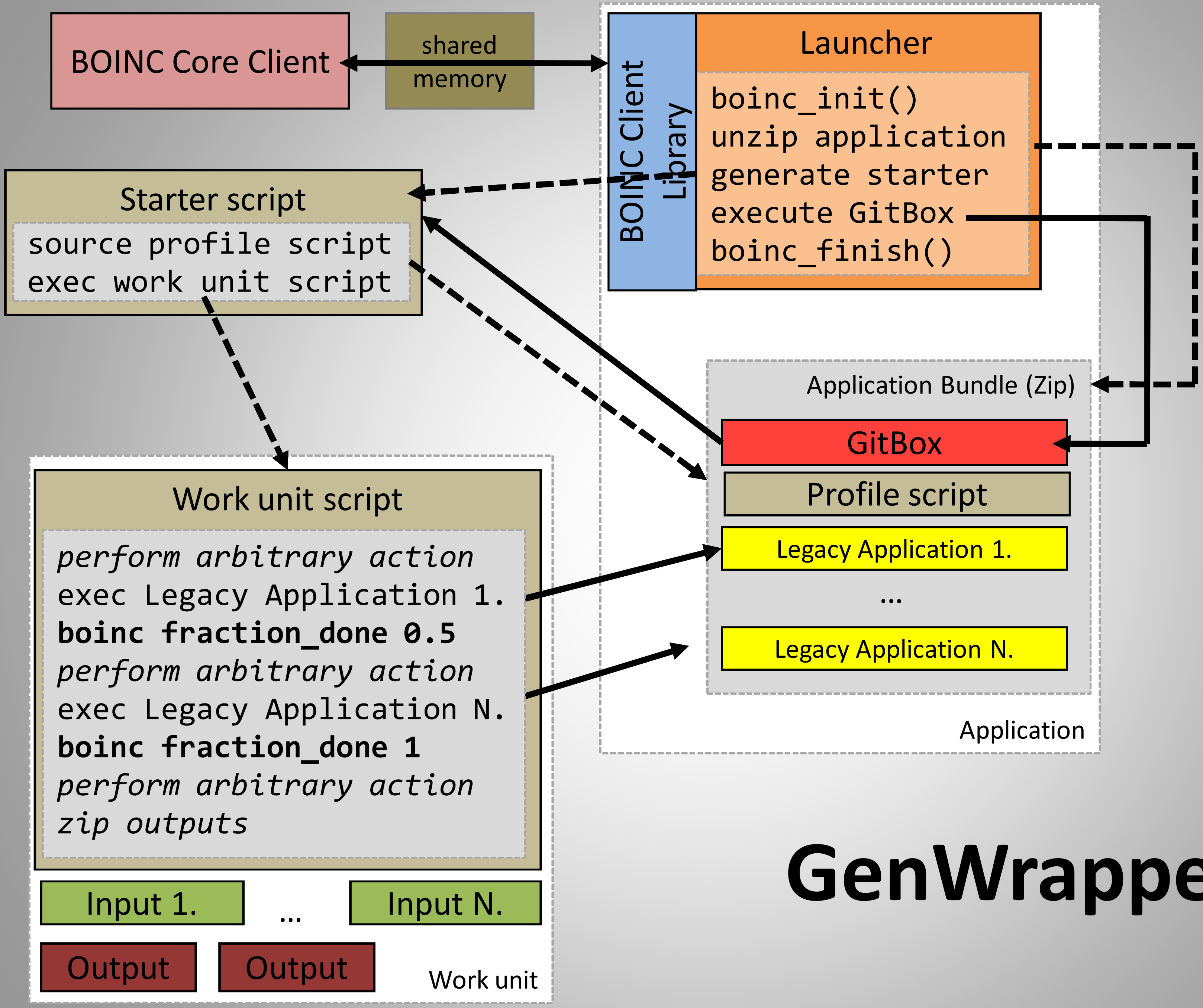
Motivation for a Generic Wrapper

- **Why did we need it?**
  - The features of the BOINC Wrapper are not enough
    - patching config files on client machines
    - input files need preparation
    - generating extra messages (log, debug)
    - independent jobs in a single WU (batching)
    - unknown number of output files
    - legacy applications may start processes themselves
    - support for DC-API and BOINC API
  - Wanted to be prepared for unknown requirements might be raised by future applications
  - We did not want to extend the BOINC Wrapper to make it an XML-based programming language, we choose to use an existing language -> Bourne shell

A Generic Wrapper

- **How did we do it ?**
  - **we took GitBox a Windows only port of BusyBox …**
    - **a single binary providing POSIX shell interpreter and essential UNIX commands (`sed`, `grep`, `tar`, `echo`, etc)**
    - **was used earlier by the git version control system on Windows (abandoned now)**
  - **… and ported it back to Linux and Mac OS X (while still runs on Windows)**
    - the name remained GitBox, but has little common with the original…
  - **extended it to…**
    - **use the BOINC API and to provide the API for POSIX shell scripting (`boinc resolve_filename`,`boinc fraction`,`boinc fraction_percent`)**
    - **have more commands available (like `unzip`, `awk`, etc) and fixed some…**
    - **handle communication with the Core Client: report CPU time; suspend, resume and kill processes started (not trivial!); CPU throttling, etc.**
- **How does it work ?**

GenWrapper



BOINC Core Client

shared memory

BOINC Client Library

Launcher

```
boinc_init()
unzip application
generate starter
execute GitBox
boinc_finish()
```

Starter script

```
source profile script
exec work unit script
```

Application Bundle (Zip)

GitBox

Profile script

Legacy Application 1.

...

Legacy Application N.

Application

Work unit script

```
perform arbitrary action
exec Legacy Application 1.
boinc fraction_done 0.5
perform arbitrary action
exec Legacy Application N.
boinc fraction_done 1
perform arbitrary action
zip outputs
```

Input 1.

...

Input N.

Output

Output

Work unit

Sample GenWrapper script

```
IN=`boinc resolve_filename in`
OUT=`boinc resolve_filename out`
NUM=`cat ${IN}`
PERCENT_PER_ITER=$((100000 / NUM))
for i in `seq $NUM`; do
    PERCENT_COMPLETE=$((PERCENT_PER_ITER * i / 1000))
    boinc fraction_done_percent ${PERCENT_COMPLETE}
    echo -e "I am ${PERCENT_COMPLETE}% complete." >> ${OUT}
    sleep 1;
done
```

- **no need to call** `boinc_init()` **or** `boinc_finish()`
  - **exit status of the script is the exit status of the work unit**
- **the script should implement checkpointing, and checkpoint itself when fits**
- **every input and output file needs to be resolved**
- **no background jobs yet (Windows lacks** `fork()` **)**
  - **but legacy applications may create new processes themselves**

Some applications and projects using GenWrapper

- **CancerGrid Project -** *Grid Aided Computer System For Rapid Anti-Cancer Drug Design*
- **EDGeS Project –** *Enabling Desktop Grids for e-Science*
  - **3D Video Rendering Service using *Blender* @** UoW
  - **Protein Molecule Simulation using *AutoDock* @** University of Westminster
    - http://wgrass.wmin.ac.uk/index.php/Desktop_Grid:Autodock
  - **Patient Readmission Application - statistical model developed in *R* @** UoW
    - http://wgrass.wmin.ac.uk/index.php/Desktop_Grid:r
- **Discrete event simulator using *Discrete Event Modelling on Simula (Demos)* @** Norwegian University of Science and Technology (NTNU)
- **EMMIL – E-commerce model to integrate logistics @** International Business School Inst. of Information Systems and Logistics, Budapest, Hungary

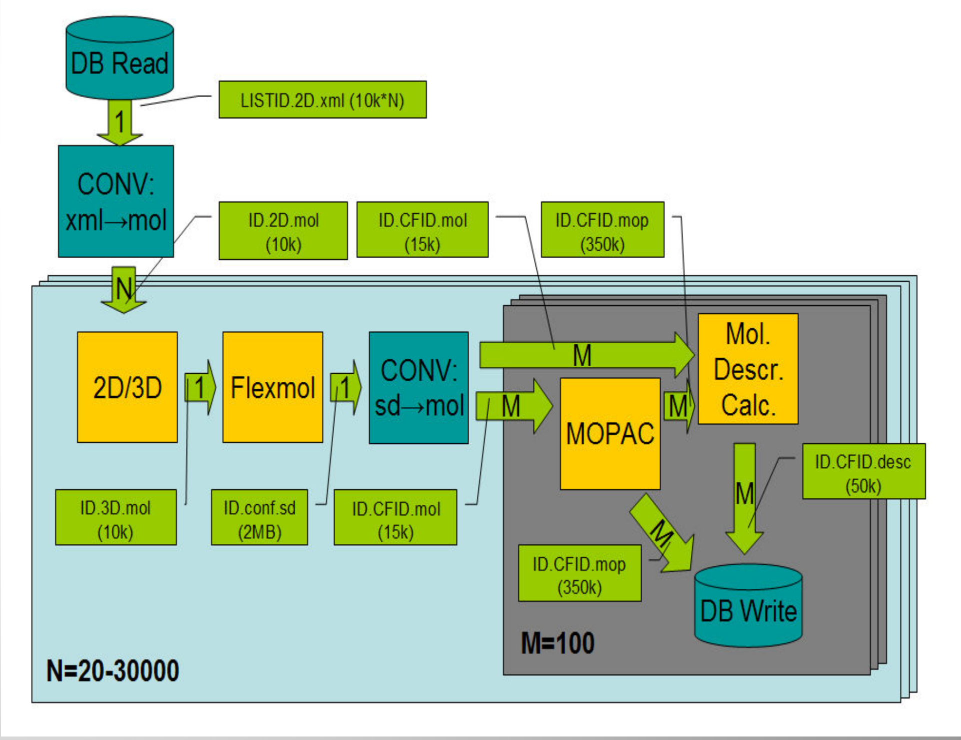
The CancerGrid project

- EU Framework Program 6 (FP-6, 2006-2009)
- Title: *Grid Aided Computer System For Rapid Anti-Cancer Drug Design*
- Project period
  - January 1, 2007 – December 31, 2009
- Goals:
  - Developing *focused libraries* with a high content of anti-cancer leads, building *models* for predicting various molecule properties
  - Developing a *computer system* based on grid technology, which helps to accelerate and automate the *in silico design* of libraries for drug discovery processes

The CancerGrid applications - Wide variety of applications in a workflow

Applications: **cmol3d**, **mopac**, **mdc**, **fmt**, **fma**, etc.

- Fortran, C, C++
- processing/ memory requirements
- multi-binary applications (already contain some wrappers), libraries
- **legacy binaries for Linux and Windows**
- config file preparation before execution
- pure logging/ debugging information
- variable run-time
  - one to one Work unit mapping not always efficient
  - **batching**
- variable number of output files
- need to be executed in a specific order
- workflows have been created
  - *molecule descriptor calculator*, *model building* and *property prediction*

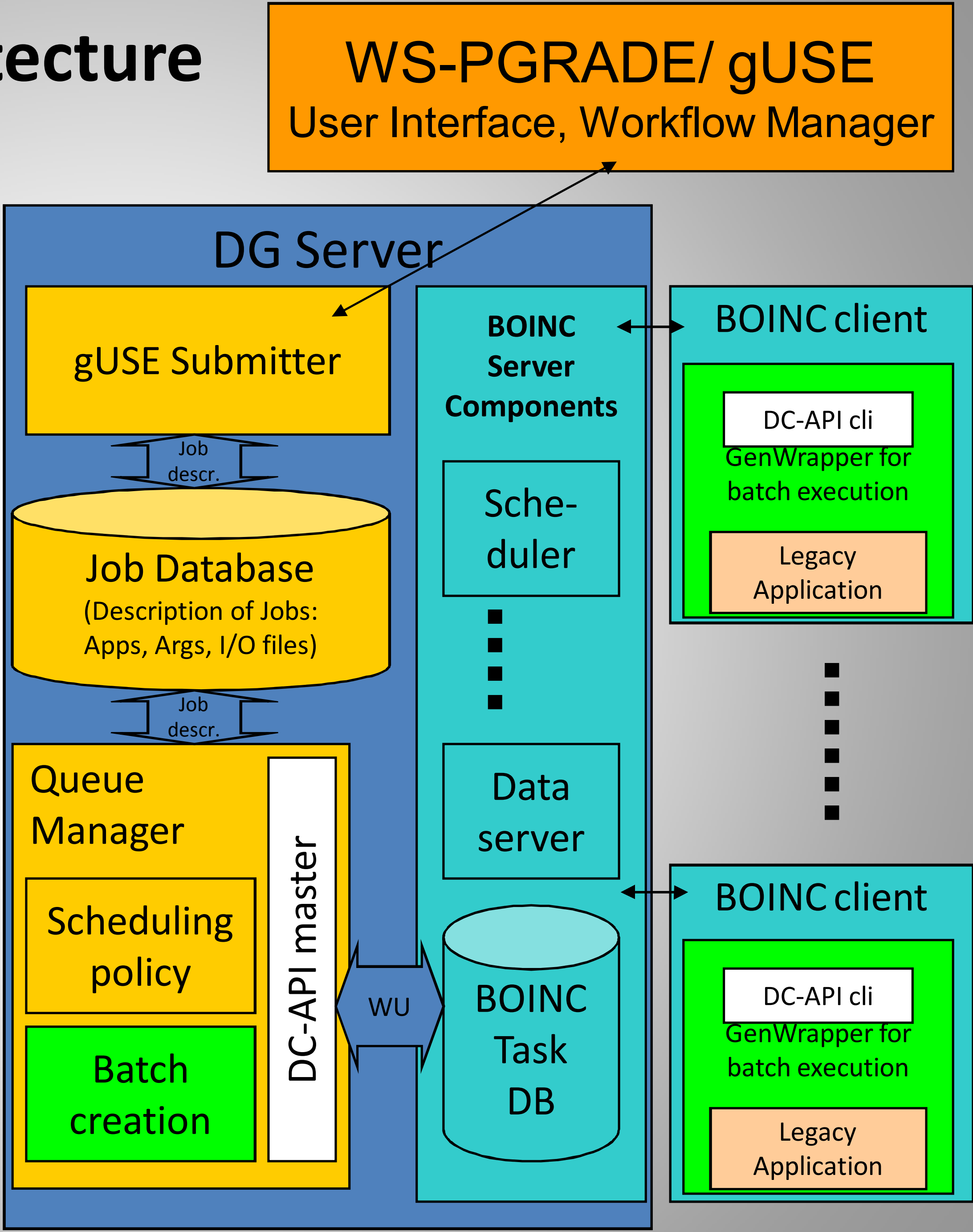


The CancerGrid applications – descriptor calculator

- **the most computation intensive workflow is the descriptor calculator**
  - 4 jobs for molecular calculations
  - 2 jobs for file format conversion
  - 3 jobs for database manipulation
- **main parameters of the workflow (from computing perspective)**
  - **`N`** : number of two dimensional input molecules
  - **`M`** : number of confirmers (variants of a molecule)
- **molecular calculation jobs are executed once for each input or once for each confirmer**
  - typical value for **`N`**`: 30,000;` for **`M`**`: 100`
  - `3,000,000` instances, total `~10,000,000` jobs
- **the granularity of the workflow is fine grained**
  - running time of one instance is a few minutes
  - not suitable for conversion to BOINC work units one to one

The CancerGrid architecture

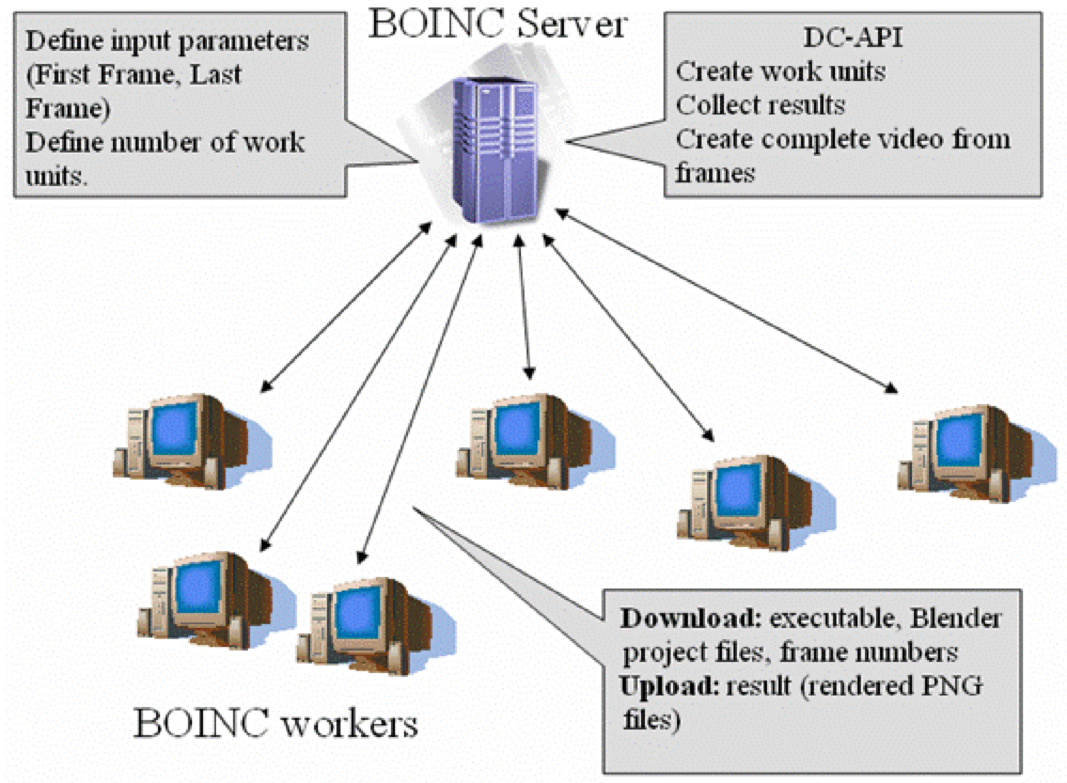
- a **Job Database**, **Job Queues** and **Queue Manager** extension has been introduced at the BOINC server.
- once a queue contains appropriate number of jobs a work unit is created using DC-API
- a shell script is created to manage the execution of the batch
  - assembled from head, body and tail fragments
  - body part is repeated for each job in the batch
  - may contain macros like `%{name}`
  - executed by GenWrapper



3D Video Rendering Service using *Blender*

University of Westminster, London, UK

- **open source rendering software**
- **Blender renders frames sequentially**
  - set of frames is sent to workers and a master creates the complete video from the pieces
- **part of an on-line distributed rendering service**



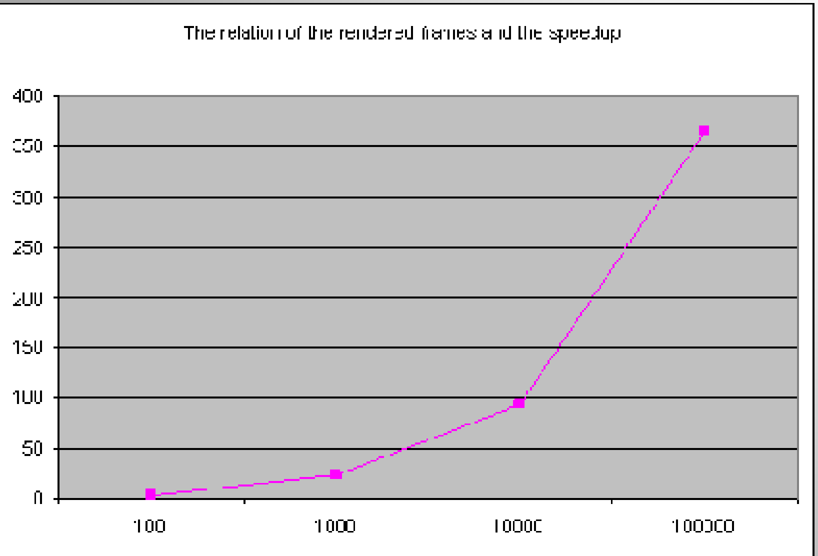
BOINC Server

Define input parameters (First Frame, Last Frame)
Define number of work units.

DC-API
Create work units
Collect results
Create complete video from frames

BOINC workers

Download: executable, Blender project files, frame numbers
Upload: result (rendered PNG files)



http://wgrass.wmin.ac.uk/index.php/Desktop_Grid:Rendering

Conclusions

- **GenWrapper offers a generic solution for wrapping and executing an arbitrary set of applications on BOINC (BOINC API or DC-API) and XtremWeb**
  - POSIX like scripting language
  - Not a silver bullet !
    - security considerations, legacy applications with lot of external dependencies
- **great flexibility and powerful tool for porting legacy applications**
- **based on a modified version of GitBox (~BusyBox)**
  - open source (GPL/ LGPL)
- **runs on Windows, Linux, Mac OS X**
- **small size**
  - Launcher and GitBox are ~400KByte each (will be integrated into a single binary)
- **many applications and projects are using it**

Thank You!

- GenWrapper
  - http://sanjuro.lpds.sztaki.hu/genwrapper
- Enabling Desktop Grids for e-Science
  - http://www.edges-grid.eu
- CancerGrid
  - http://www.cancergrid.eu

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