

# Setting up a Galaxy Instance as a Service

**Nikolay Vazov**

**Jochen Bick**

**Hans-Rudolf Hotz**

**You are given the task  
to set up a Galaxy instance for others  
(i.e. as a core service in your institute)  
and you are not really familiar  
with Galaxy.**

**this is not an ordinary training session**

**...more like a workshop, with presentations**

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**Hans-Rudolf Hotz**    '10 rules'

**Jochen Bick**            starting problems and experiences

**Nikolay Vazov**        how can we make simple  
things more complicated

...and a panel discussion at the end

***though we are flexible***

## **What this training session is not about:**

- writing tool wrappers
- how to use galaxy

**this is not an ordinary training session**

# '10 rules' for Setting up a Galaxy Instance as a Service

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Friedrich Miescher Institute for Biomedical Research  
Basel, Switzerland

6. July 2015

**some info about me:**



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**some info about me:**

## **Friedrich Miescher Institute**

**317 employees**

(incl. 95 PhD students, 99 Post Docs)

**Epigenetics**

(7 research groups)

**Cancer**

(9 research groups)

**Neurobiology**

(8 research groups)

### **Technology Platforms**

**Computational Biology** – Cell Sorting – Imaging and Microscopy – *C. elegans*

Functional Genomics – Histology – Mass Spectrometry – Protein Structure

- funded by the Novartis Research Foundation
- affiliated institute of Basel University

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**The Computational Biology platform is providing support for....**



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# The Computational Biology platform is providing support for....

the “average” lab scientist, using computers to:

draw plasmids  
do BLAST searches  
use Excel

the “modern” lab scientist, using computers to:

analyze NGS data  
with R/Bioconductor  
scripts

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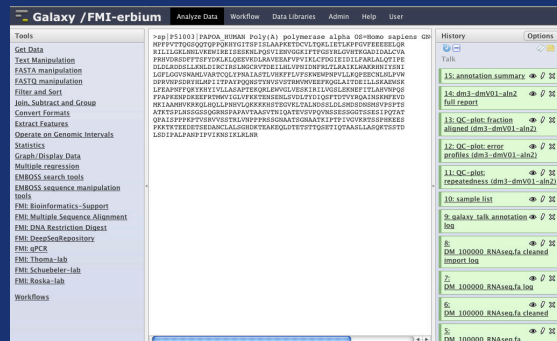
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<http://galaxyproject.org/>

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## **why are we using Galaxy**

- **open source software / no license fee**
- **it provides a standard set of Bioinformatics tools**
- **we can add our own scripts and tools**
- **in addition to the ~15 core developers, there is a huge world wide community**
- **a local installation is simple to set up**
- **it is flexible (you can adjust it to your needs)**



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*in use at the FMI since early 2008 (2007)*

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# Galaxy as a stepping stone

the “average” lab scientist, using computers to:

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with R/Bioconductor  
scripts

<http://galaxyproject.org/>

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# Galaxy as a teaching tool

*for learning Bioinformatics....*

the “average” lab scientist, using computers to:

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<http://galaxyproject.org/>

*... which is more than pressing a red button*

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# the FMI Galaxy Server

**single (dedicated) multi-core box**

- 16 cpu (four quad-core Intel X7350)
- 128GB RAM
- python 2.6.5
- 34 TB local attached storage

**connected to a MySQL database**

**external authentication**



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# the FMI Galaxy Server

## users

- 238 registered users
- 20 'heavy users'
- 30 'occasional users'

## jobs

- ~ 500 jobs/month
- NGS and MA analysis



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# disclaimer

**I will talk about my experience over the last 7 years**



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# disclaimer

**I will talk about my experience over the last 7 years**

- this might not be up-to-date**
- our Galaxy server is heavily adjusted to our need**



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# 10 rules for setting up a galaxy instance as a service



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# **10 rules for setting up a galaxy instance as a service**

**Check: what are you actually asked for**

**Check: what resources do you have / need**

**Follow the suggestion on the wiki**

**Set up only what you have been asked to**

**Know the tools you offer**

**Prevent data duplication**

**Set up 'reports'**

**Offer training**

**Keep the Galaxy software (and you) up to date**

**Adjust your Galaxy server to changes in requirements**



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# 1) Check: what are you actually asked for



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# 1) Check: what are you actually asked for

- talk to the person(s) who contacted you
  - why Galaxy ?



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# 1) Check: what are you actually asked for

- talk to the people who will use your service
  - using Galaxy for what?
  - do they know [use.galaxy.org](http://use.galaxy.org) ?
  - alternatives ?

# 1) Check: what are you actually asked for

- talk to the people who will use your service
  - using Galaxy for what?
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**define the tools**

# 1) Check: what are you actually asked for

- talk to the people who will use your service
  - using Galaxy for what?
  - do they know [use.galaxy.org](http://use.galaxy.org) ?
  - alternatives ?



**define the tools**



**use the toolshed**



**develop your own tools**

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# 1) Check: what are you actually asked for

- talk to potential users
  - what are they using now ?
  - do they know [use.galaxy.org](https://use.galaxy.org) ?
  - are there overlaps with the initial request ?

# **1) Check: what are you actually asked for**

- is Galaxy the right tool ?**
  - Galaxy is not Bioinformatician**
  - Galaxy might be too 'big' for the task**
  - Galaxy is not (yet) a LIMS**
- (- Galaxy is not good for 1000 of repeated jobs)**
  - another system is already in place**

# **1) Check: what are you actually asked for**

## **Visibility**

- internal web site**
- public web site**

## **Access**

- everybody can create an account**
- accounts are created for the users**
- external authentication**



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## 2) Check: what resources do you need / have ?



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## 2) Check: what resources do you need / have ?

- hardware
  - cpu / memory
  - storage
    - fast (local) storage
    - slow (network) storage

## **2) Check: what resources do you need / have ?**

- people / knowledge**
  - system administration for the Galaxy server**
  - Bioinformatics background**

## **select the option(s) which fits your requirements and resources**

- use Main (usegalaxy.org)
- use another public galaxy server  
*<https://wiki.galaxyproject.org/PublicGalaxyServers>*
- install galaxy locally
- use galaxy on the cloud
- get 'SlipStream' galaxy appliance

*<https://wiki.galaxyproject.org/BigPicture/Choices>*



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### 3) Follow the suggestion on the wiki



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read them first.....before you set up  
a production server

*<https://wiki.galaxyproject.org/Admin>*

*[https://wiki.galaxyproject.org/Admin/Config/  
Performance/ProductionServer](https://wiki.galaxyproject.org/Admin/Config/Performance/ProductionServer)*



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switching to a database server

SQLite  PostgreSQL

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### 3) Follow the suggestion on the wiki

make sure you are admin

*<https://wiki.galaxyproject.org/Admin/Interface>*



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### 3) Follow the suggestion on the wiki

remove 'deleted' datasets

*<https://wiki.galaxyproject.org/Admin/Config/Performance/Purge%20Histories%20and%20Datasets>*



set up a cron job

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### 3) Follow the suggestion on the wiki

setup 'Trackster'

*<https://wiki.galaxyproject.org/VisualizationSetup>*



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### **3) Follow the suggestion on the wiki**

**check other installations:**

**<https://wiki.galaxyproject.org/Community/Deployments>**

**Galaxy Community Log Board:**

**(a place to share how you addressed a particular task)**

**<https://wiki.galaxyproject.org/Community/Logs>**

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### 3) Follow the suggestion on the wiki

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**Galaxy Community Log Board:**

(a place to share how you addressed a particular task)

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and add your stuff as well

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## 4) Set up only what you have been asked to



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## **4) Set up only what you have been asked to**

**.....at least in the beginning:  
don't confuse your clients with too many tools**



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## 4) Set up only what you have been asked to

.....at least in the beginning:  
don't confuse your clients with too many tools

offer group/user specific tools

*<https://wiki.galaxyproject.org/UserDefinedToolboxFilters>*

*<https://wiki.galaxyproject.org/Admin/Config/Access%20Control>*



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good for testing

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## **4) Set up only what you have been asked to**

**.....but make sure you have:**

**production server / development server**



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## **4) Set up only what you have been asked to**

**.....but make sure you have:**

**production server / development server**

**and the production server backed-up  
(including the database server)**



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## 5) Know the tools you offer



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## 5) Know the tools you offer

First, make sure you know how to use galaxy

*<https://wiki.galaxyproject.org/Learn>*



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## 5) Know the tools you offer

First, make sure you know how to use galaxy

*<https://wiki.galaxyproject.org/Learn>*

Second, understand the tools you offer

- can you execute them on the command line

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## 6) Set up 'reports'



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## 6) Set up 'reports'

*<https://wiki.galaxyproject.org/Admin/UsageReports>*



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## 6) Set up 'reports'

it is a second web site



## 6) Set up 'reports'

Today's jobs

All unfinished jobs

Jobs per tool

Jobs per user

User disk usage





## 6) Set up 'reports'

....learn about the database



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## 6) Set up 'reports'

....learn about the database:

- execute queries which are not covered by 'reports'



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## 6) Set up 'reports'

....learn about the database:

- execute queries which are not covered by 'reports'
- *fix* the database

## 6) Set up 'reports'

....learn about the database:

- execute queries which are not covered by 'reports'

- *fix the database*

**I have not recommended this to you**

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## 7) Prevent data duplication



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## 7) Prevent data duplication

a quote from a bioinformatics mailing list:

*“We don’t want to use Galaxy because it produces to much data”*



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## 7) Prevent data duplication

a quote from a bioinformatics mailing list:

*“We don’t want to use Galaxy because it produces too much data”*

**Galaxy can help you reducing the storage requirements**

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## 7) Prevent data duplication

use 'Data Libraries'

*<https://wiki.galaxyproject.org/Admin/DataLibraries>*

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## 7) Prevent data duplication

use 'Data Libraries'

*<https://wiki.galaxyproject.org/Admin/DataLibraries>*

- *'Link to files without copying into Galaxy,*
- *enable 'Upload files from filesystem paths'*

*[https://wiki.galaxyproject.org/Admin/  
DataLibraries/UploadingLibraryFiles](https://wiki.galaxyproject.org/Admin/DataLibraries/UploadingLibraryFiles)*

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## 7) Prevent data duplication

promote history sharing

promote Galaxy 'pages'



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## 7) Prevent data duplication

promote history sharing

promote Galaxy 'pages'

allow user to see the full path of datasets  
( `expose_dataset_path = True` )

## 7) Prevent data duplication

use 'external' data

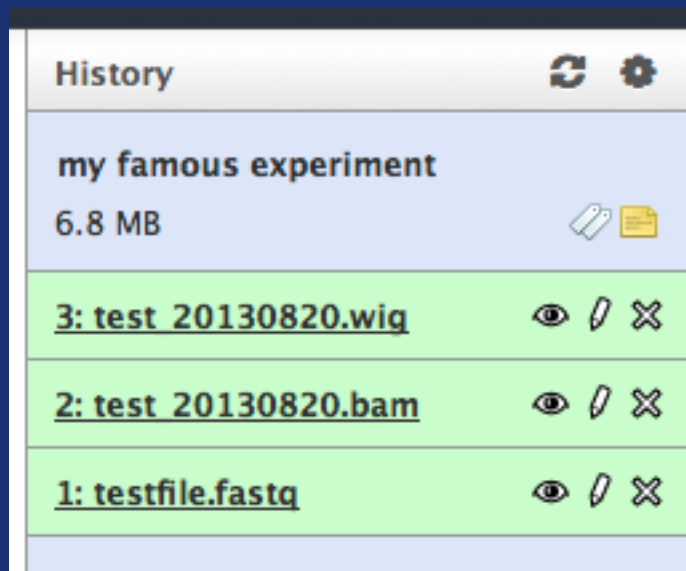


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## 7) Prevent data duplication

a simple NGS analysis:

fastq file → BAM file → wig file



The screenshot shows a 'History' window with a list of files. The first entry is 'my famous experiment' with a size of '6.8 MB' and a tag icon. Below it are three files: '3: test 20130820.wig', '2: test 20130820.bam', and '1: testfile.fastq'. Each of these three files has an eye icon, a pencil icon, and a close (X) icon to its right.

History	
my famous experiment 6.8 MB	
<u>3: test 20130820.wig</u>	
<u>2: test 20130820.bam</u>	
<u>1: testfile.fastq</u>	

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## 7) Prevent data duplication

storing data outside of Galaxy:

- raw data (fastq) files are in central/group specific repositories
- the Galaxy 'aligner' knows the location of the fastq files and stores the BAM file again in a group specific repository and creates just a 'log file' as history item
- the Galaxy 'count' tool uses the 'log file' as input

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storing data outside of Galaxy:

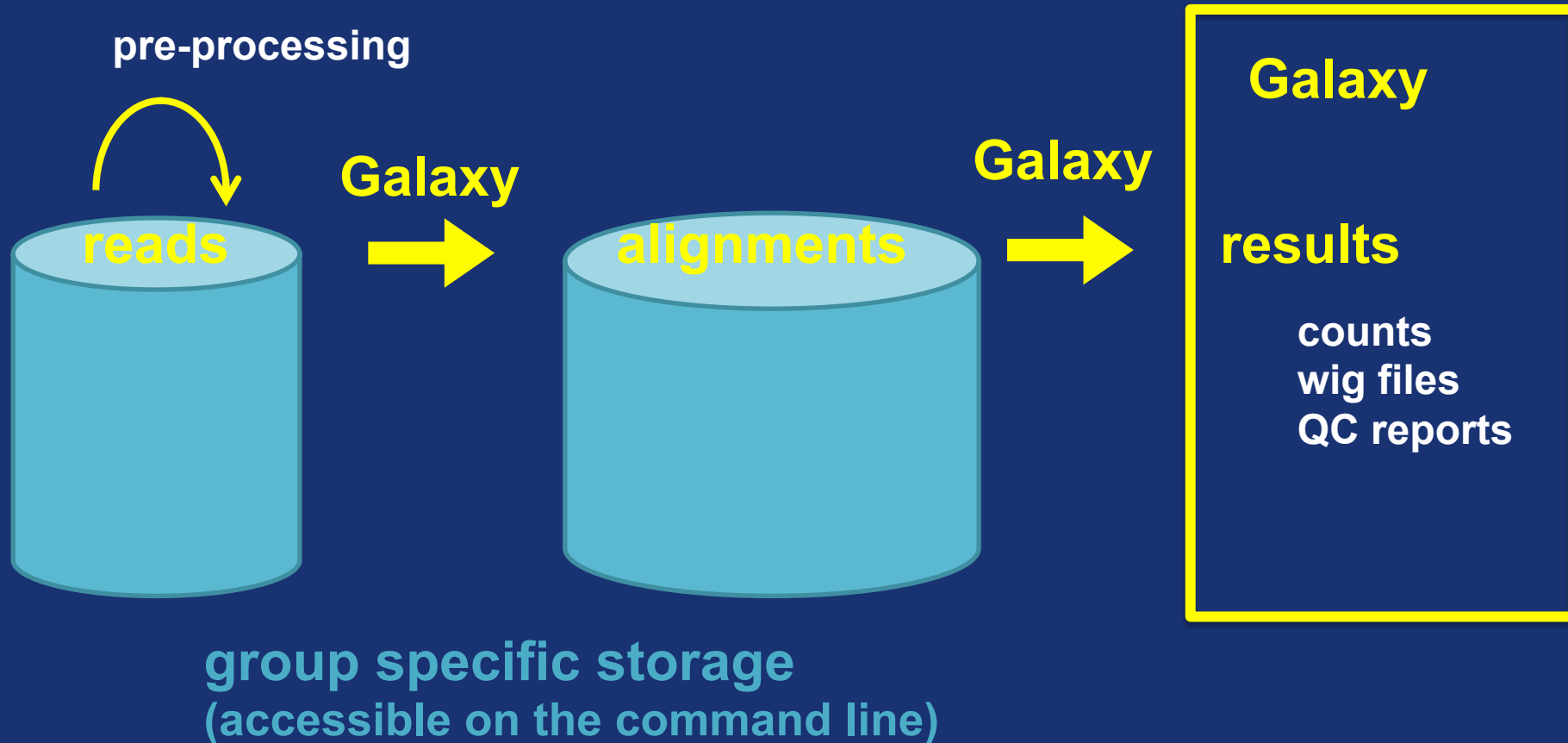
- raw data (fastq) files are in central/group specific repositories
- the Galaxy 'aligner' knows the location of the fastq files and stores the BAM file again in a group specific repository and creates just a 'log file' as history item
- the Galaxy 'count' tool uses the 'log file' as input

**this is not really best (Galaxy) practice, but it allows to collaborate with non-Galaxy users ....and reproducibility is still guaranteed**

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## 7) Prevent data duplication



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## 8) Offer training



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## 8) Offer training

individual training

run training courses

*<https://wiki.galaxyproject.org/Teach>*

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 stress testing for the server

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## 9) Keep your server (and you) up to date



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## 9) Keep your server up to date

unless you have a very good reason, make sure you are running the latest (or at least a recent) code version

- it is easier for others to help you
- the reported issue might already be fixed in the current release



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## 9) Keep your server up to date

unless you have a very good reason, make sure you are running the latest (or at least a recent) code version

- it is easier for others to help you
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find a balance between updates (with new or different features) and continuity

*we do 3 update per year*

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## 9) Keep your server up to date

doing an update is easy



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## 9) Keep your server up to date

doing an update is easy ....most of the time



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## 9) Keep your server up to date

doing an update is easy ....most of the time

- announce the down time one week in advance
- install a new server
- update the 'new server' from last time
- update the development server
- update the production server



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## 9) Keep your server up to date

doing an update is easy ....most of the time

- announce the down time one week in advance
- install a new server
- update the 'new server' from last time
- update the development server
- update the production server

***goal: minimize the down time***

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## 9) Keep yourself up to date



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## 9) Keep yourself up to date

- read the DevNewsBriefs

<https://wiki.galaxyproject.org/DevNewsBriefs>

- follow the mailing lists

<https://wiki.galaxyproject.org/MailingLists>

- join the "Galaxy Admins"

<https://wiki.galaxyproject.org/Community/GalaxyAdmins>

BOF: Tuesday, 7 July, 18:20 Franklin Room, JICCC

- go to GCC2016

- form regional communities



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## 9) Keep yourself up to date

take the time to look at new features



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## 10) Adjust your Galaxy server to changes in requirements



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## 10) Adjust your Galaxy server

you don't need a cluster to set up different queues



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## 10) Adjust your Galaxy server

you don't need a cluster to set up different queues



`job.conf.xml`

`job_conf.xml.sample_advanced`

*<https://wiki.galaxyproject.org/Admin/Config/Jobs>*

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## 10) Adjust your Galaxy server

you can change the hardware



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## 10) Adjust your Galaxy server

you can change the hardware, as long as you keep the 'database/' directory and the SQL DB in sync.



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## 10) Adjust your Galaxy server

you can change the hardware, as long as you keep the 'database/' directory and the SQL DB in sync.

### old recipe:

- make a copy of the SQL DB
- copy the complete galaxy directory to the new server (make sure you keep the path)
- point the new galaxy server to the MySQL DB copy and start it
  - > due to the higher Python version, news eggs were downloaded
  - > all python code was re-compiled
- test the new server (while the old one is still in use)
- stop the old server
- rsync ~/galaxy\_dist/database/files/
- point the new galaxy server to the 'live' MySQL DB and re-start it



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## 10) Adjust your Galaxy server

you can change the database server



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## 10) Adjust your Galaxy server

you can change the database server

MySQL → PostgreSQL

## 10) Adjust your Galaxy server

you can change the database server

MySQL → PostgreSQL

recipe will be posted on

*<https://wiki.galaxyproject.org/Community/Logs>*

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# Acknowledgment

## *Computational Biology*

- Michael Stadler / Christian Hundsruicker

## *Functional Genomics*

- Tim Roloff

## *IT Support*

- Stefan Grzybeck

***....and all the people from the “Galaxy”***

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