Scaling bio-analyses from computational clusters to grids

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molgenis

Content

- Bio-workflows
- Workflow
  - Modeling
  - Job Generation
  - Tool deployment
  - Data management
  - Workflow execution
  - Implementation detail
  - Recent developments
- Conclusion and further steps

Bio-workflows

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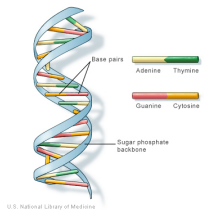
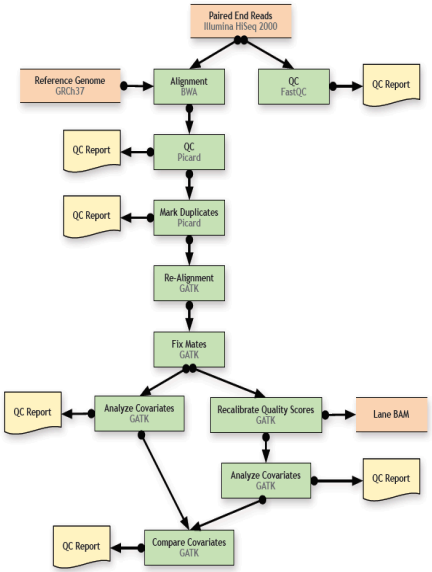
Example: NGS alignment workflow



HiSeq



Per Project:
1. Aligned reads
2. QC-reports
3. SNP lists

Raw data → ***alignment workflow*** → Result data

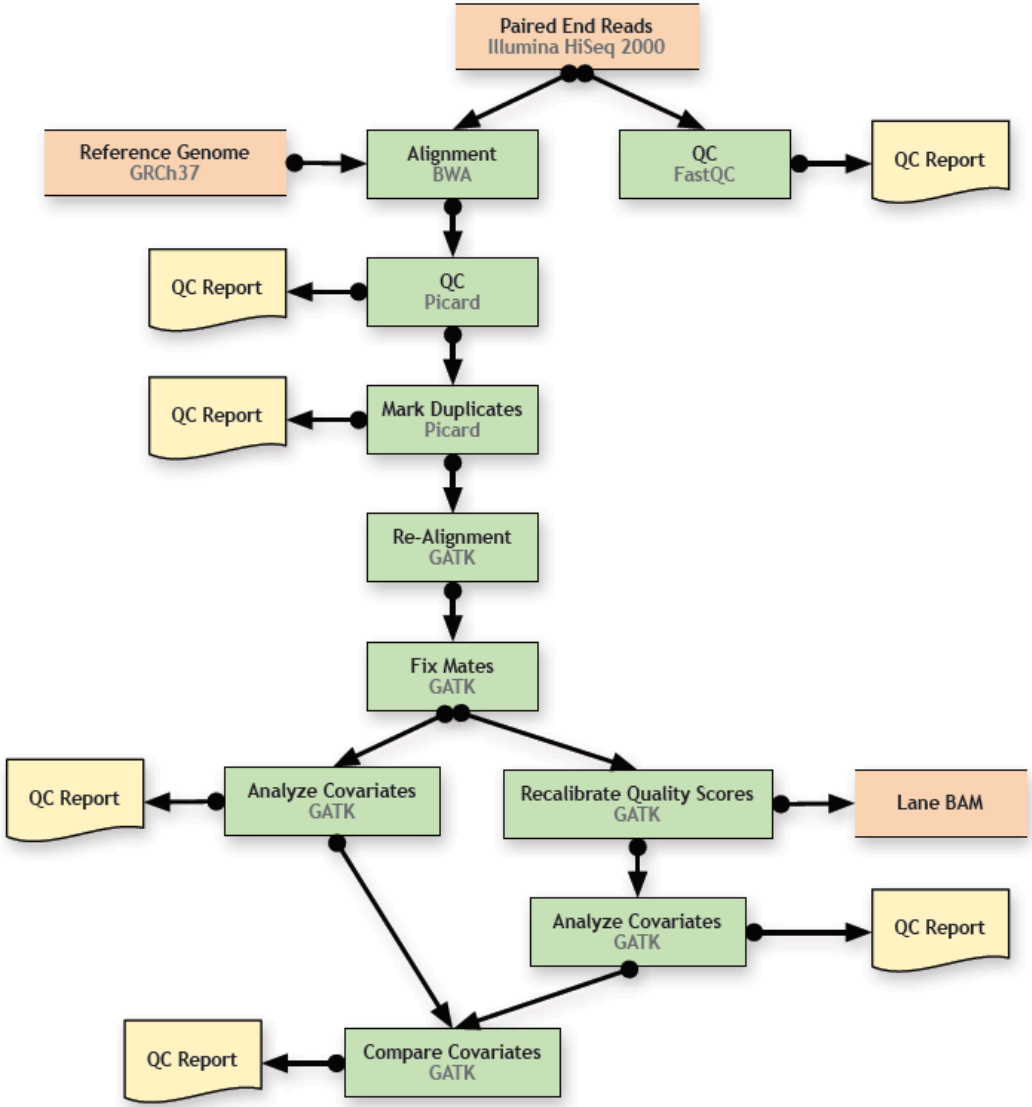
10-100 samples

20 – 200 days

80 – 800 GB

Alignment & SNP calling workflow

31 steps, ≥ 2 days per sample



- Input
  - Analysis protocols
  - Sample DNA data
  - Reference DNA data
- Analysis
  - Scripts are generated and executed
- Output
  - Aligned DNA and QC reports

An analysis job (script) generated from a protocol

backend specific

```
#!/bin/bash
#PBS -q test
#PBS -l nodes=1:ppn=4
#PBS -l walltime=08:00:00
#PBS -l mem=6gb
#PBS -e $GCC/test_compute/projects/batch4/intermediate/test1/err/err_test1_BwaElement1A102a_FC81D90ABXX_L7.err
#PBS -o $GCC/test_compute/projects/batch4/intermediate/test1/out/out_test1_BwaElement1A102a_FC81D90ABXX_L7.out
mkdir -p $GCC/test_compute/projects/batch4/intermediate/test1/err
mkdir -p $GCC/test_compute/projects/batch4/intermediate/test1/out
printf "test1_BwaElement1A102a_FC81D90ABXX_L7_started " >>$GCC/test_compute/projects/batch4/intermediate/test1/log_test1.txt
date "+DATE: %m/%d/%y%tTIME: %H:%M:%S" >>$GCC/test_compute/projects/batch4/intermediate/test1/log_test1.txt
date "+start time: %m/%d/%y%t %H:%M:%S" >>$GCC/test_compute/projects/batch4/intermediate/test1/
test1_BwaElement1A102a_FC81D90ABXX_L7.txt
echo running on node: `hostname` >>$GCC/test_compute/projects/batch4/intermediate/test1/
test1_BwaElement1A102a_FC81D90ABXX_L7.txt
```

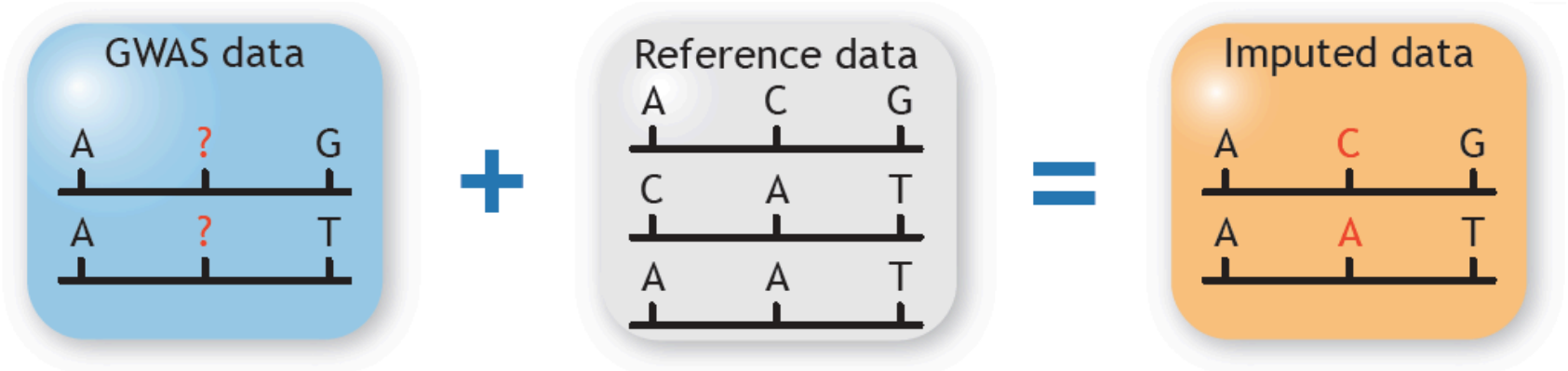
analysis specific

```
/target/gpfs2/gcc/tools//bwa-0.5.8c_patched/bwa aln \
/target/gpfs2/gcc/resources/hg19/indices/human_g1k_v37.fa \
$GCC/test_compute/projects/batch4/rawdata/110121_I288_FC81D90ABXX_L7_HUMrutRGADIAAPE_1.fq.gz \
-t 4 \
-f $GCC/test_compute/projects/batch4/intermediate/A102a_110121_I288_FC81D90ABXX_L7_HUMrutRGADIAAPE_1.fq.gz.sai
```

```
printf "test1_BwaElement1A102a_FC81D90ABXX_L7_finished " >>$GCC/test_compute/projects/batch4/intermediate/test1/log_test1.txt
date "+finish time: %m/%d/%y%t %H:%M:%S" >>$GCC/test_compute/projects/batch4/intermediate/test1/
test1_BwaElement1A102a_FC81D90ABXX_L7.txt
date "+DATE: %m/%d/%y%tTIME: %H:%M:%S" >>$GCC/test_compute/projects/batch4/intermediate/test1/log_test1.txt
```

Imputation workflow

- Imputation:



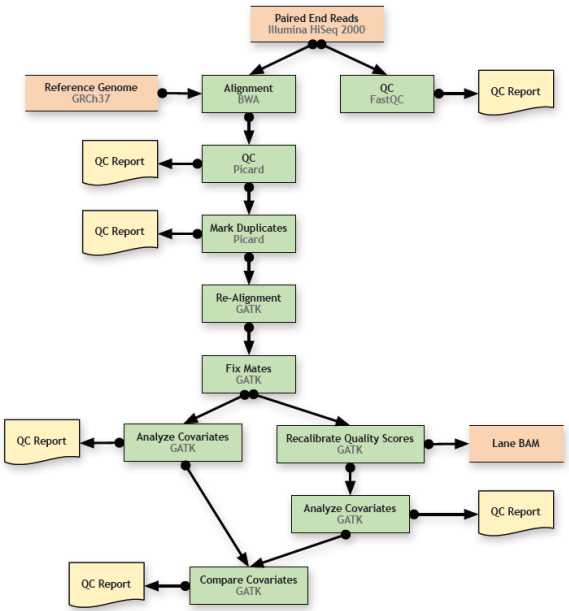
- Number of jobs

$$number\_jobs = \sum_{chr=1..22} \frac{Lenght_{chr}}{5\_megabase} * \frac{number\_of\_samples}{500}$$

- One run:

Bio-workflow complexity

- Many analysis steps
  - Many analysis jobs
  - Different analysis tools and their dependencies
- Large various data involved
- Heterogeneous resources



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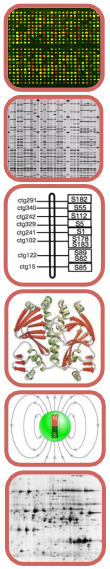
Workflow design and generation

MOLGENIS approach

- Model
- Generate
- Use

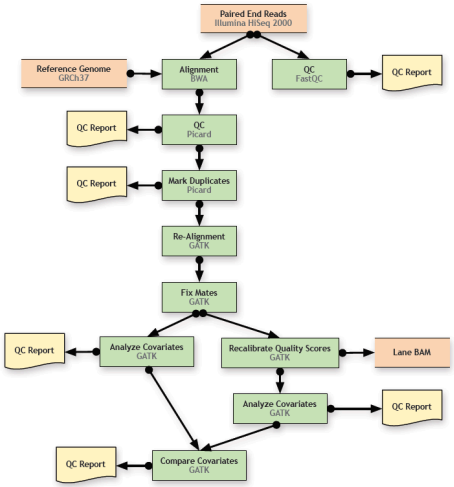
Species...

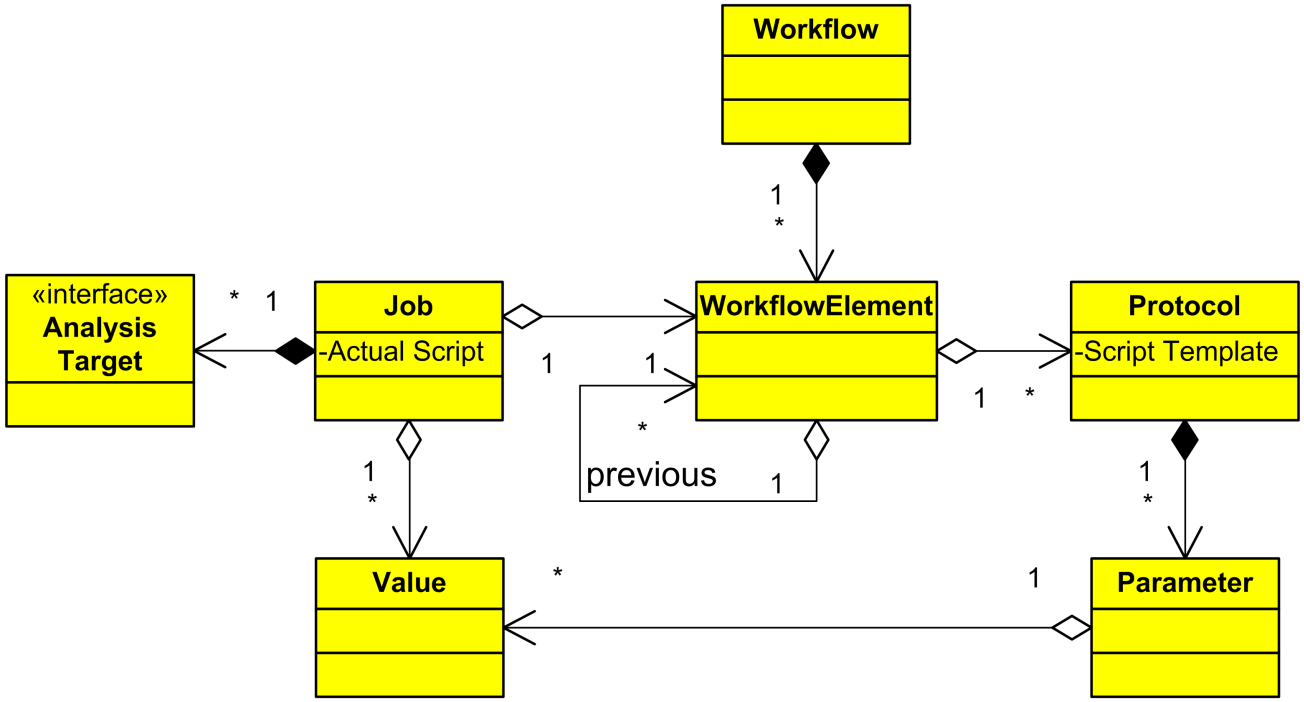


Analyses...

Projects ...

Workflow design





- Jobs are generated from the model
- Every job has an analysis target (*e.g.* Genome region)

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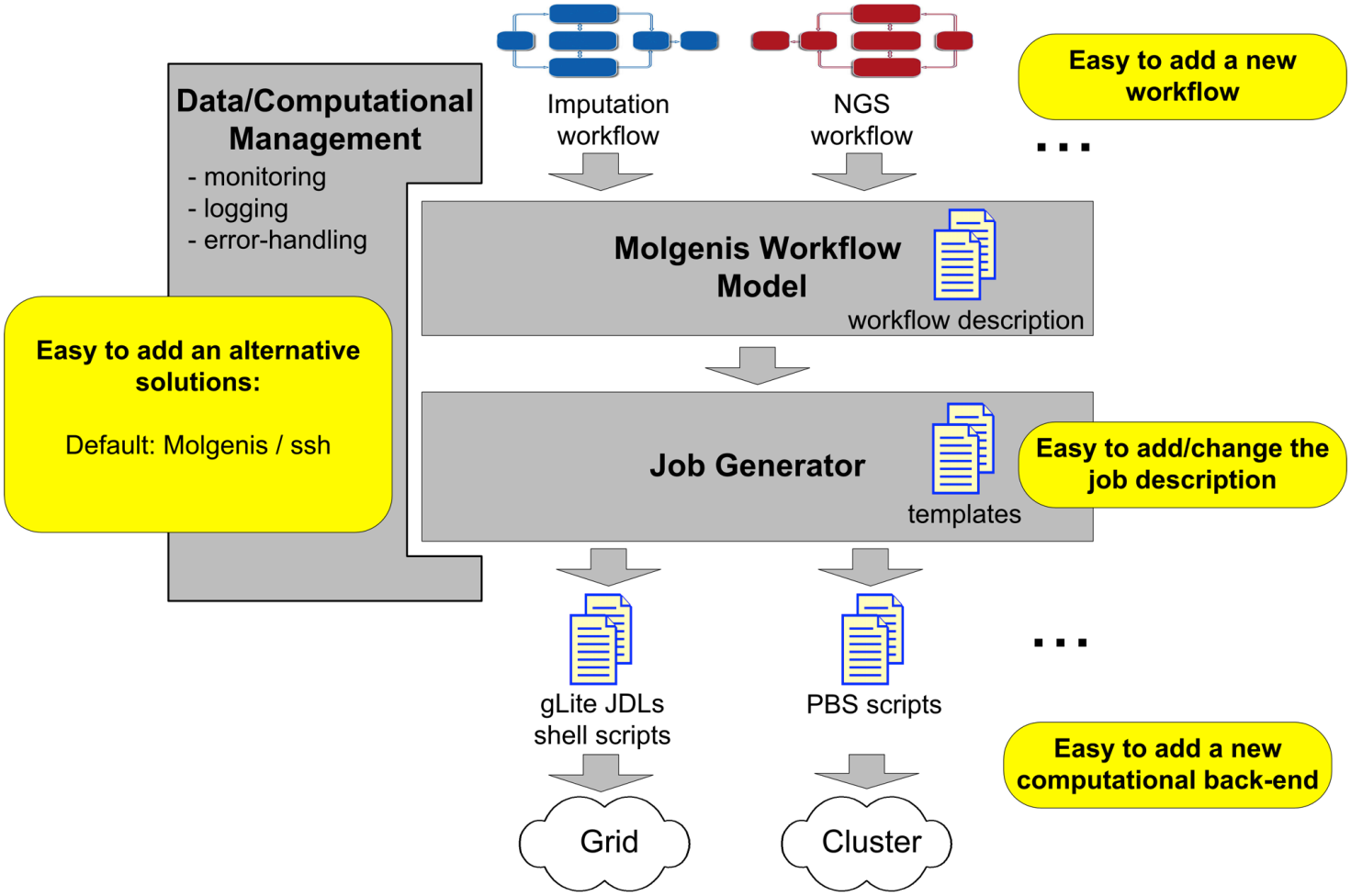
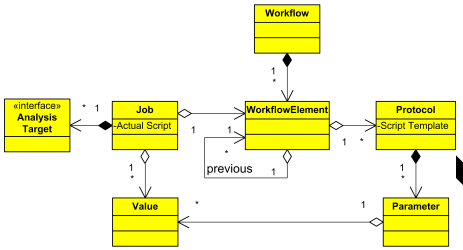
Command-line generator (Demo @ IWSG-2012)



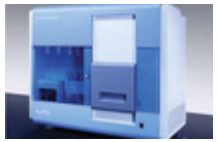
- Generates jobs (scripts) from model described in files
- Suitable for workflows (PBS cluster) and single jobs (gLite grid)

Database solution with MOLGENIS software toolkit (1)

Model (xml)



Workflow



NextGenSeq

Model organisms

Generator (java)

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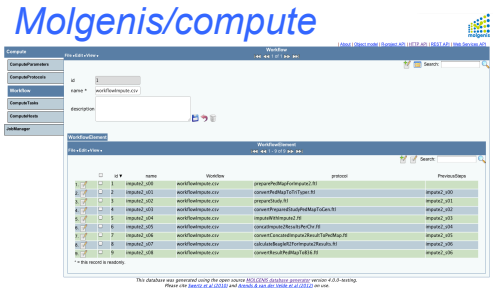
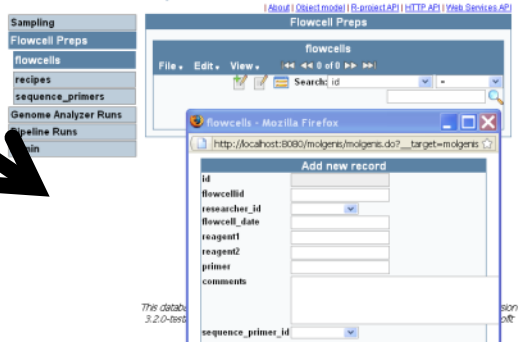
Use (web)

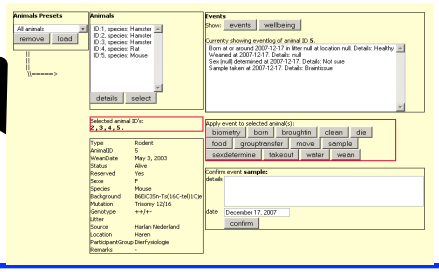
Molgenis/compute



Solexa Sequencer LIMS

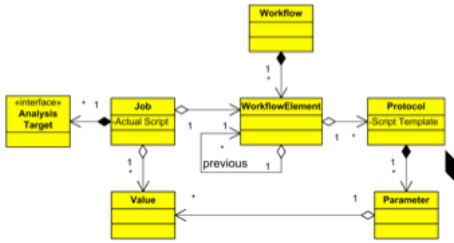


Animal Observatory



Database solution with MOLGENIS software toolkit (2)

Model (xml)



Workflow

NextGenSeq

Model organisms

- Model
  - workflow.xml / 100 loc
  - ui.xml / 25 loc

Generator (java)

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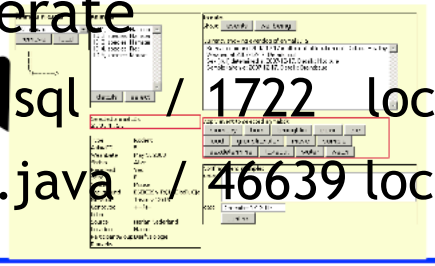
Use (web)

Molgenis/compute

Solexa Sequencer LIMS

Animal Observatory



- Generate
  - sql / 1722 loc
  - *.java / 46639 loc

1 : 400!

Workflow design view in the generated Molgenis web-UI

Compute Testing

molgenis

| About | Object model | R-project API | HTTP API | REST API | Web Services API

Compute

- ComputeParameters
- ComputeProtocols
- Workflow
- ComputeTasks
- ComputeHosts
- JobManager

File ▾ Edit ▾ View ▾ — **Workflow** — 1 of 1

Search:

id: 1

name *: workflowImpute.csv

description:

WorkflowElement

File ▾ Edit ▾ View ▾ — **WorkflowElement** — 1 - 9 of 9

Search:

	id ▼	name	Workflow	protocol	PreviousSteps
1.	1	impute2_s00	workflowImpute.csv	preparePedMapForImpute2.ftl	
2.	2	impute2_s01	workflowImpute.csv	convertPedMapToTriTyper.ftl	impute2_s00
3.	3	impute2_s02	workflowImpute.csv	prepareStudy.ftl	impute2_s01
4.	4	impute2_s03	workflowImpute.csv	convertPreparedStudyPedMapToGen.ftl	impute2_s02
5.	5	impute2_s04	workflowImpute.csv	imputeWithImpute2.ftl	impute2_s03
6.	6	impute2_s05	workflowImpute.csv	concatImpute2ResultsPerChr.ftl	impute2_s04
7.	7	impute2_s06	workflowImpute.csv	convertConcatedImpute2ResultToPedMap.ftl	impute2_s05
8.	8	impute2_s07	workflowImpute.csv	calculateB[illegible]gleR2ForImpute2Results.ftl	impute2_s06
9.	9	impute2_[illegible]08	workflowImpute.csv	conver[illegible]ultPedMapToB36.ftl	impute[illegible]06

* = this record is readonly.

This [illegible] was generated [illegible] [illegible]base generator version 4.0.0-testing. [illegible] cite Sw[illegible] [illegible]de et al (2012) on use.

workflow step

analysis protocol

previous steps

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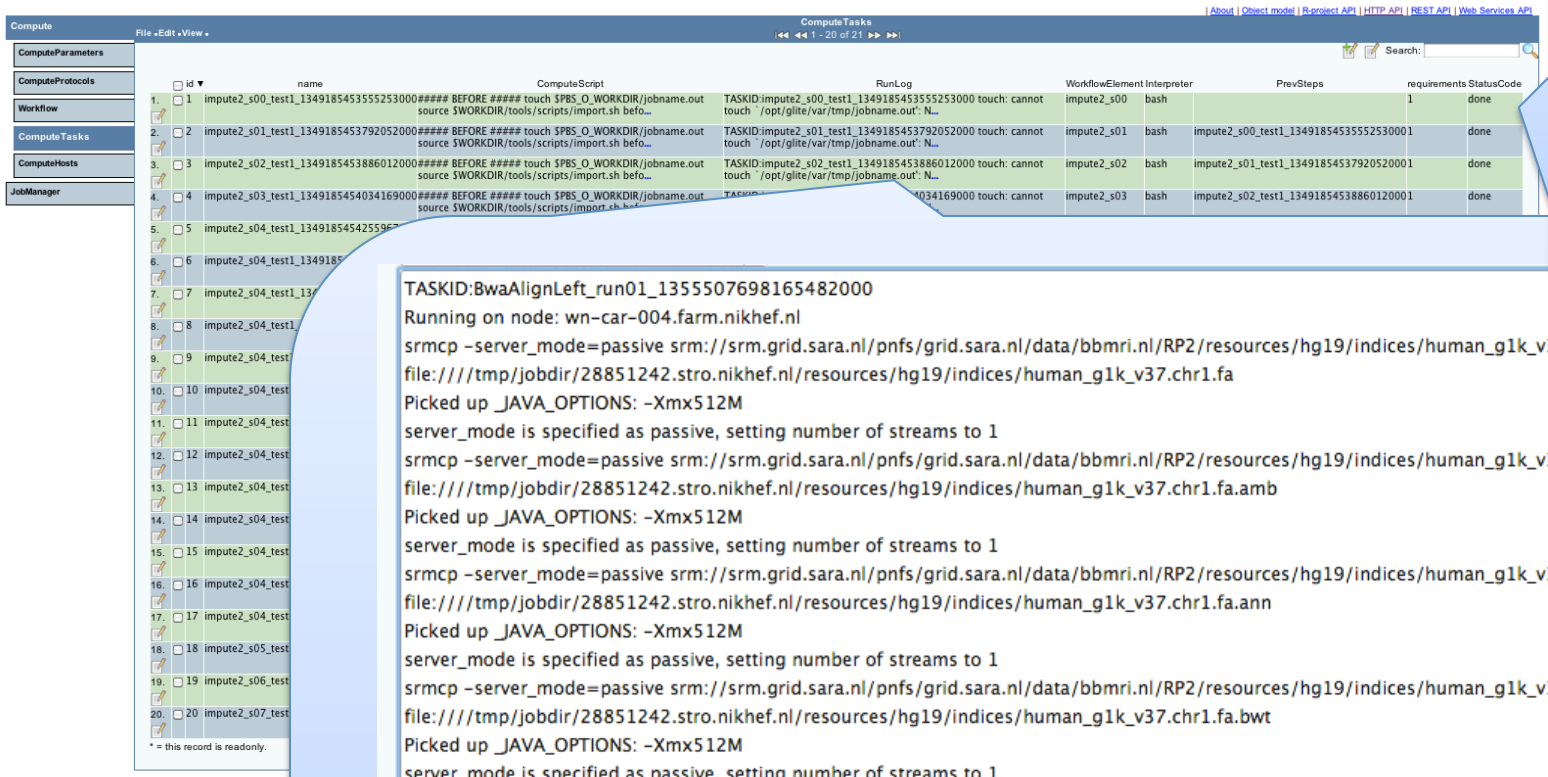
Workflow run-time view (analysis jobs)



StatusCode
done
done
done
done
done

```
TASKID:BwaAlignLeft_run01_1355507698165482000
Running on node: wn-car-004.farm.nikhef.nl
srmcp -server_mode=passive srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2/resources/hg19/indices/human_g1k_v37.chr1.fa
file:////tmp/jobdir/28851242.stro.nikhef.nl/resources/hg19/indices/human_g1k_v37.chr1.fa
Picked up _JAVA_OPTIONS: -Xmx512M
server_mode is specified as passive, setting number of streams to 1
srmcp -server_mode=passive srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2/resources/hg19/indices/human_g1k_v37.chr1.fa.amb
file:////tmp/jobdir/28851242.stro.nikhef.nl/resources/hg19/indices/human_g1k_v37.chr1.fa.amb
Picked up _JAVA_OPTIONS: -Xmx512M
server_mode is specified as passive, setting number of streams to 1
srmcp -server_mode=passive srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2/resources/hg19/indices/human_g1k_v37.chr1.fa.ann
file:////tmp/jobdir/28851242.stro.nikhef.nl/resources/hg19/indices/human_g1k_v37.chr1.fa.ann
Picked up _JAVA_OPTIONS: -Xmx512M
server_mode is specified as passive, setting number of streams to 1
srmcp -server_mode=passive srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2/resources/hg19/indices/human_g1k_v37.chr1.fa.bwt
file:////tmp/jobdir/28851242.stro.nikhef.nl/resources/hg19/indices/human_g1k_v37.chr1.fa.bwt
Picked up _JAVA_OPTIONS: -Xmx512M
server_mode is specified as passive, setting number of streams to 1
srmcp -server_mode=passive srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2/resources/hg19/indices/human_g1k_v37.chr1.fa.fai
file:////tmp/jobdir/28851242.stro.nikhef.nl/resources/hg19/indices/human_g1k_v37.chr1.fa.fai
Picked up _JAVA_OPTIONS: -Xmx512M
server_mode is specified as passive, setting number of streams to 1
srmcp -server_mode=passive srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2/resources/hg19/indices/human_g1k_v37.chr1.fa.pac
file:////tmp/jobdir/28851242.stro.nikhef.nl/resources/hg19/indices/human_g1k_v37.chr1.fa.pac
Picked up _JAVA_OPTIONS: -Xmx512M
server_mode is specified as passive, setting number of streams to 1
srmcp -server_mode=passive srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2/resources/hg19/indices/human_g1k_v37.chr1.fa.rbwt
file:////tmp/jobdir/28851242.stro.nikhef.nl/resources/hg19/indices/human_g1k_v37.chr1.fa.rbwt
Picked up _JAVA_OPTIONS: -Xmx512M
server_mode is specified as passive, setting number of streams to 1
```

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Failed jobs overview

Search results where: StatusCode = failed

Interpreter	PrevSteps	requirements	StatusCode
bash		1	failed

chr: 4 from: 185000001 to: 190000001

Running on node: v33-45.gina.sara.nl

TaskHistory 1 - 10 of 16

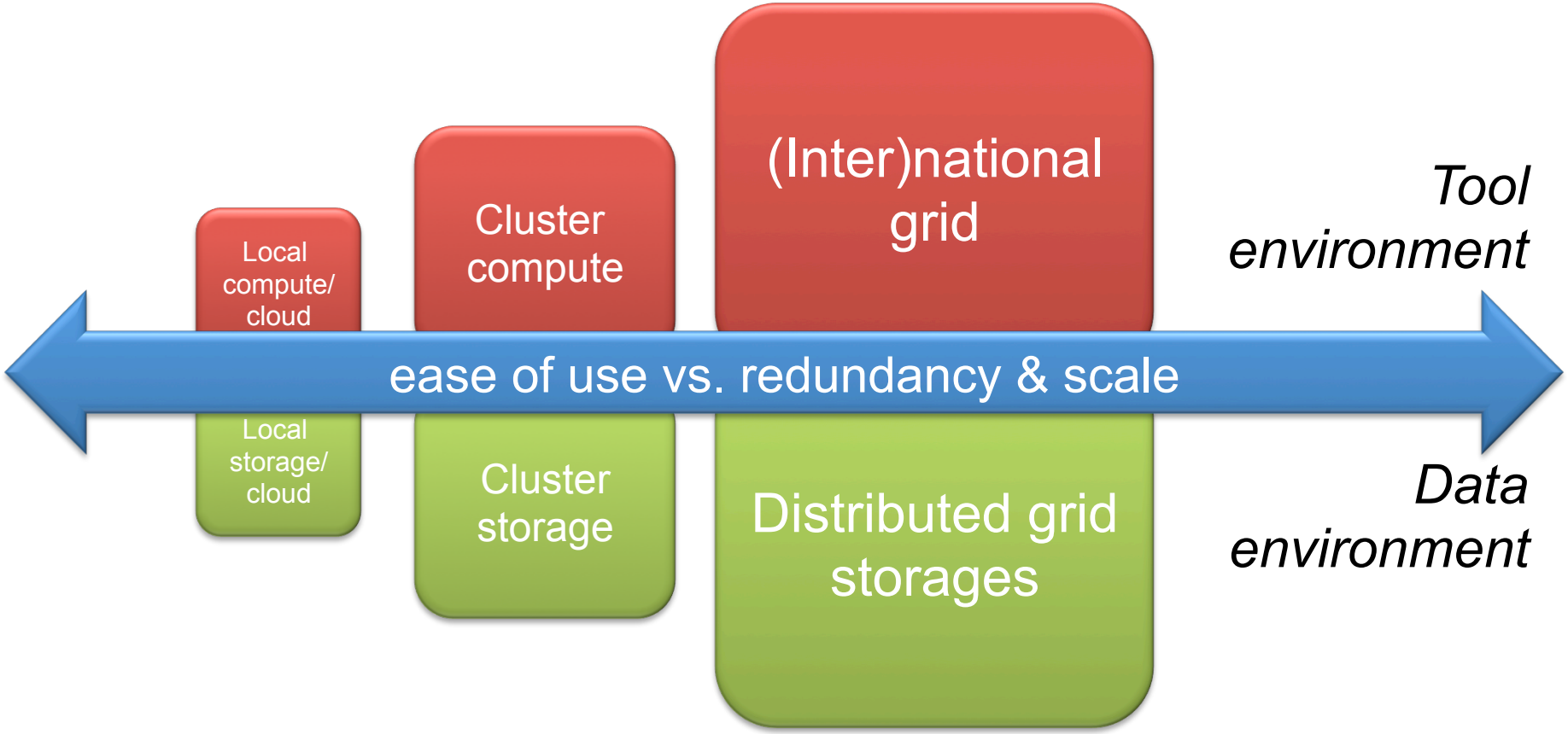
	id	ComputeTask	ComputeWorker	StatusCode	StatusTime	
					09:31:23	TASKID:imputation_run01_6664677
					21:31:50	TASKID:imputation_run01_6664677
					07:32:04	TASKID:imputation_run01_6664677
					11:33:11	TASKID:imputation_run01_6664677
					14:43:57	TASKID:imputation_run01_6664677
					07:21:26	TASKID:imputation_run01_6664677
					13:22:14	TASKID:imputation_run01_6664677
8.	6740	imputation_run01_6664677232470394		failed	April 6, 2013, 07:47:18	TASKID:imputation_run01_6664677
9.	6951	imputation_run01_6664677232470394		failed	April 6, 2013, 14:31:48	TASKID:imputation_run01_6664677
10.	7134	imputation_run01_6664677232470394		failed	April 6, 2013, 19:04:43	TASKID:imputation_run01_6664677

Error: terminate called after throwing an instance of 'std::bad_alloc'
what(): St9bad_alloc

How much memory:
virtual memory (kbytes, -v) 4194304

Workflow deployment

Computational environments



“Harmonized” tool management

Tool in input sandbox
“getFile(‘tool.zip’)”

In $WORKDIR
- Download

Tool deployed as
“load module”

In $VO_BBMRI_NL_SW_DIR
- Download
- Build
- Configure

Simple download vs. On-site build deployment

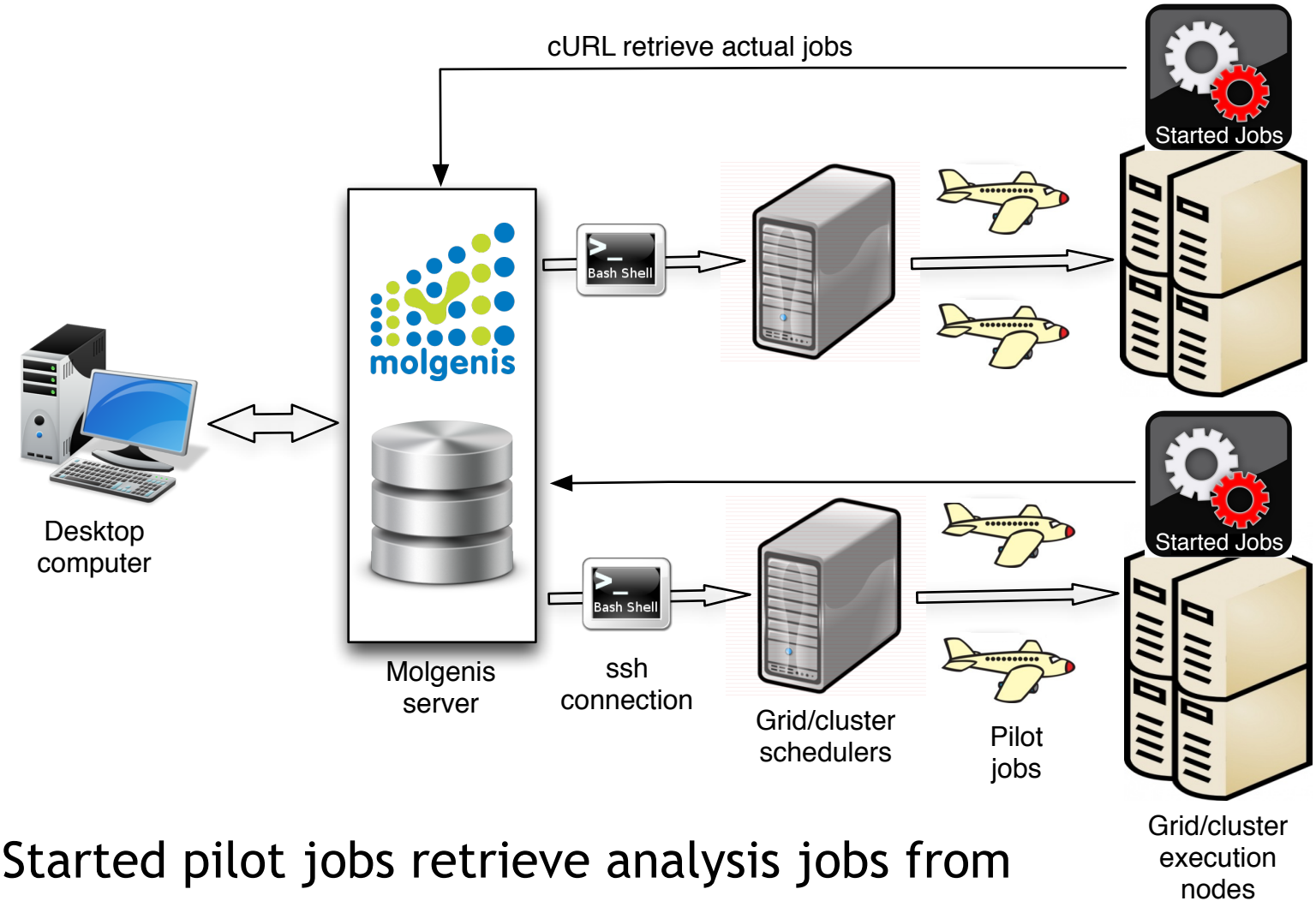
‘Harmonized’ tool management: modules

- Build using standard ‘modulecmd’ tool
- Software should be deployed at all grid sites
- Module file should be added to all sites
- http://www.bbmriwiki.nl/svn/ebiogrid/modules/

```
#
%Module1.0#################################################################
##
## bwa 0.5.8c_patched modulefile
##

proc ModulesHelp { } {
        global toolversion
        global toolname

        puts stderr "Set up the environment for $toolname version $toolversion
\n"
}

# for Tcl script use only
set toolname          bwa
set toolversion       0.5.8c_patched
set tooldir           "$env(VO_BBMRI_NL_SW_DIR)/tools/$toolname-$toolversion"
```

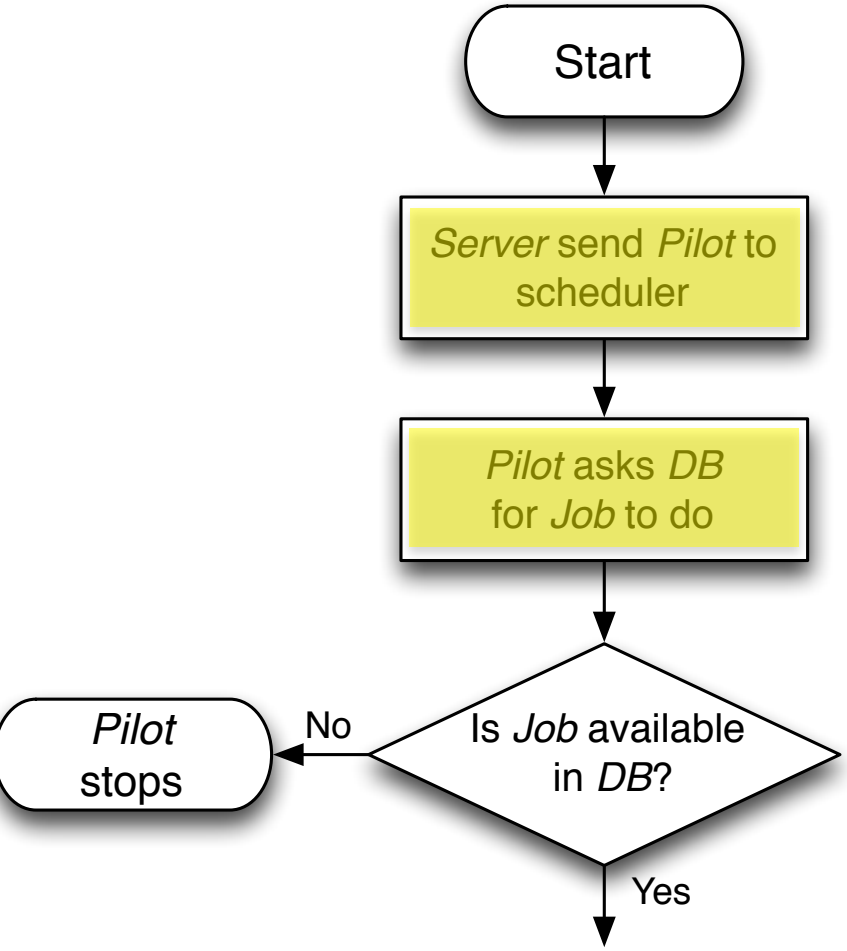
Workflow execution

Execution topology



- Started pilot jobs retrieve analysis jobs from Molgenis server

Workflow execution with pilots (1)



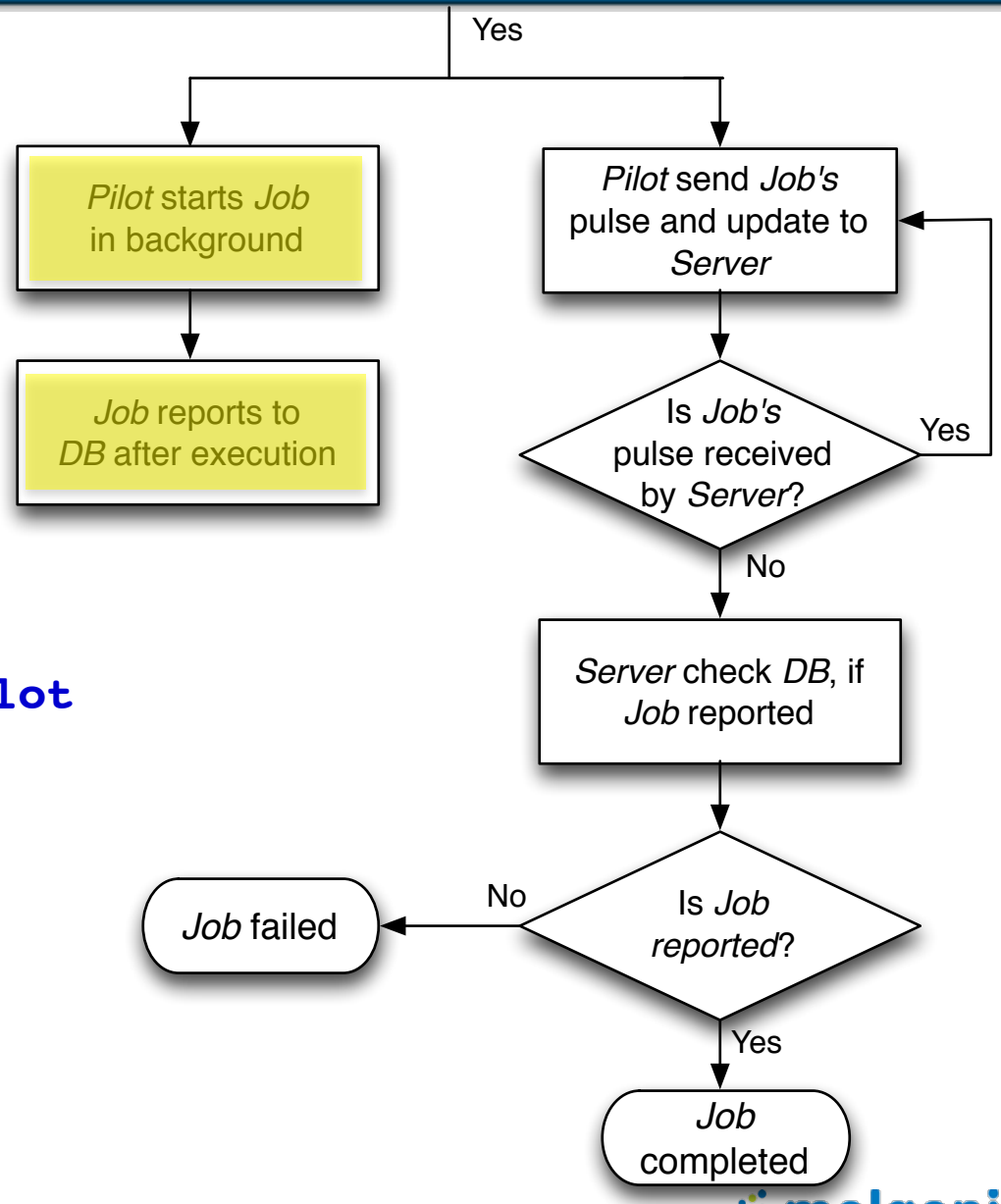

```
glite-wms-job-submit \
-d $USER … $HOME/maverick.jdl
```

```
curl  … -F status=started \
-F backend=ui.grid.sara.nl \
http://$SERVER:8080/api/pilot > scri
```

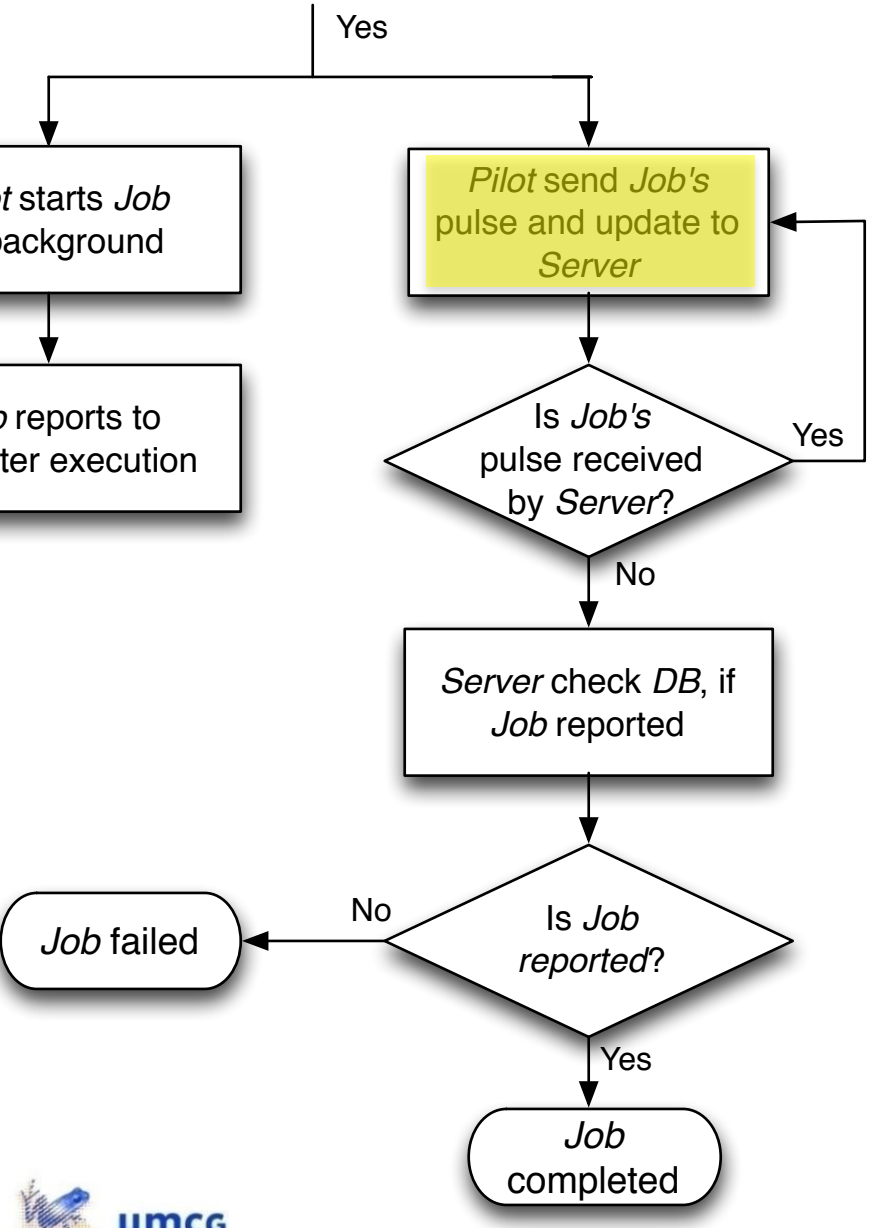
Workflow execution with pilots (2)

```
bash -l script.sh 2>&1 \
| tee -a log.log &
```

```
curl … -F status=done \
-F log_file=@done.log \
http://$SERVER:8080/api/pilot
```



Workflow execution with pilots (3)




```
while [ 1 ] ; do
…
check_process "script.sh"
CHECK_RET=$?
if [ $CHECK_RET -eq 0 ];
then
        …
        curl … -F status=nopulse \
        -F log_file=@inter.log …
        …
elif
        …
        curl … -F status=pulse \
        -F log_file=@inter.log …
        …
```

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Back-end independent analysis templates

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Template structure

```
//header
      #MOLGENIS walltime=15:00 nodes=1 cores=4 mem=6
//tool management
      module load bwa/${bwaVersion}
//data management
      getFile ${indexfile}
      getFile ${leftbarcodefqgz}
//template of the actual analysis
      bwa aln \
      ${indexfile} ${leftbarcodefqgz} \
      -t ${bwaaligncores} -f ${leftbwaout}
//data management
      putFile ${leftbwaout}
```

Data transfer

- getFile and p
  - are back-e
  - now, we
    - check i
    - do srm/
- Input

```
getFile $
```

- Generated o

```
getFile $V
imputatio
chr20.map
```

```
#------- data transfer

getRemoteLocation()
{
    ARGS=($@)
    myFile=${ARGS[0]}
    remoteFile=srm://srm.grid.sara.nl/pnfs/grid.sara.nl/data/bbmri.nl/RP2${myFile:`expr length $TMPDIR`}
    echo $remoteFile
}

getFile()
{
    ARGS=($@)
    NUMBER="${#ARGS[@]}";
    if [ "$NUMBER" -eq "1" ]
    then

    myFile=${ARGS[0]}
    remoteFile=`getRemoteLocation $myFile`

    # 1. myPath = getPath( myFile ) will strip off the file name and return the path
    mkdir -p $(dirname "$myFile")

    # 2. cp srm:.../remoteFile myFile
    echo "srmcp -server_mode=passive $remoteFile file:///$myFile"
    srmcp -server_mode=passive $remoteFile file:///$myFile
    chmod 755 $myFile

    else
    echo "Example usage: getData \"\$TMPDIR/datadir/myfile.txt\""
    fi
}

putFile()
{
    ARGS=($@)
    NUMBER="${#ARGS[@]}";
    if [ "$NUMBER" -eq "1" ]
    then
    myFile=${ARGS[0]}
    remoteFile=`getRemoteLocation $myFile`
    echo "srmrm $remoteFile"
    srmrm $remoteFile
    echo "srmcp -server_mode=passive file:///$myFile $remoteFile"
    srmcp -server_mode=passive file:///$myFile $remoteFile
        returnCode=$?

        echo "srmcopy: ${returnCode}"

        if [ $returnCode -ne 0 ]
        then
            exit 1
        fi
    else
    echo "Example usage: putData \"\$TMPDIR/datadir/myfile.txt\""
    fi
}
```

Generated back-end independent script

```
//header
#MOLGENIS walltime=15:00 nodes=1 cores=4 mem=6
//tool management
module load bwa/0.5.8c_patched
//data management
getFile $WORKDIR/resources/hg19/indices/human_g1k_v37.fa
getFile $WORKDIR/groups/gcc/projects/cardio/run01/rawdata/
121128_SN163_0484_AC1D3HACXX_L8_CAACCT_1.fq.gz
//template of the actual analysis
bwa aln \
human_g1k_v37.fa 121128_SN163_0484_AC1D3HACXX_L8_CAACCT_1.fq.gz -t 4 \
-f 121128_SN163_0484_AC1D3HACXX_L8_CAACCT_1.bwa_align.human_g1k_v37.sai
//data management
putFile $WORKDIR/groups/gcc/projects/cardio/run01/results/
121128_SN163_0484_AC1D3HACXX_L8_CAACCT_1.bwa_align.human_g1k_v37.sai
```

Current developments

Pilots Dashboard

- During execution

run08@ui.grid.sara.nl (May 31, 2013 11:31:31 AM)

Active

Inactivate

Stop Submitting Pilots

Jobs generated	0	Jobs done	4
Jobs ready	2	Jobs failed	0
Jobs running	0		
Pilots submitted	17	Pilots started	10

- Workflow is completed

run08@ui.grid.sara.nl (May 31, 2013 11:31:31 AM)

Completed

Jobs generated	0	Jobs done	6
Jobs ready	0	Jobs failed	0
Jobs running	0		
Pilots submitted	21	Pilots started	12

Dash-board for jobs monitoring (work-in-progress)

Pilot dashboard

run05@ui.grid.sara.nl (May 30, 2013 3:43:51 PM)
Not active
Activate

Jobs generated	6	Jobs done	0
Jobs ready	0	Jobs failed	0
Jobs running	0		
Pilots submitted	0	Pilots started	0

run04@ui.grid.sara.nl (May 30, 2013 3:43:33 PM)
Active
Inactivate
Username Password Submit Pilots

Jobs generated	6	Jobs done	0
Jobs ready	0	Jobs failed	0
Jobs running	0		
Pilots submitted	0	Pilots started	0

run03@ui.grid.sara.nl (May 30, 2013 3:43:18 PM)
Active
Inactivate
Stop Submitting Pilots

Jobs generated	2	Jobs done	0
Jobs ready	4	Jobs failed	0
Jobs running	0		
Pilots submitted	0	Pilots started	0

run02@ui.grid.sara.nl (May 30, 2013 3:43:02 PM)
Not active
Activate
Resubmit failed jobs

Jobs generated	5	Jobs done	0
Jobs ready	0	Jobs failed	1
Jobs running	0		
Pilots submitted	0	Pilots started	0

run01@ui.grid.sara.nl (May 30, 2013 3:42:45 PM)
Completed

Jobs generated	0	Jobs done	6
Jobs ready	0	Jobs failed	0
Jobs running	0		
Pilots submitted	0	Pilots started	0

Enhancements and further steps

- What if not all parameters are known at the generation time
  - Run-time parameters passing to DB from previous steps (implemented)
- Advanced pilot management
  - Pilots re-using
- Better workflow visualization
  - Showing workflow elements and their properties

H. Byelas and M. Swertz, "Visualization of bioinformatics workflows for ease of understanding and design activities," *Proceedings of the BIOSTEC BIOINFORMATICS-2013 conference*, pp. 117–123, 2013.

Conclusion

Conclusion

- One protocol template style that is suitable for different back-ends
- Workflow tools deployment using module system
- Hidden in scripts data management
- Workflow execution using pilot jobs

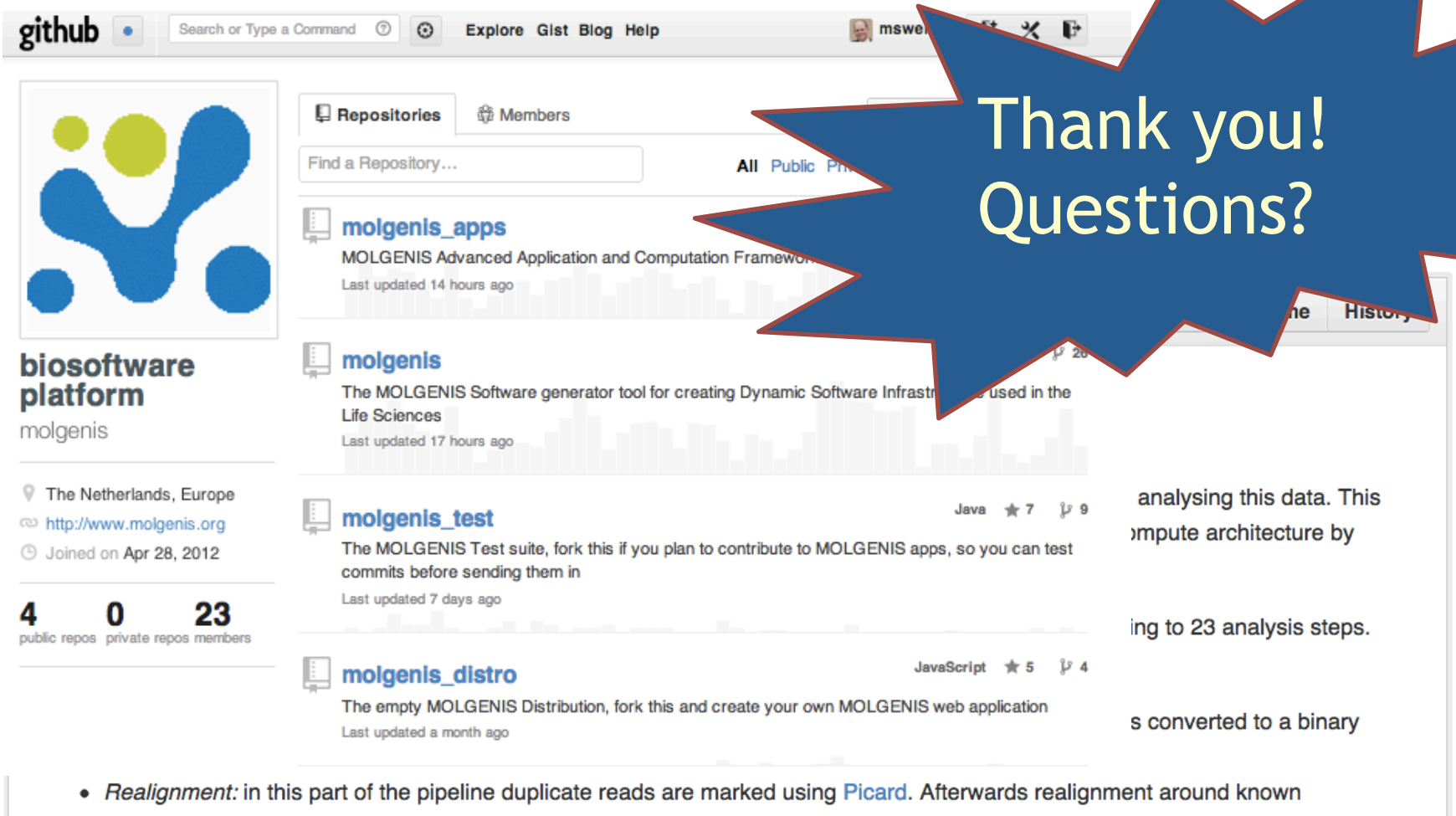
All available as open source

Fork me on GitHub

http://www.molgenis.org

http://www.molgenis.org/wiki/ComputeStart

h.v.byelas@gmail.com m.a.swertz@gmail.com



Thank you!
Questions?

nis