

Secure and practical computational reproducibility in the life sciences

Bioconda, BioContainers, Galaxy
& the de.NBI Galaxy-Docker-Technology

Rolf Backofen, Björn Grüning & The RBC Team

Center for RNA Bioinformatics (RBC)



Rolf Backofen



Uwe
Ohler



Nikolaus
Rajewksy



Peter Stadler

RBC



Björn
Grüning

Altuna
Akalin

de.NBI-epi

Partner Projects



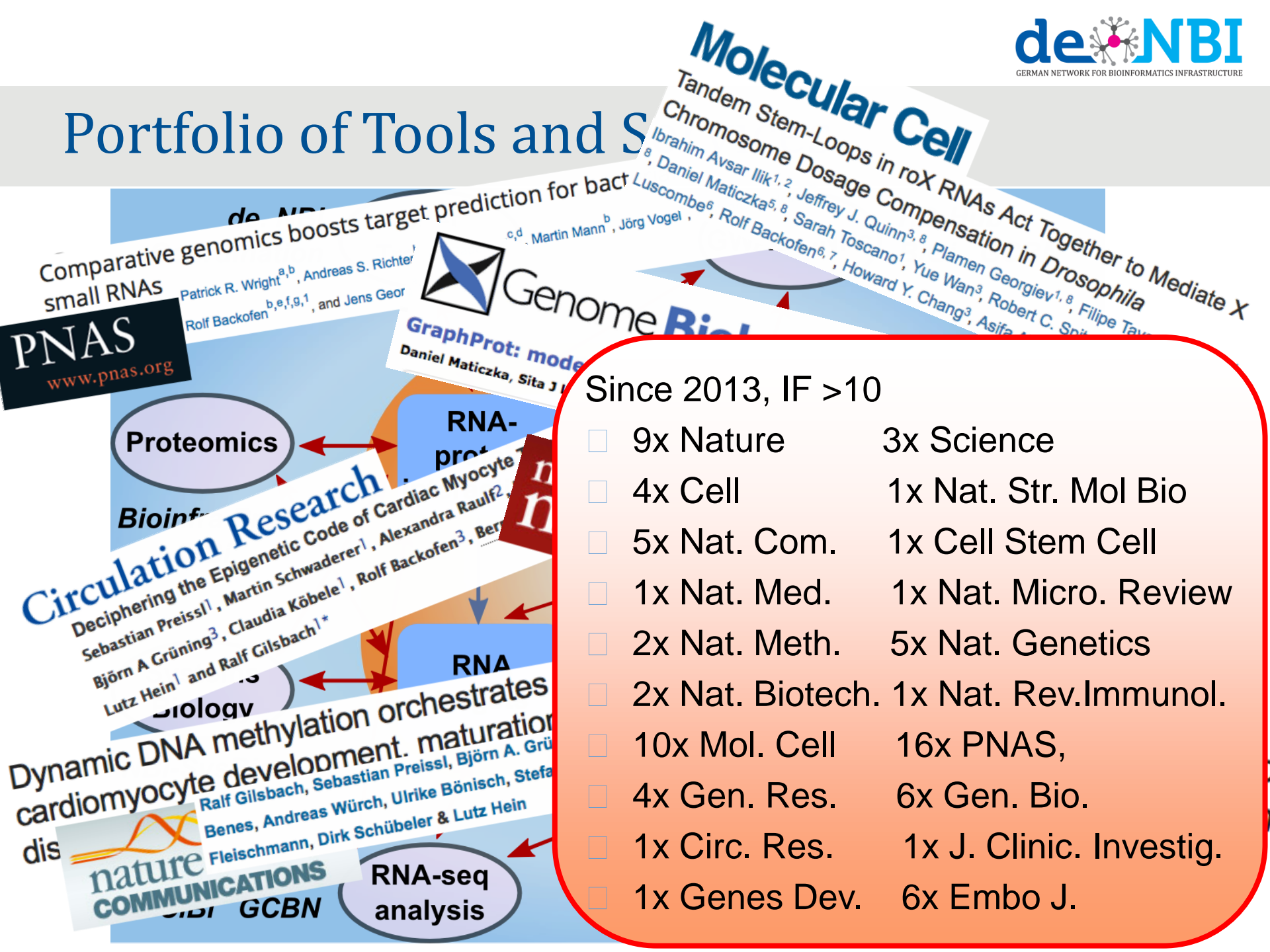
Wolfgang
Hess

Steve
Hoffmann

Olaf
Wolkenhauer

de.STAIR

Portfolio of Tools and S



Since 2013, IF >10

- 9x Nature
- 4x Cell
- 5x Nat. Com.
- 1x Nat. Med.
- 2x Nat. Meth.
- 2x Nat. Biotech.
- 10x Mol. Cell
- 4x Gen. Res.
- 1x Circ. Res.
- 1x Genes Dev.
- 3x Science
- 1x Nat. Str. Mol Bio
- 1x Cell Stem Cell
- 1x Nat. Micro. Review
- 5x Nat. Genetics
- 1x Nat. Rev.Immunol.
- 16x PNAS,
- 6x Gen. Bio.
- 1x J. Clinic. Investig.
- 6x Embo J.

Service

- knowledge transfer in RNA bioinformatics



- we can't do all analysis ourselves!
- solutions:
 - **Galaxy**
 - *standard workflows*
 - *FR server: 600+ users*
 - **virtualization**
 - *distribute computation*
 - **training, training, training**

Galaxy: Accessible Research

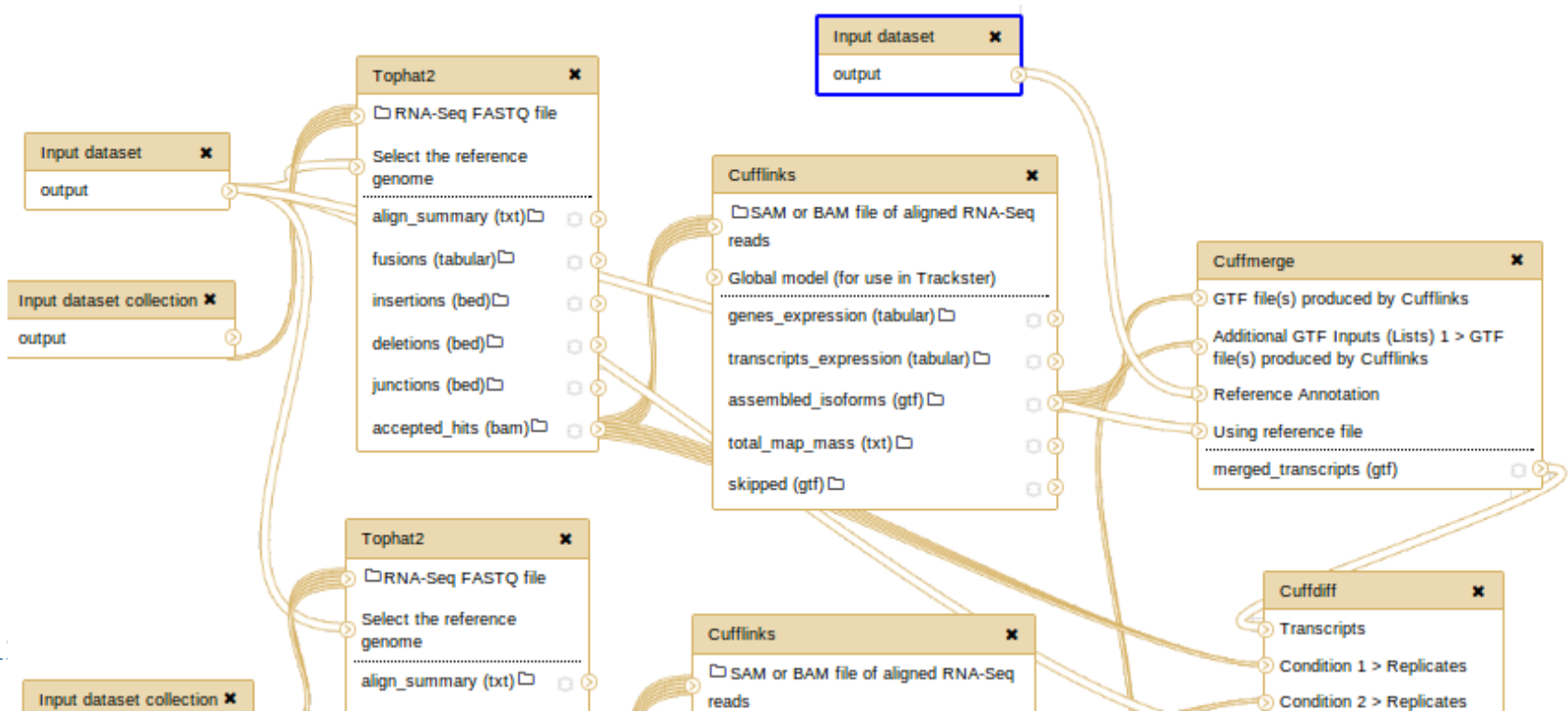
□ reproducibility

- experimental details
- transparency

□ scalable

□ easy deployment

- tools available to users
- minimal installation overhead



What is Galaxy?

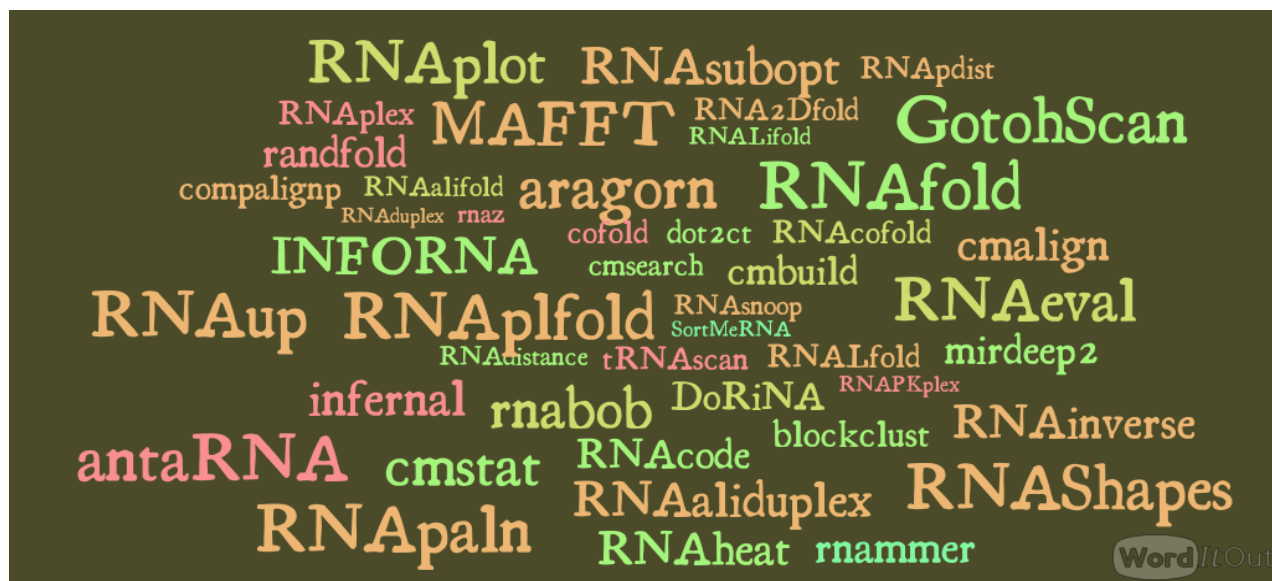
- Omics data analysis platform
- Accessible via normal web browser
- Every single step is recorded and reproducible
- 5000 citations so far
- 150.000 known user

The screenshot displays the Galaxy web interface. The top navigation bar includes 'Analyze Data', 'Workflow', 'Shared Data', 'Visualization', 'Cloud', 'Help', and 'User'. A 'Tools' sidebar on the left lists various categories like 'Get Data', 'Send Data', 'Text Manipulation', etc. The main workspace shows the 'Unified Genotyper (version 0.0.6)' tool configuration. The 'Choose the source for the reference list' dropdown is set to 'History'. Under 'BAM files', 'BAM file 1' is selected with the file '56: (hidden) Map with BWA for Illumina on data 2, data 7, and data 3: mapped reads'. The 'Using reference file' dropdown is set to '3: AgamP3 assembly'. The 'Binding for reference-ordered datas' dropdown is set to 'BOTH'. The 'Genotype likelihoods calculation model to employ' dropdown is set to 'BOTH'. Two input fields for confidence thresholds are both set to '30.0'. The right-hand 'History' panel shows a list of previous jobs, including 'Infravec: imported from Dan Lawson', '89: AgamP3.7 GTF for mat', '86: Pasted Entry', '85: SAM-to-BAM on data 3 and data 57: converted BAM', '81: Filter on data 67', '80: 2Lfa', '79: 2L arm coord', and '69: Unified Genotyper on data 3 and data 56 (log)'. The '69' job is selected, showing details like '340 lines' and 'format: txt, database: ?'.

Galaxy RNA Workbench

- already integrated: >4000 tools, ~800 by RBC
 - *We are one of 3 groups worldwide with direct Galaxy commit*

- RNA-specific tools and packages: **60+**



- RBC-specific:
 - *Vienna RNA package, doRiNA, Freiburger RNA Tools*

Services of Freiburg Galaxy Server

Workflows

General

- Build, Test, Use, Share, FAIR

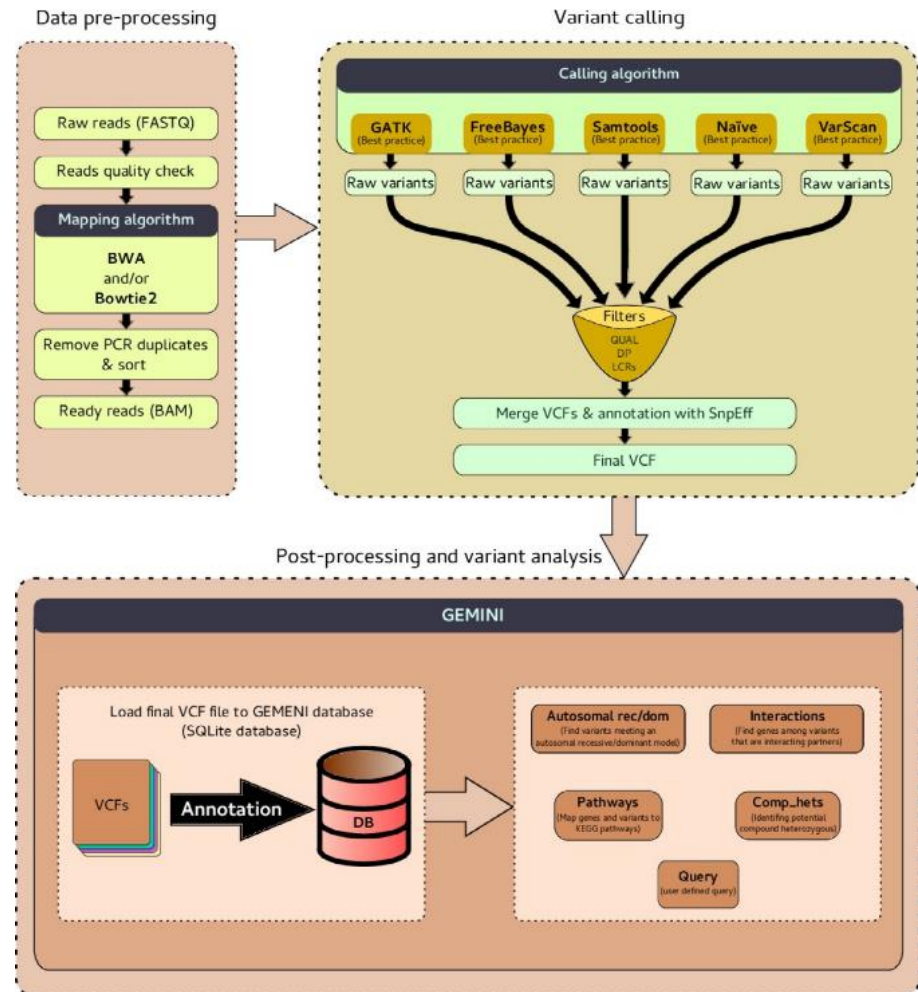
RNA-seq

- Quality Control
- Differential Expression Analysis

ChIP-seq, MethylC-seq

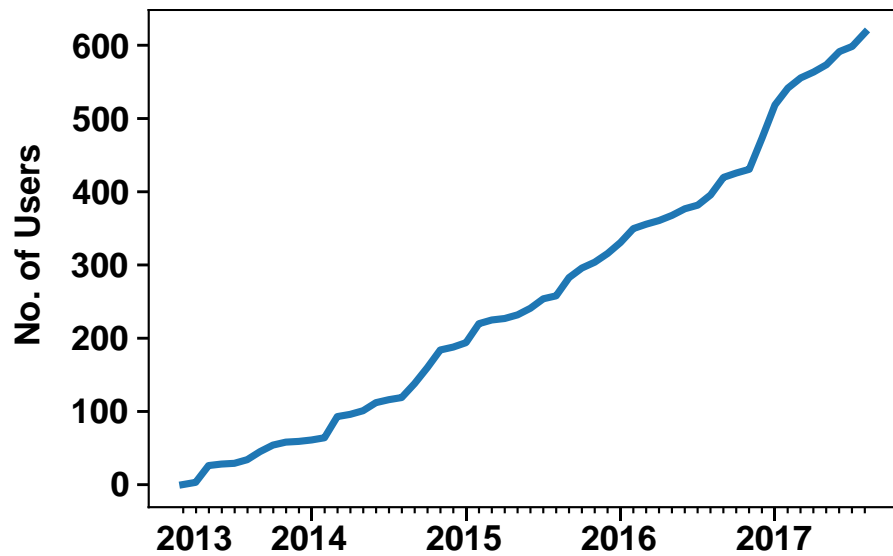
Additionally

- Exome-seq
- Proteomics, Metabolomics
- Imaging, Textmining

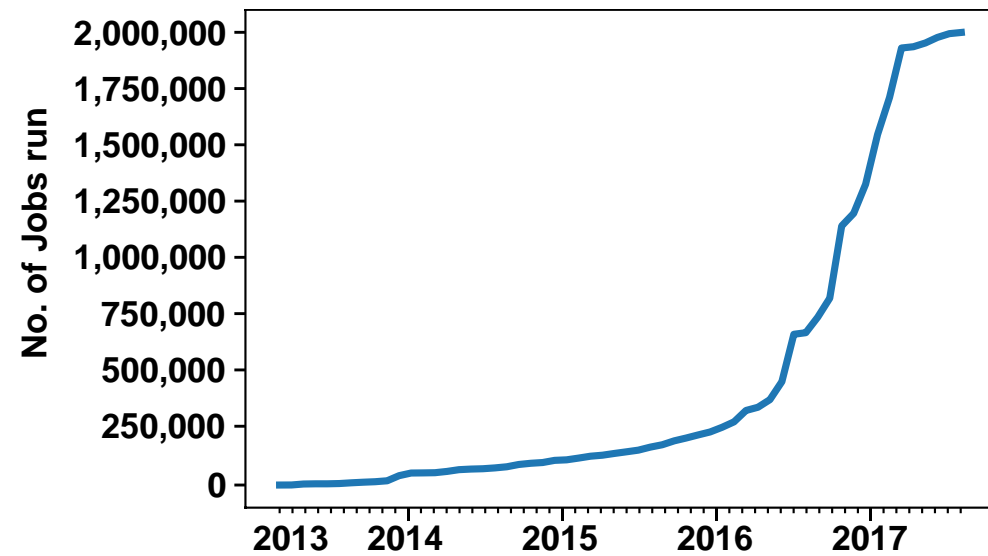


Impact Measurements

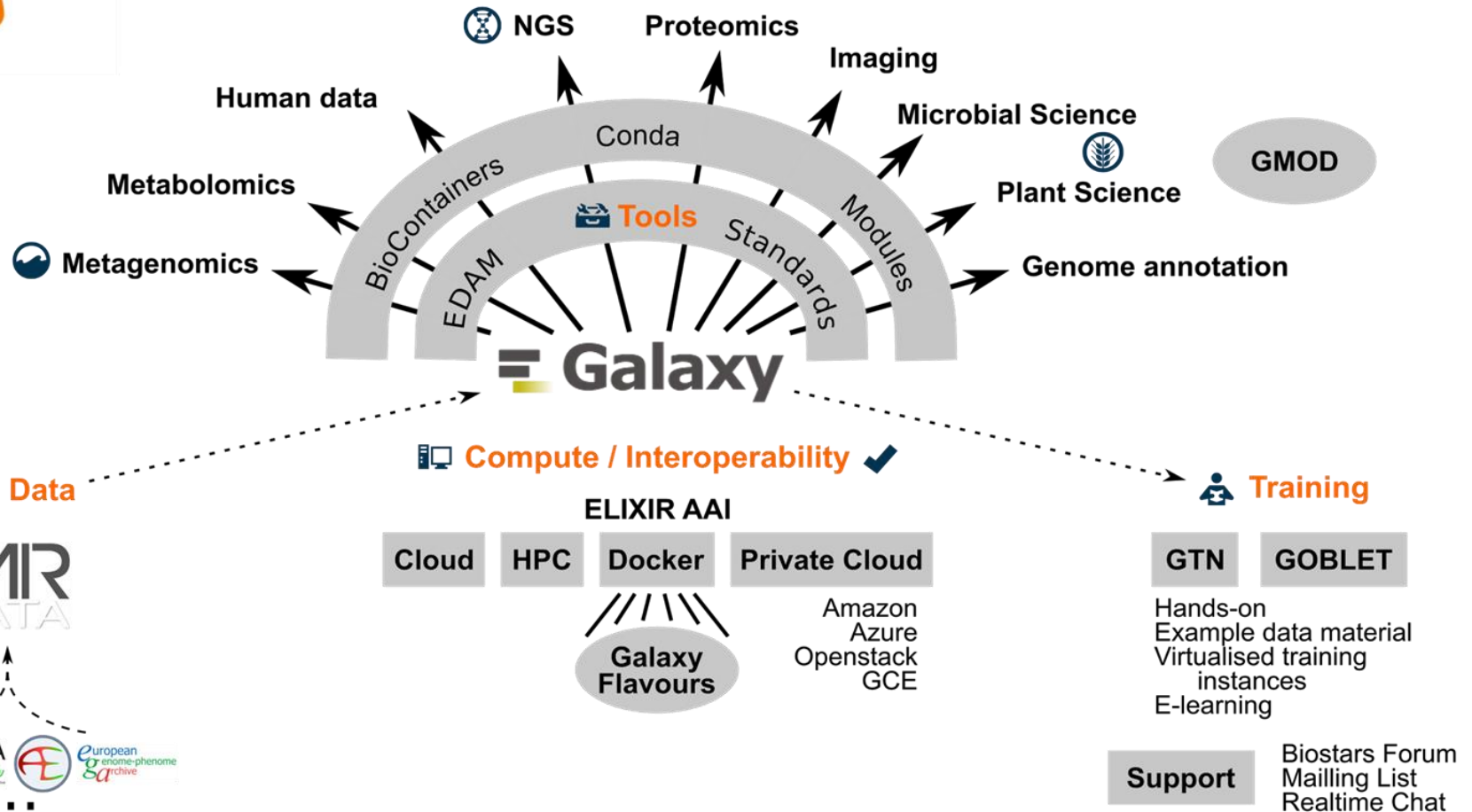
- users



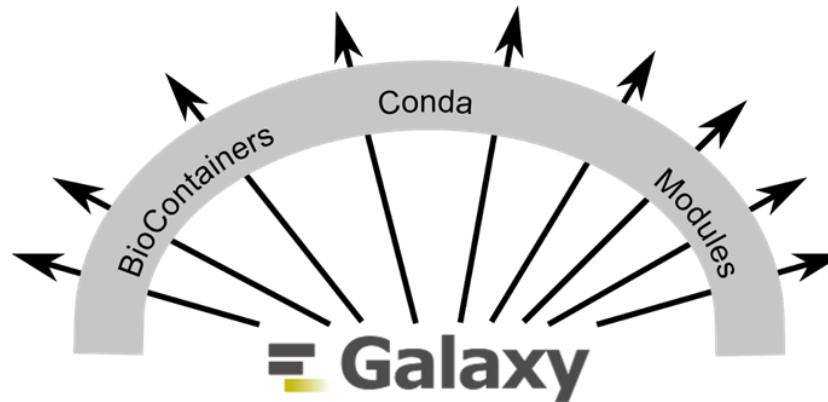
- jobs run



Building a sustainable virtualized infrastructure



Building a secure virtualized infrastructure



- Isolate every single tool
 - from all other data
 - from other tools
 - from the Operating System
- Isolate the analysis workbench

adjustable reproducibility and security

Least reproducible → Most reproducible

www.icorexperience.com

Easy ← Hard / Impossible ?

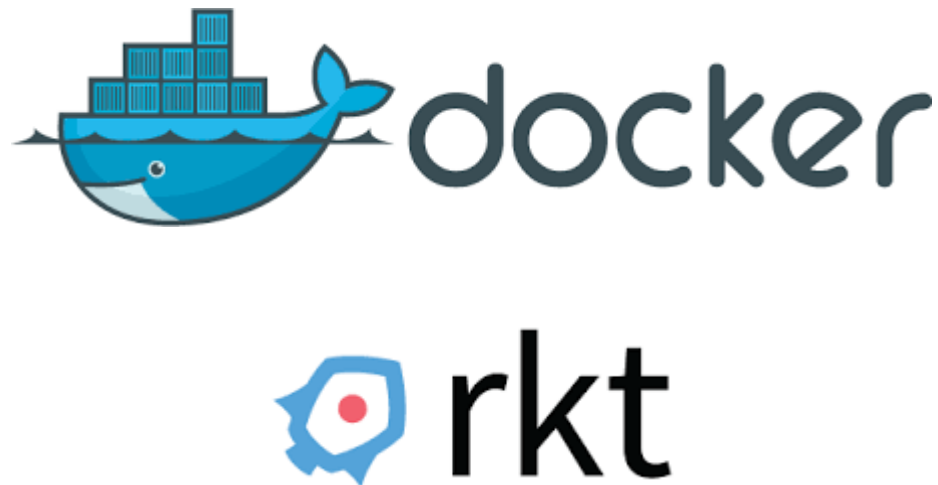


Less secure → Most secure

www.icorexperience.com

Easy ← Hard / Impossible ?

Linux Containers for advanced isolation



If there is no standard*, embrace new technologies and make them interconvertible.

* Open Container Initiative (OCI) has released 1.0 of the container and runtime specification 3 days ago.

Sustainable community-based infrastructure

BIOCONDA®

provides software for biomedical research.

- 14,400 commits on GitHub
- 287 contributors
- >2,700 packages



provides system-agnostic executable environments for bioinformatics tools

- Uses Docker & rkt
- >2,800 Images
- Automatic builds from BioConda



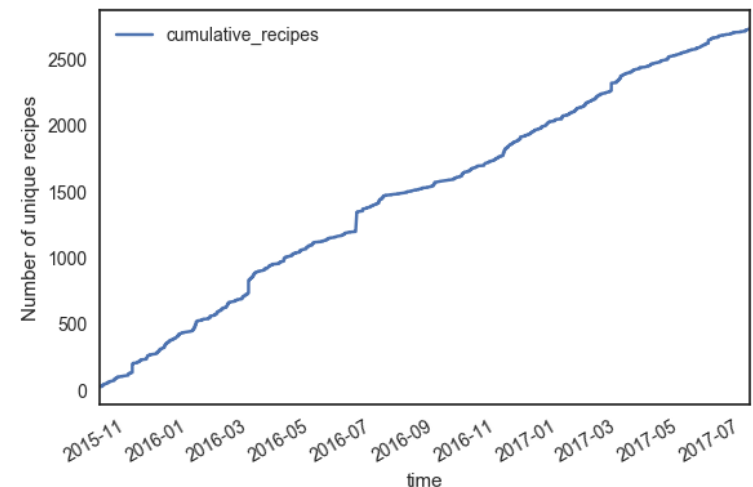
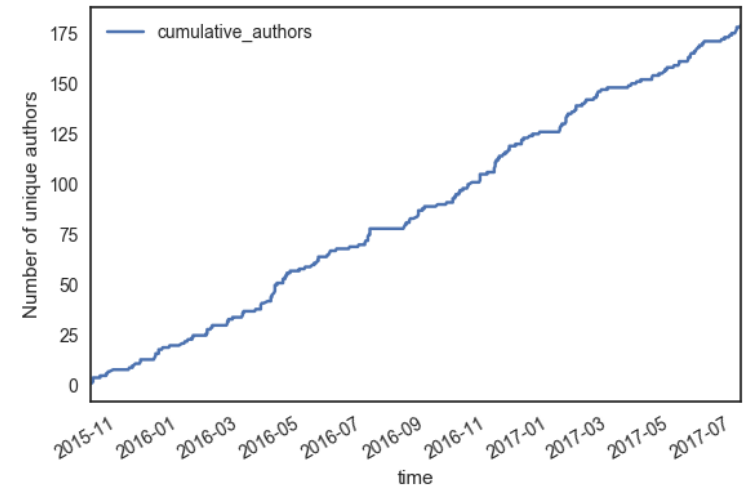
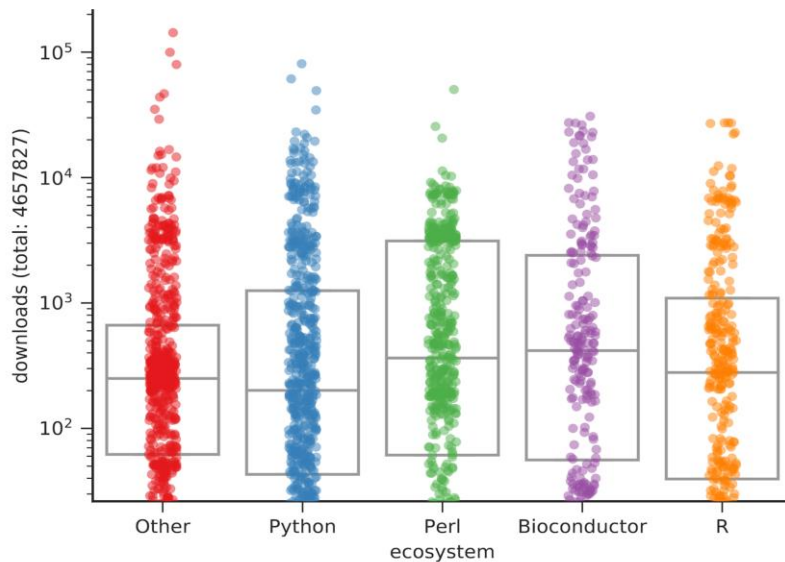
Galaxy is an open web-based platform for data intensive research

- 29,500 commits
- 163 contributors
- RBC is one of the biggest instances

Our achievement: Cloud-Ready, all integrated into Galaxy

Biocontainers

- build out of **conda** package
- all tested automatically
- bioconda-utils / galaxy-lib



Community



330 Contributors

6200 merged PR

in 2 years

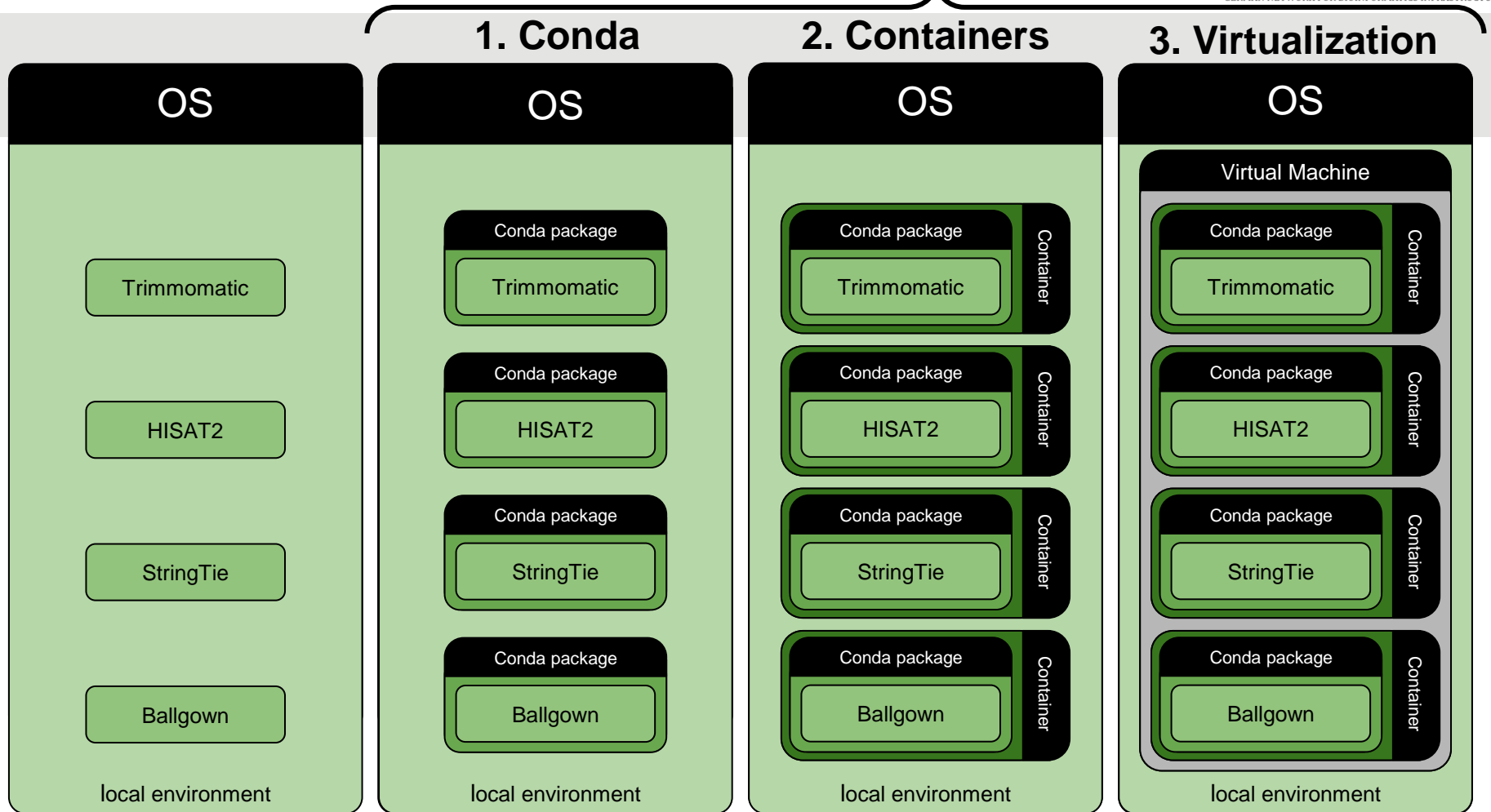
www.iconexperience.com

www.iconexperience.com



www.iconexperience.com

www.iconexperience.com



1. Conda

2. Containers

3. Virtualization

OS

OS

OS

OS

Trimmomatic

Conda package

Trimmomatic

Conda package

Trimmomatic

Container

Virtual Machine

Conda package

Trimmomatic

Container

HISAT2

Conda package

HISAT2

Conda package

HISAT2

Container

Conda package

HISAT2

Container

StringTie

Conda package

StringTie

Conda package

StringTie

Container

Conda package

StringTie

Container

Ballgown

Conda package

Ballgown

Conda package

Ballgown

Container

Conda package

Ballgown

Container

local environment

local environment

local environment

local environment

Least reproducible /
secure

Most reproducible /
secure

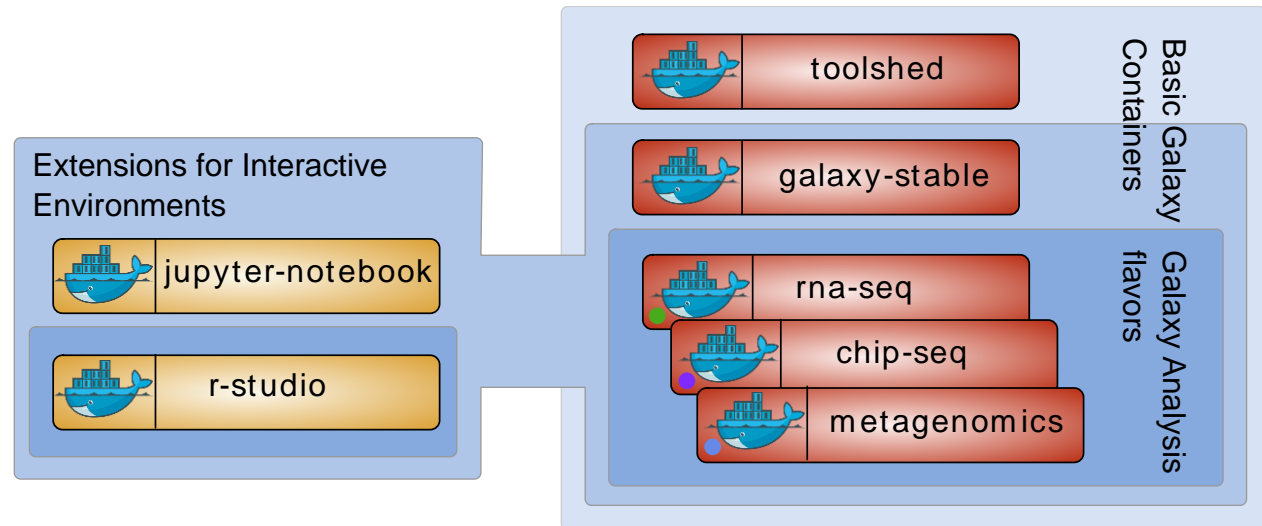
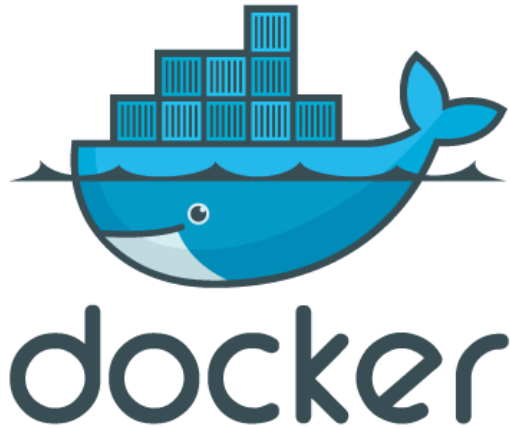
```
> git clone hisat2
> make
> sudo make install
> hisat2 --version
```

```
> conda install hisat2
> hisat2 --version
```

```
> docker run --rm
quay.io/biocontainers/
hisat2 --version
```

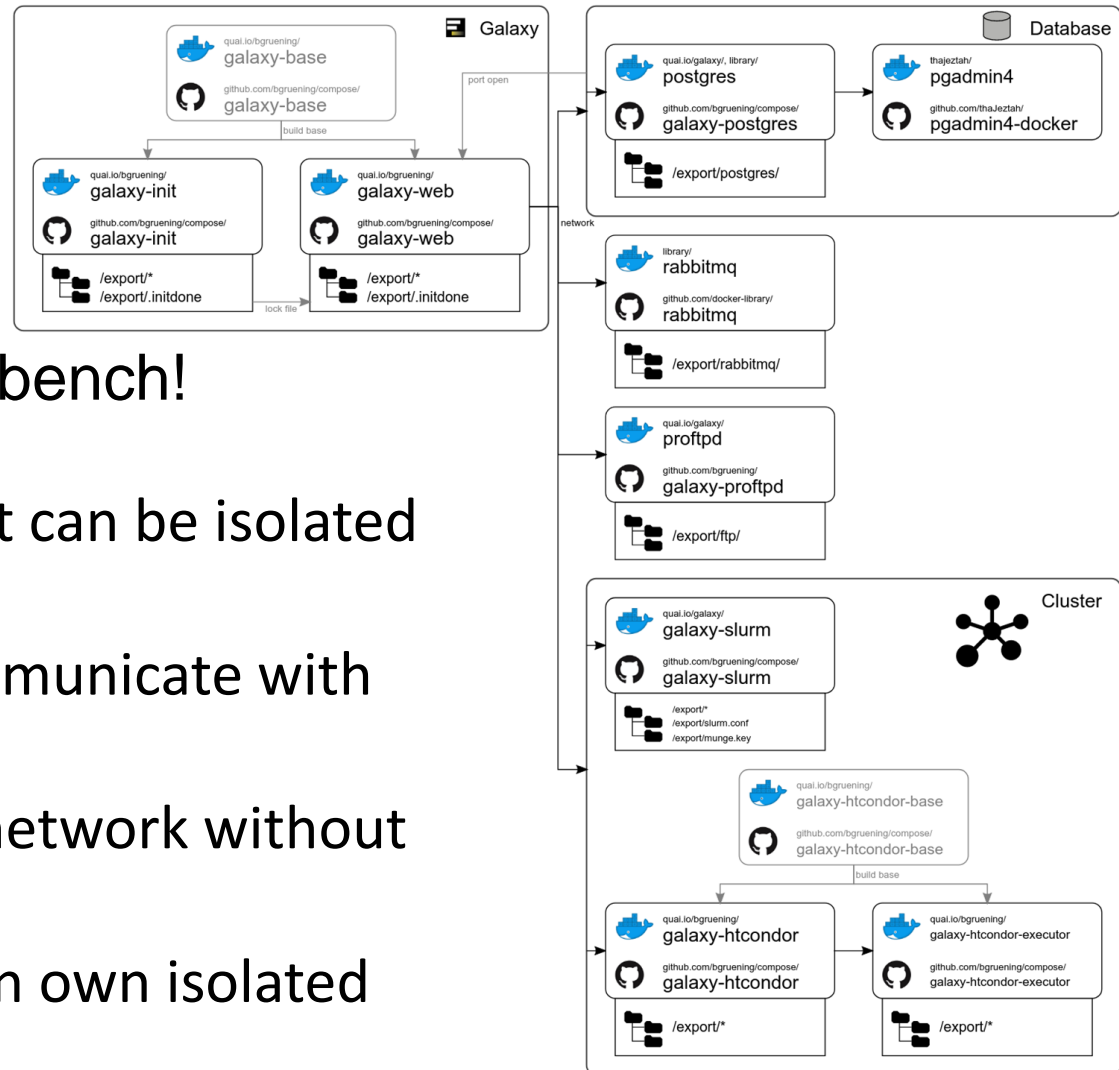

Galaxy in Docker

- Idea: tools to data, not data to tools -> virtualization



- drag & drop based Galaxy flavor generator
- Widely used: >28.000 downloads, ELIXIR (Tjenester for Sensitive Data 2.0 Norway), Cancer Center Amsterdam ...

Galaxy in Docker: Microservices

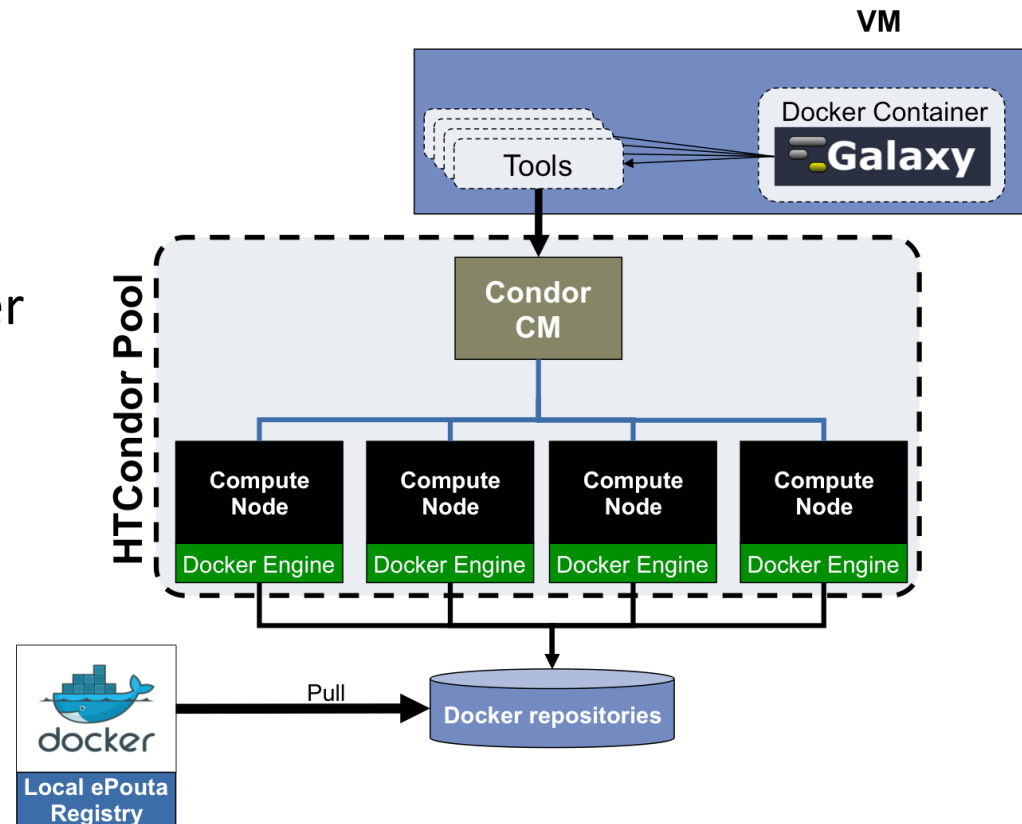


Isolate the analysis workbench!

- Every single component can be isolated and hardened
- Microservices that communicate with each other
- Can run in an isolated network without Internet
- executes analysis jobs in own isolated containers

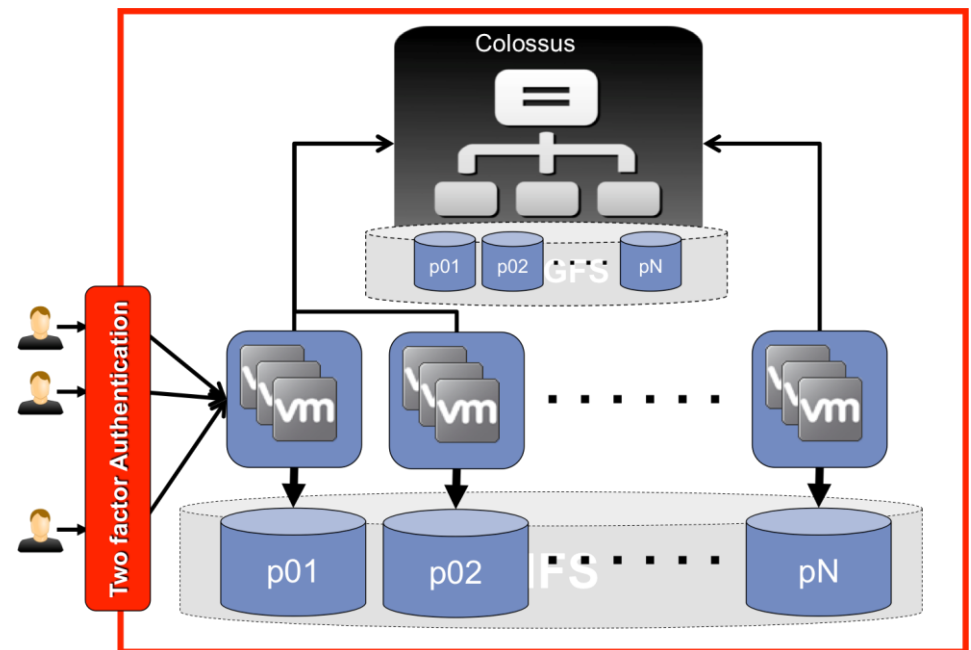
Real world deployments with sensitive data: Version 1

- central Galaxy server
- job submission to a hardened HTCondor pool
- Galaxy server runs in Docker
- every single job runs in Docker
- every job is isolated from all other data
- one job has only read access to the input data it needs
- entire stack can run in an isolated network

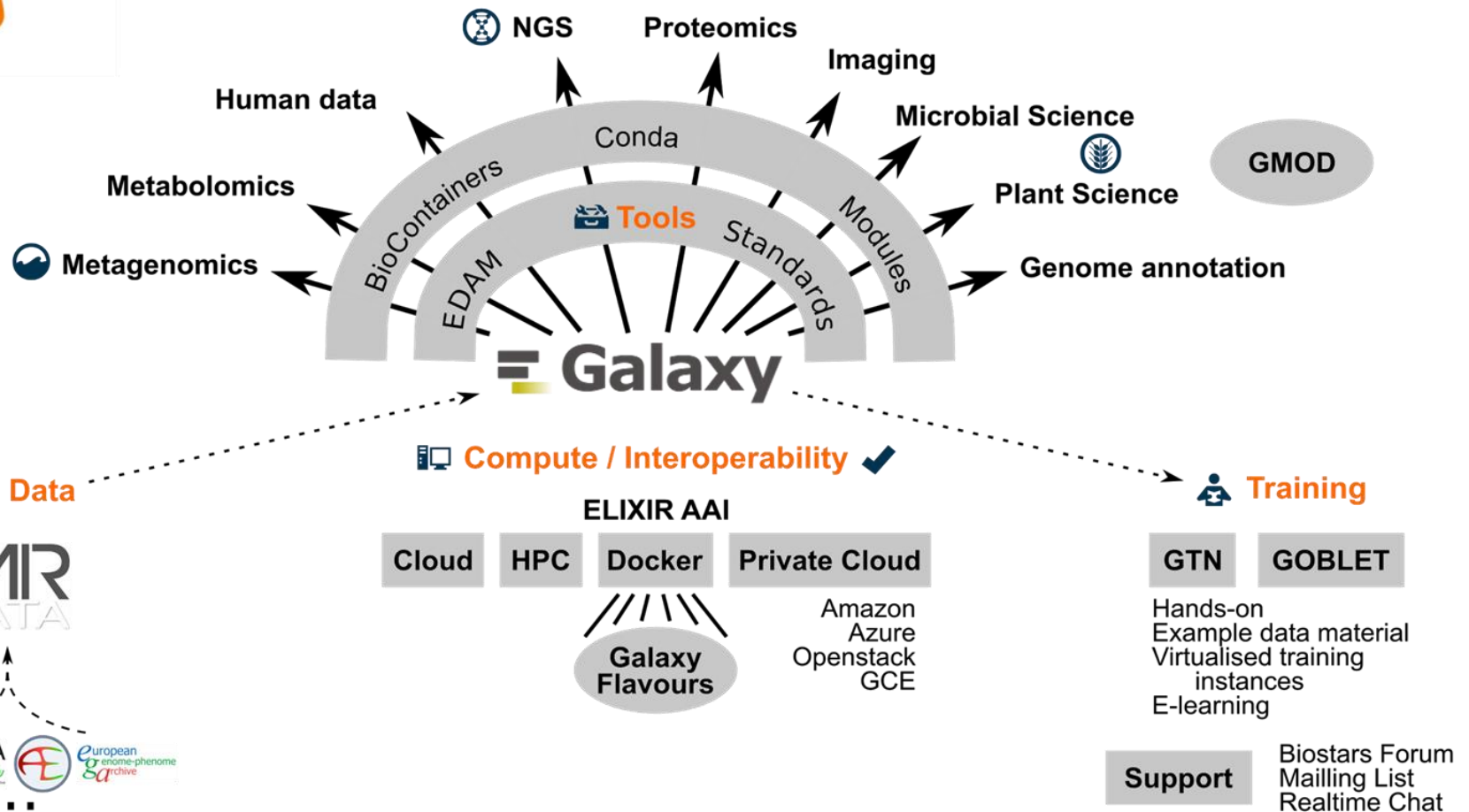


Real world deployments with sensitive data: Version 2

- 2 factor Authentication into virtual machines (VM)
- VMs are isolated
- every VM starts its own Galaxy instance
- data is saved encrypted to the local network
- Users can not interact with each other (share workflows, histories etc ...)
- every VM can run Version 1 as well



Building a sustainable infrastructure





bioRxiv
beta
THE PREPRINT SERVER FOR BIOLOGY

New Results

Practical computational reproducibility in the life sciences

Björn Grüning, John Chilton, Johannes Köster, Ryan Dale, Jeremy Goecks, Rolf Backofen, Anton Nekrutenko, James Taylor

doi: <https://doi.org/10.1101/200683>

This article is a preprint and has not been peer-reviewed [what does this mean?].



bioRxiv
beta
THE PREPRINT SERVER FOR BIOLOGY

New Results

Bioconda: A sustainable and comprehensive software distribution for the life sciences

Björn Grüning, Ryan Dale, Andreas Sjödin, Jillian Rowe, Brad A. Chapman, Christopher H. Tomkins-Tinch, Renan Valieris, The Bioconda Team, Johannes Köster

doi: <https://doi.org/10.1101/207092>

This article is a preprint and has not been peer-reviewed [what does this mean?].



bioRxiv
beta
THE PREPRINT SERVER FOR BIOLOGY

HOME |
| CHAN

Search

New Results

Community-driven data analysis training for biology

Bérénice Batut, Saskia Hiltmann, Andrea Bagnacani, Dannon Baker, Vivek Bhardwaj, Clemens Blank, Anthony Bretaudeau, Loraine Guéguen, Martin Čech, John Chilton, Dave Clements, Olivia Doppelt-Azeroual, Anika Erxleben, Mallory Freeberg, Simon Gladman, Youri Hoogstrate, Hans-Rudolf Hotz, Torsten Houwaart, Pratik Jagtap, Delphine Larivière, Gildas Le Corguillé, Thomas Manke, Fabien Mareuil, Fidel Ramirez, Devon Ryan, Florian Sigloch, Nicola Soranzo, Joachim Wolff, Pavankumar Videm, Markus Wolfen, Aisanjiang Wubuli, Dilmurat Yusuf, Rolf Backofen, Anton Nekrutenko, Björn Grüning

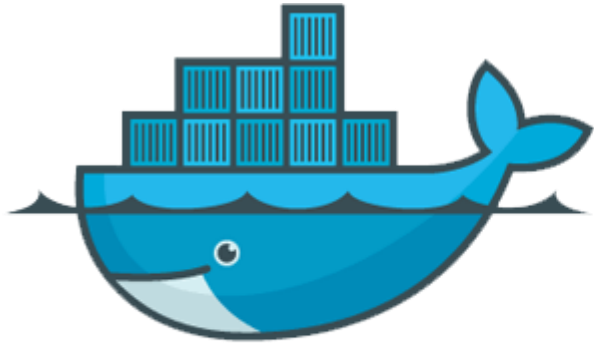
doi: <https://doi.org/10.1101/225680>

HOME
| CHA

Conclusion

- **Galaxy**
 - Every single step is recorded and reproducible
 - 5000 citations so far, 150.000 known user
 - Freiburg Server: largest in Europe with 600 users.
- **Deployments with Sensitive data.**
 - Reproducibility stack:
 - OS -> Packages -> Containers -> VM*
 - Galaxy Docker Flavour Concept
 - Community-based effort:
 - Bioconda, Biocontainers & Galaxy*

Thanks!



docker



TRAVIS



Yasset Perez-Riverol
Felipe Leprevost ...



GitHub

Björn Grüning & the RBC team

BIOCONDA[®]

Johannes Köster
Ryan Dale ...

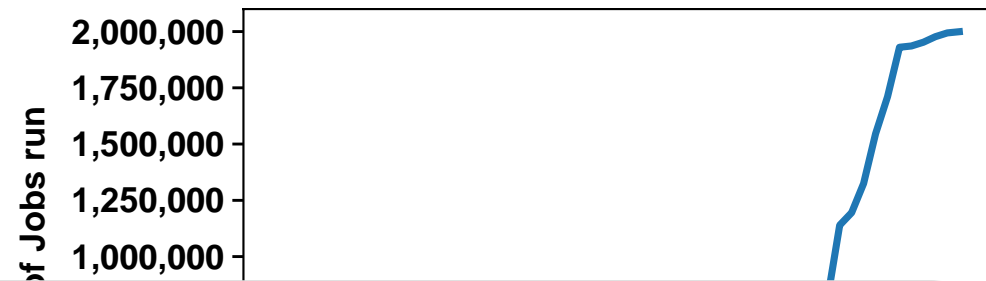
Thank you for your attention

Impact Measurements

- users



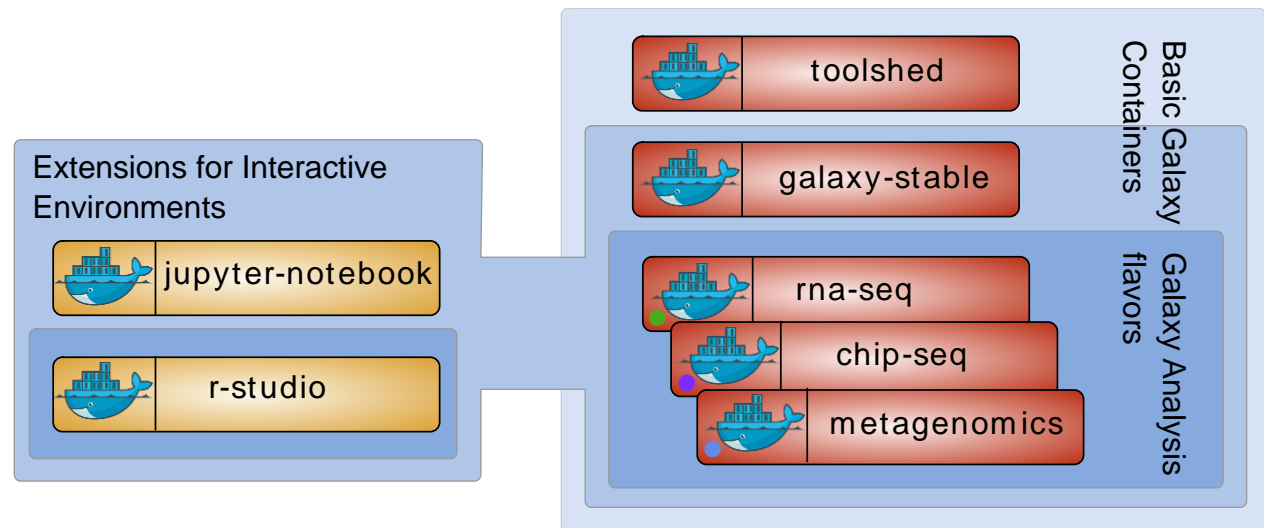
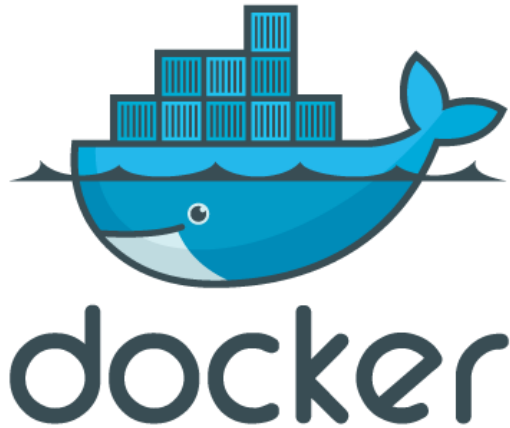
- jobs run



Measurement (from SIG2 report)	Total
Citations/links to website/acknowledgements	9,589
Supporttickets / GitHub issues	4,942
Number of downloads	3,474,974
Web app & database hits	170,411

Overcoming computational limitations

- Idea: tools to data, not data to tools -> virtualization



- drag & drop based Galaxy flavor generator
- Widely used: >28.000 downloads, ELIXIR (Tjenester for Sensitive Data 2.0 Norway), Cancer Center Amsterdam ...

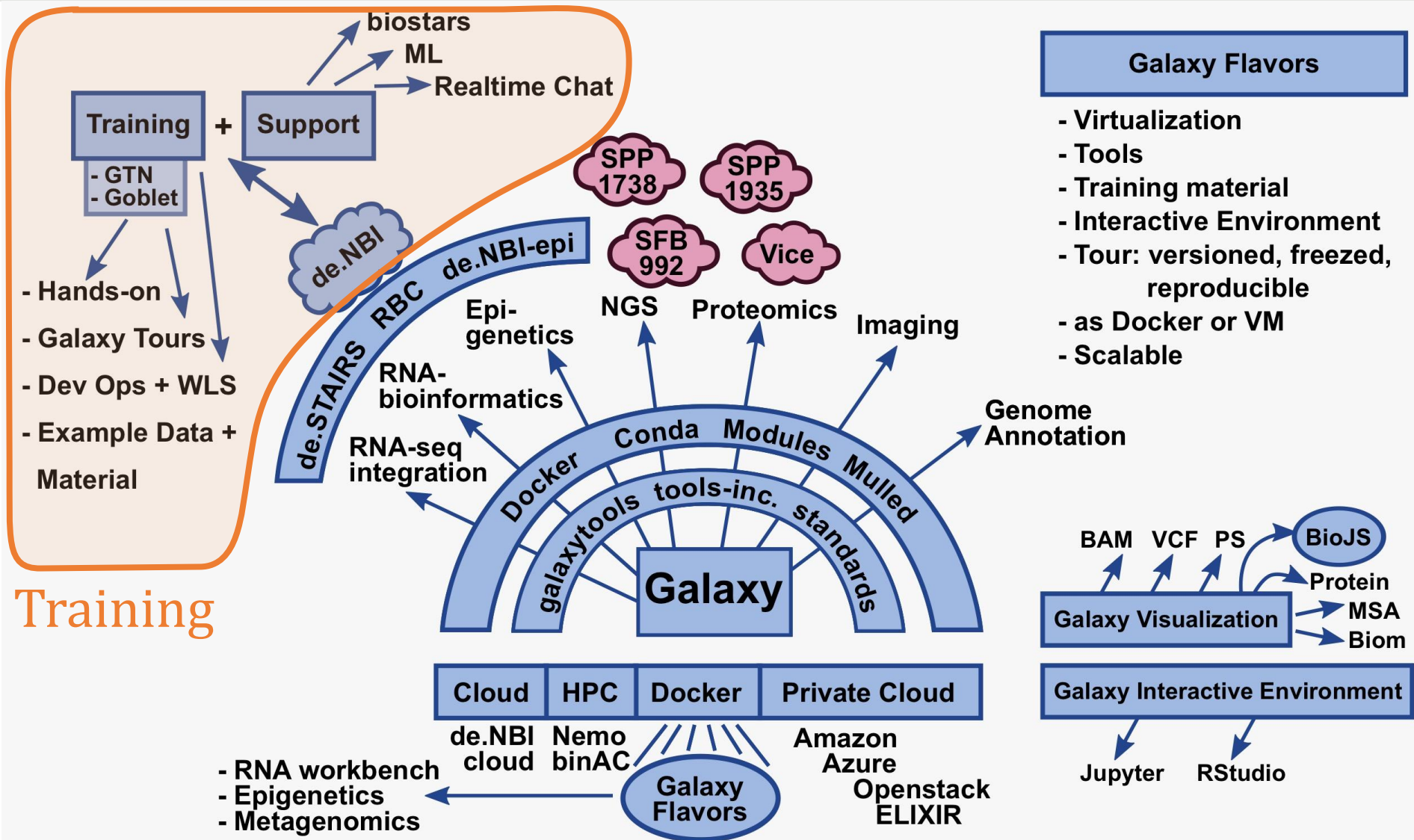
My Appliances

This page is a log of the appliances you have launched. ▾

- Usable clouds:
 - Amazon
 - de.NBI-cloud (FR)
 -
- Our contributions:
 - Virtual container via the flavor generator
 - Can be started world-wide
 - Interface to RBC Galaxy server (user with account can use it)

Cloud: bwcloud

Masterplan



Training by RBC

- 28 training courses, ~500 participants
- 12 locations across the world



2016 events

19 th – 20 th Jan	ELIXIR EDAM codefest	Freiburg
22 nd – 26 th Feb	Galaxy HTS data analysis workshop	Freiburg
07 th – 08 th Mar	RAD-Seq tools and workflows codefest	Online
04 th Apr	Conda codefest	Online
06 th – 07 th Apr	Galaxy DevOps workshop	Heidelberg
27 th – 29 th Apr	HPC workshop	Oslo, Norway
25 th – 29 th Jun	Galaxy Community Conference workshop	Indiana
27 th Jul	RBC Kick-Off meeting	Freiburg
19 th – 23 rd Sep	Galaxy HTS data analysis workshop	Freiburg
27 th – 28 th Sep	GalaxyP codefest	Online
06 th – 07 th Oct	Galaxy training material codefest	Online
20 th – 21 st Oct	Swiss German Galaxy workshop	Freiburg
24 th – 26 th Oct	NETTAB hackathon	Rom, Italy
02 nd – 03 rd Nov	BioConda codefest	Online
30 th Nov – 01 st Dec	Galaxy Docker workshop	Barcelona, Spain
01 st – 02 nd Dec	FAIRDOM/de.NBI Foundry workshop	Frankfurt
15 th – 16 th Dec	Galaxy RNA-seq data analysis workshop	Freiburg

2017 events

09 th – 10 th Jan	Galaxy QIIME codefest	Online
16 th – 19 th Jan	European Galaxy developer workshop	Strasbourg, France



Galaxy Tours – Bioinformatics Training 2.0

The image shows a screenshot of the Galaxy web interface. At the top, there is a navigation bar with 'Galaxy' on the left and 'Upload your data', 'Analyze Data', 'Workflow', 'Shared Data', 'Visualization', and 'Help' on the right. Below the navigation bar, there is a 'Tools' section with a search bar. A tooltip is visible over the 'Upload your data' button, stating: 'Galaxy supports many ways to get in your data. Use this button to upload your data.' The main content area is titled 'Download from web or upload from disk' and has two tabs: 'Regular' and 'Composite'. Under the 'Regular' tab, there is a 'Name' section with a 'New File' button and a text area containing the URL 'https://raw.githubusercontent.com/human_augustus.f'. Below this, there are dropdown menus for 'Type (set all):' (set to 'Auto-detect') and 'Genome (set all):' (set to '---- Addit'). At the bottom, there are several buttons: 'Choose local file', 'Choose FTP file', 'Paste/Fetch data', 'Pause', 'Reset', 'Start', and 'Close'. A large grey overlay box with a green border is positioned in the center, containing the text 'Galaxy Tours' and a bulleted list. To the right, a 'manager' window is partially visible with 'Prev' and 'Next' buttons. At the bottom right, there is a 'View on Twitter' link and a 'TAC' logo.

Galaxy Tours

- Analysis in a box
- Real execution of code
- User can just use the tour or change parameters/input

Thank you for your attention

Galaxy Tours – Bioinformatics Training 2.0

The screenshot displays the Galaxy web interface with a tour overlay. The main content area shows the 'Filter data on any column' tool configuration. The 'Filter' section includes a search for 'filter', a 'Dataset missing?' warning, and a filter expression 'c1=='chr22''. The 'Number of header lines' is set to 0. A green tooltip above the tool says 'error' if problems were encountered. The 'History' panel on the right shows a search for 'Galaxy tours' with 4 results, including links to GitHub repositories. A dialog box titled 'Enjoy Galaxy' is centered, displaying 'Thanks for taking this tour! Happy research with Galaxy!' and 'End tour' button. The background shows the Galaxy tool menu on the left and a data table on the right.

De.NBI cloud



- Recently opened: Supercomputer NEMO
 - **15,000** cores, **position 214** in TOP 500
- we got
 - **1,500,000 €** hardware extension for GALAXY
 - Additionally **5% of existing NEMO resources**
 - **IMPORTANT: cloud knowledge of BW-CLOUD**

Trainings -Material

Galaxy Training!

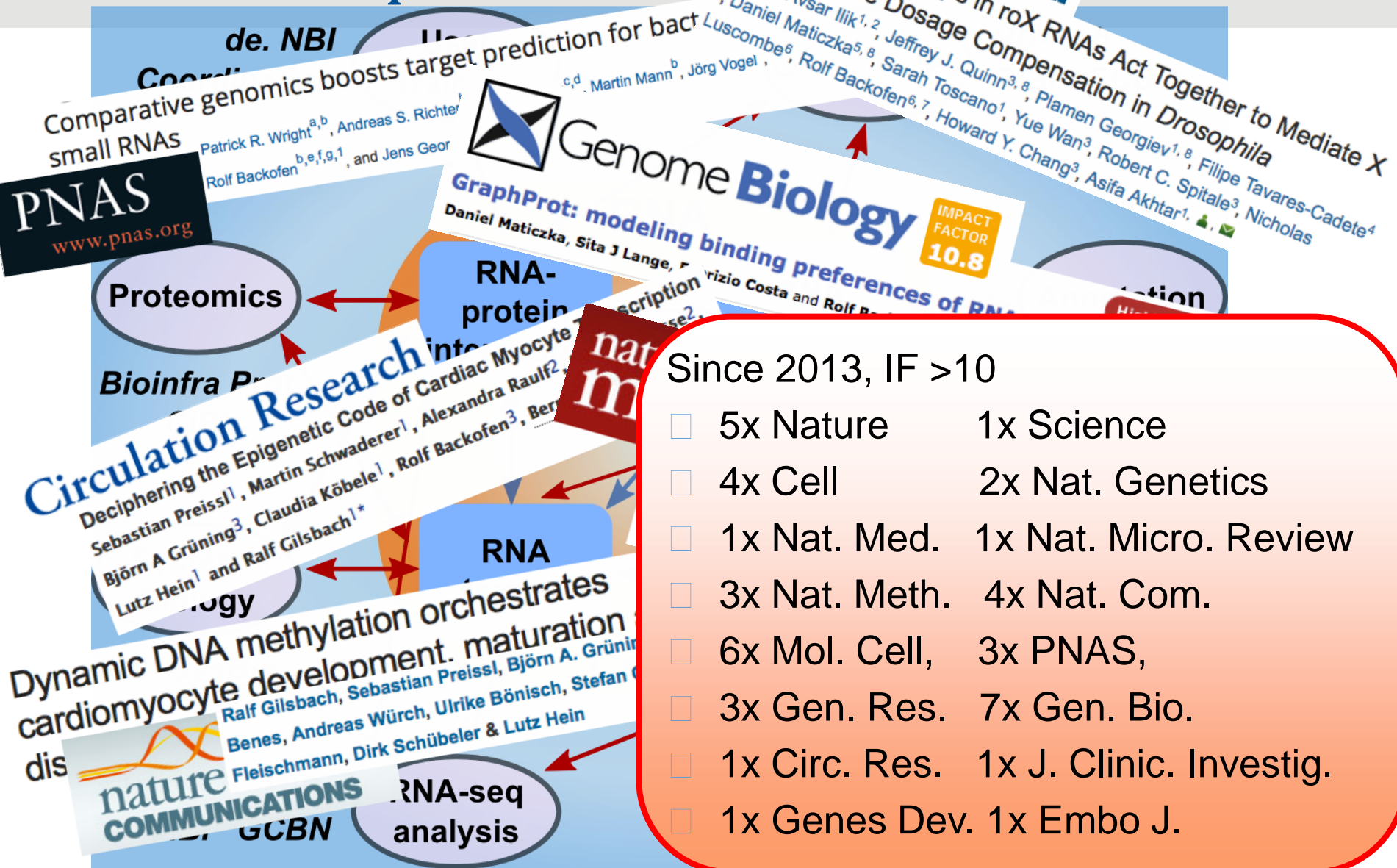
Help on Gitter

- 11 topics with 68 tutorials for 3 different target audiences
- 51 contributors, 3 contribution feasts
 - Online in October 2016
 - Cambridge in May 2017, organized with ELIXIR and GOBLET
 - Montpellier in June 2017 during the Galaxy Community Conference
- Integration with ELIXIR's training platform (TeSS)

Conclusion

- **RNA-Bioinformatics Center (RBC):**
 - RNA-mediated post-transcriptional regulation
 - integrates all international renowned German RNA bioinformatics groups
- **Important aspects of our service:**
 - RNA workbench based on Galaxy
 - Virtualization for distribution of computational burden
 - Strong interaction with ELIXIR
 - training, training, training (user, user, user)
future: eLearning!!

Areas of Expertise



Since 2013, IF >10

- 5x Nature 1x Science
- 4x Cell 2x Nat. Genetics
- 1x Nat. Med. 1x Nat. Micro. Review
- 3x Nat. Meth. 4x Nat. Com.
- 6x Mol. Cell, 3x PNAS,
- 3x Gen. Res. 7x Gen. Bio.
- 1x Circ. Res. 1x J. Clinic. Investig.
- 1x Genes Dev. 1x Embo J.