The Genomics Virtual Laboratory

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University of Melbourne

What is the Genomics Virtual Lab?

Nationally distributed platform for *genomics*, built on the federal *Research Cloud*

RDSI
Research Data Storage Infrastructure

nectar

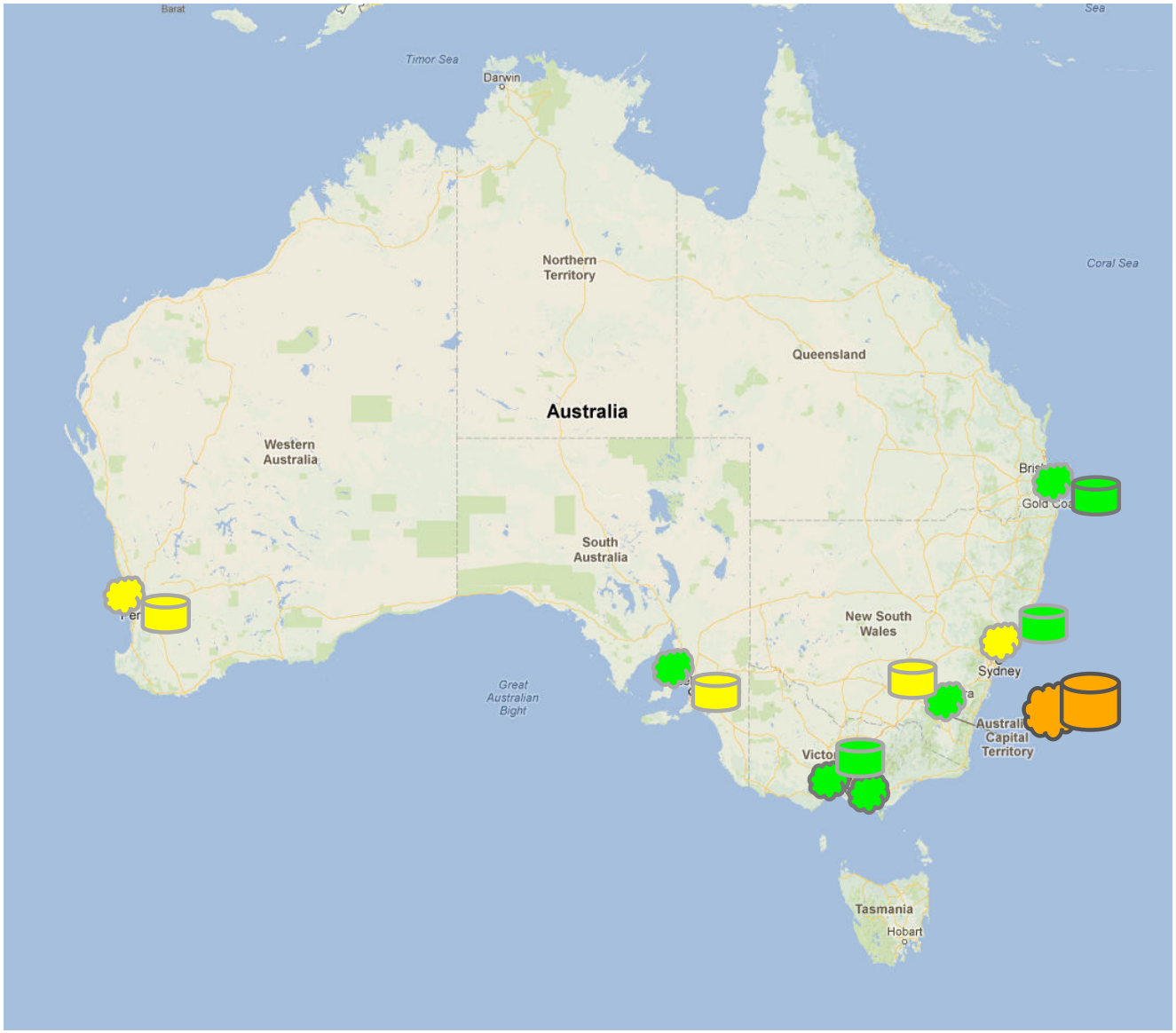
http://nectar.org.au

The Australian Research Cloud

Cloud node:
3-6000 cores

Data node:
1-5 PB

Coming 2014-15



GVL: Drivers

To provide a genomics analysis platform with:

1. ***Reproducibility***
2. ***Accessibility***
3. ***Performance***
4. ***Flexibility***
5. ***Consistency***
6. ***Functionality***

for as many researchers as possible

GVL: Design principles

Criteria	Design Implication
Accessible	Minimal client-side requirements
Reproducible	Workflow support + software & tool management process
Performance	User-managed scaling of compute resources + high availability resources
Flexible	User configurable + administrable Multiple interaction modes
Consistent	Single platform from training to analysis
Functional	Pre-populated with suite of tools for common use cases + required reference data + visualisation options

GVL: Design implications

Criteria	Design Implication	Technical implication
Accessible	Minimal client-side requirements	**Web based** tool and management interfaces
Reproducible	Workflow support + software & tool management process	**Workflow platforms** + automated process for **deployable underlying environment**
Performance	User-managed scaling of compute resources + high availability resources	**Cloud-based architecture** + interface for managing resources
Flexible	User configurable + administrable	**Per-user instances** accessible through web and command line; user-administrable environment
Consistent	Single platform from training to analysis	**Tutorials and guides** for training using best practice tools + **scalability**
Functional	Pre-populated with suite of tools for common use cases + required reference data + visualisation options	Process for **building underlying images** Automated configuration of **reference datasets**

For as many researchers as possible...

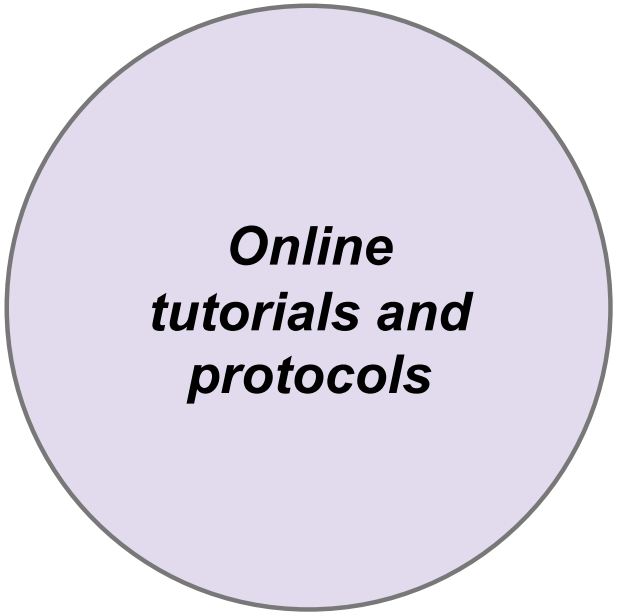
Galaxy Main

GVL: Philosophy

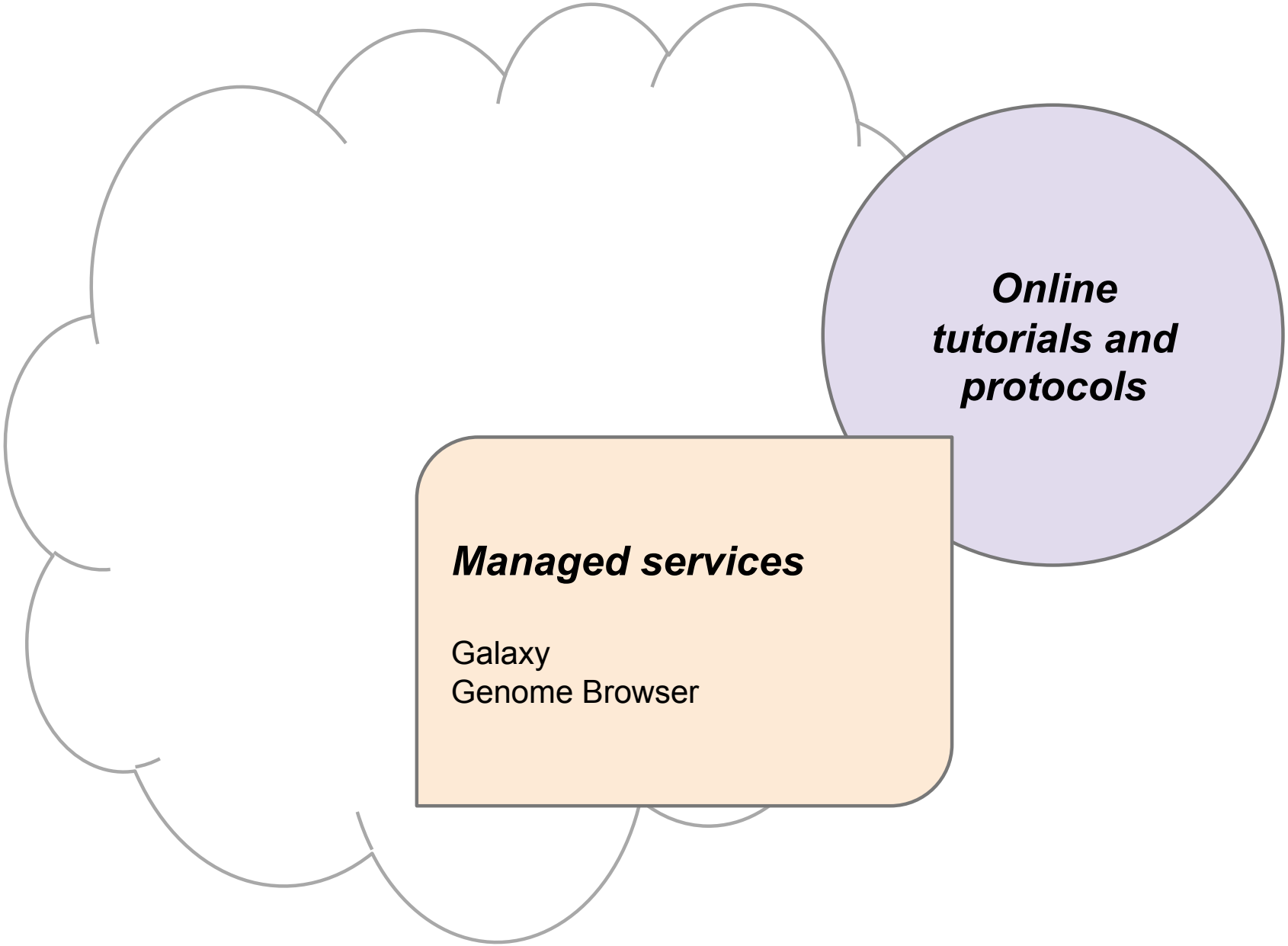
Genomics Virtual Lab

Galaxy Main

GVL: In practice



GVL: In practice



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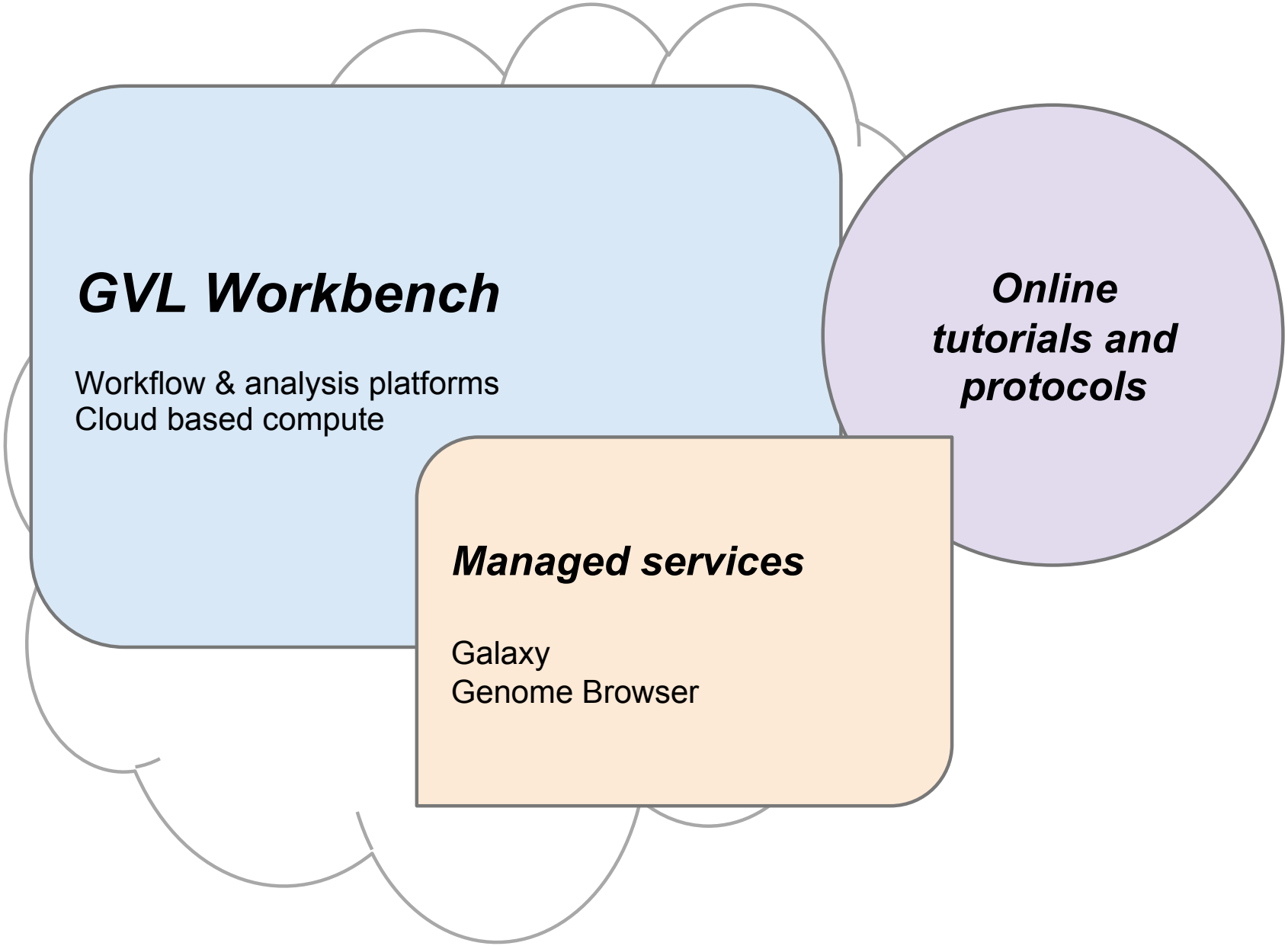
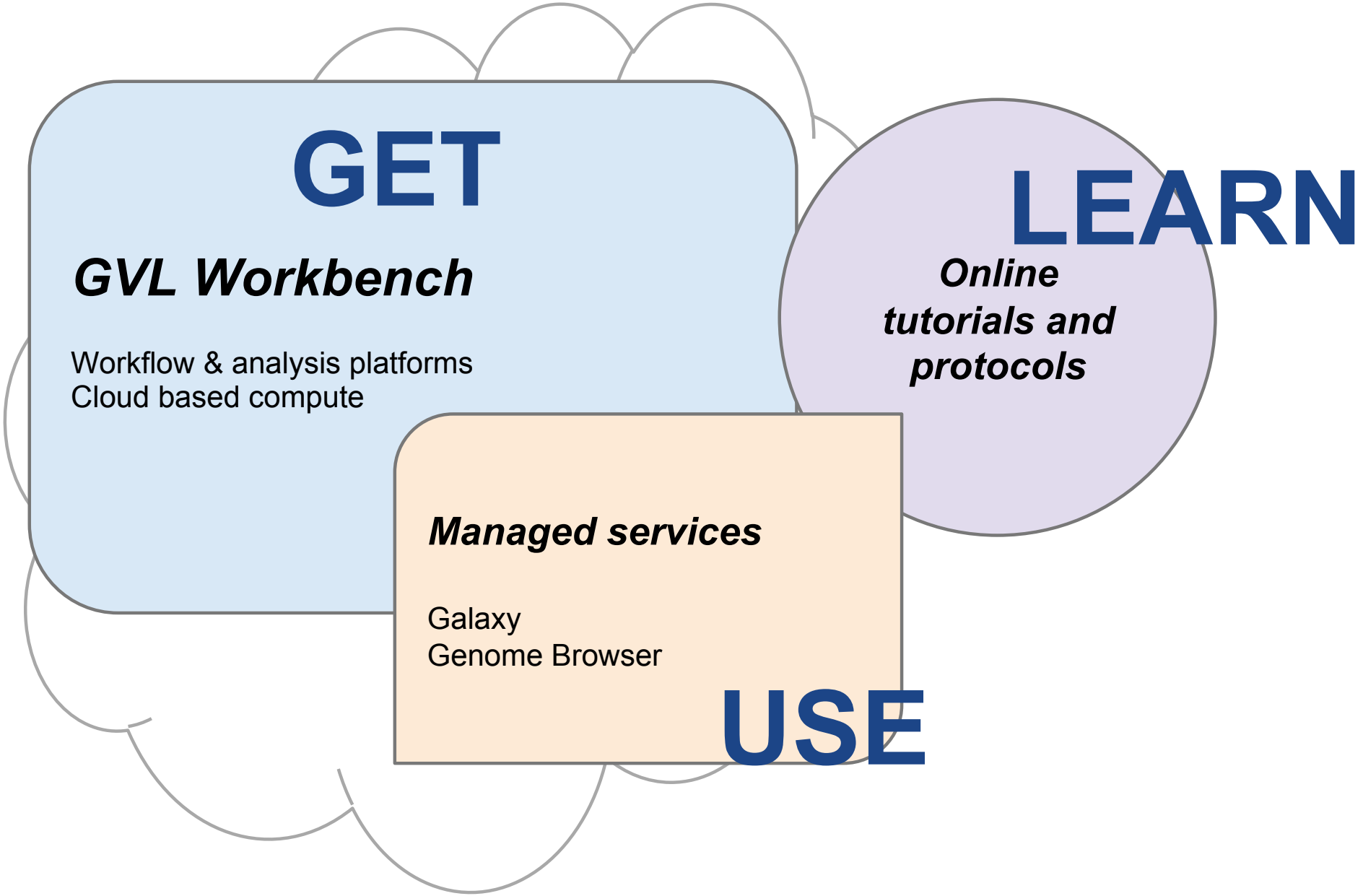
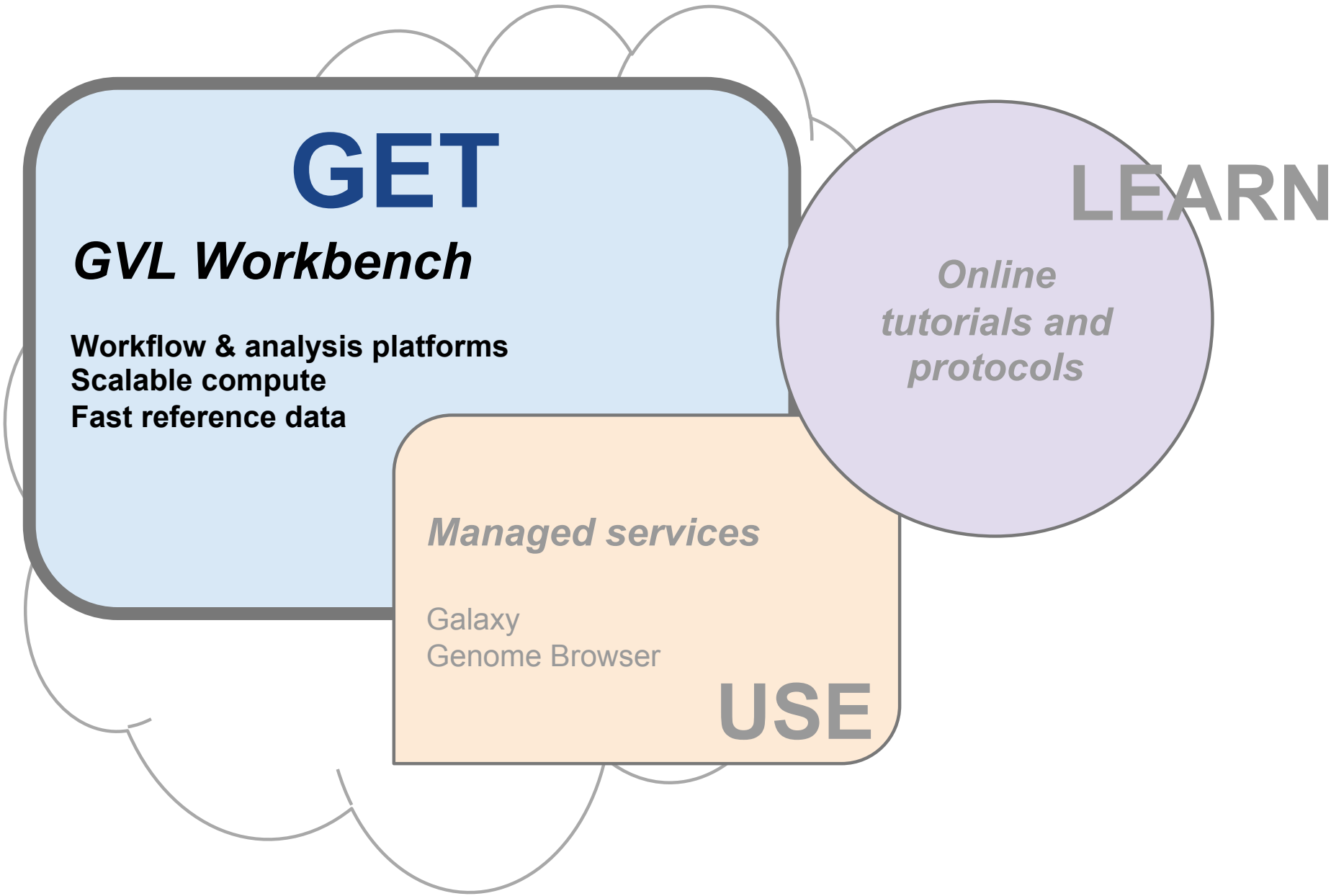


GVL: http://genome.edu.au

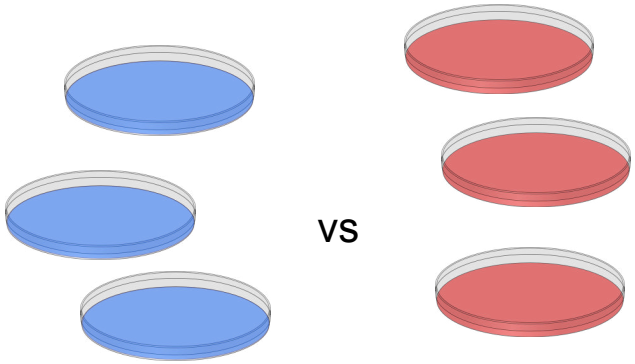


GVL: Developer's perspective



What characterises genomic analysis?

eg: Differential Gene Expression

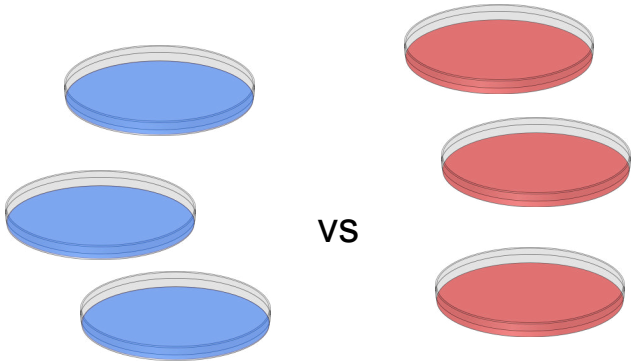


"What genes are turned on in blue cells and turned off in red cells?"

Differential Gene Expression

2E7 observations
over 1E5 genes
for 6 samples

(30GB raw data)



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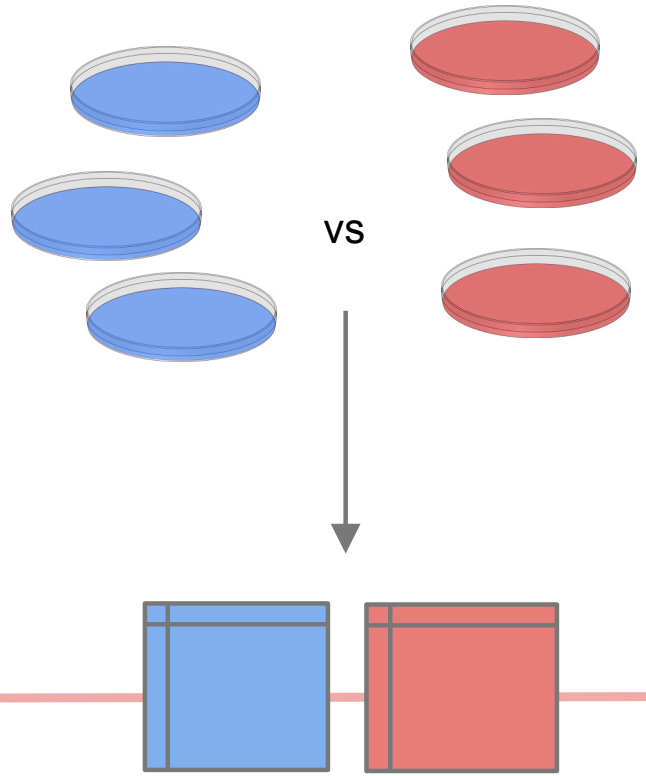
Differential Gene Expression

DATA REDUCTION

Workflows
Large reference data
High compute

2E7 observations over 1E5 genes for 2x3 samples



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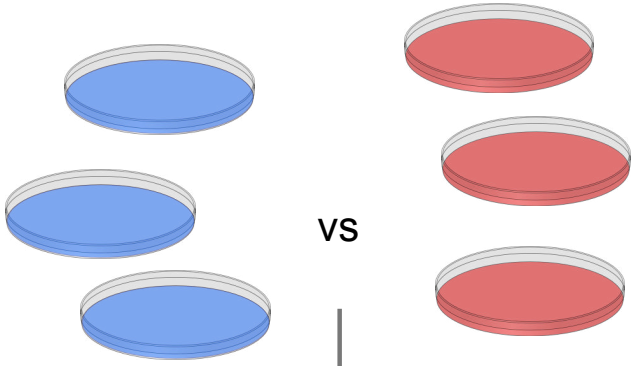
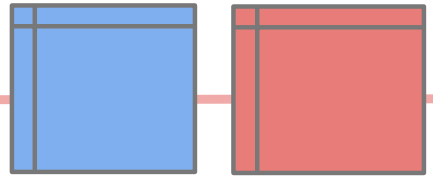
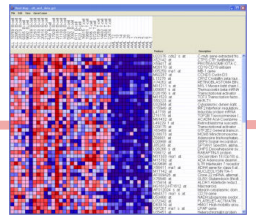




DATA ANALYSIS

Interactive
Flexibility

Test difference: [1,2,3] vs [4,5,6]



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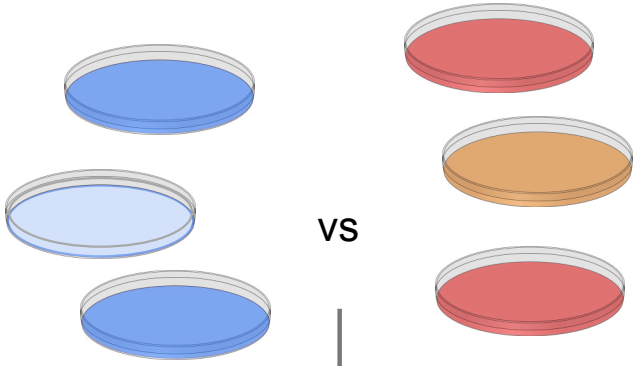

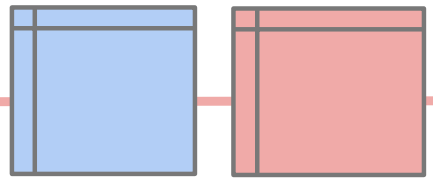

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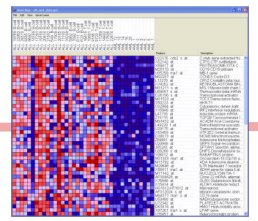

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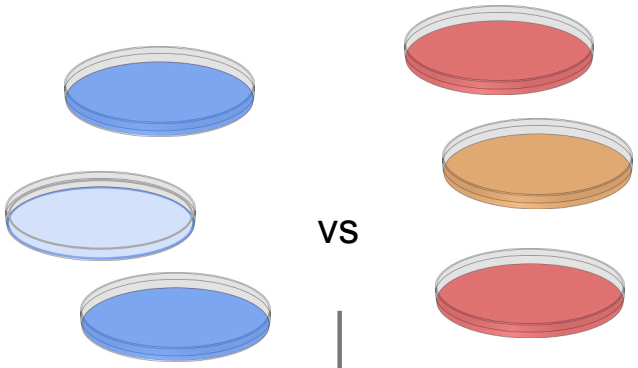

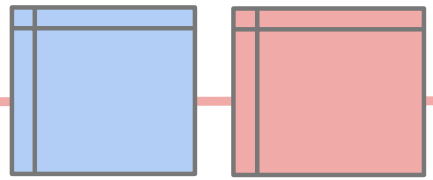

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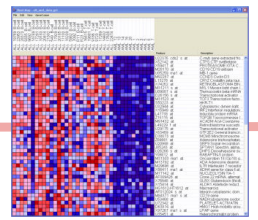
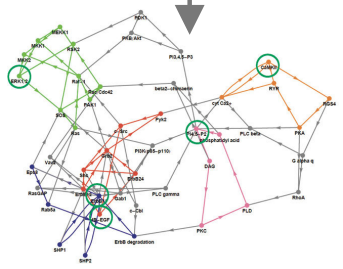


DATA INTERPRETATION

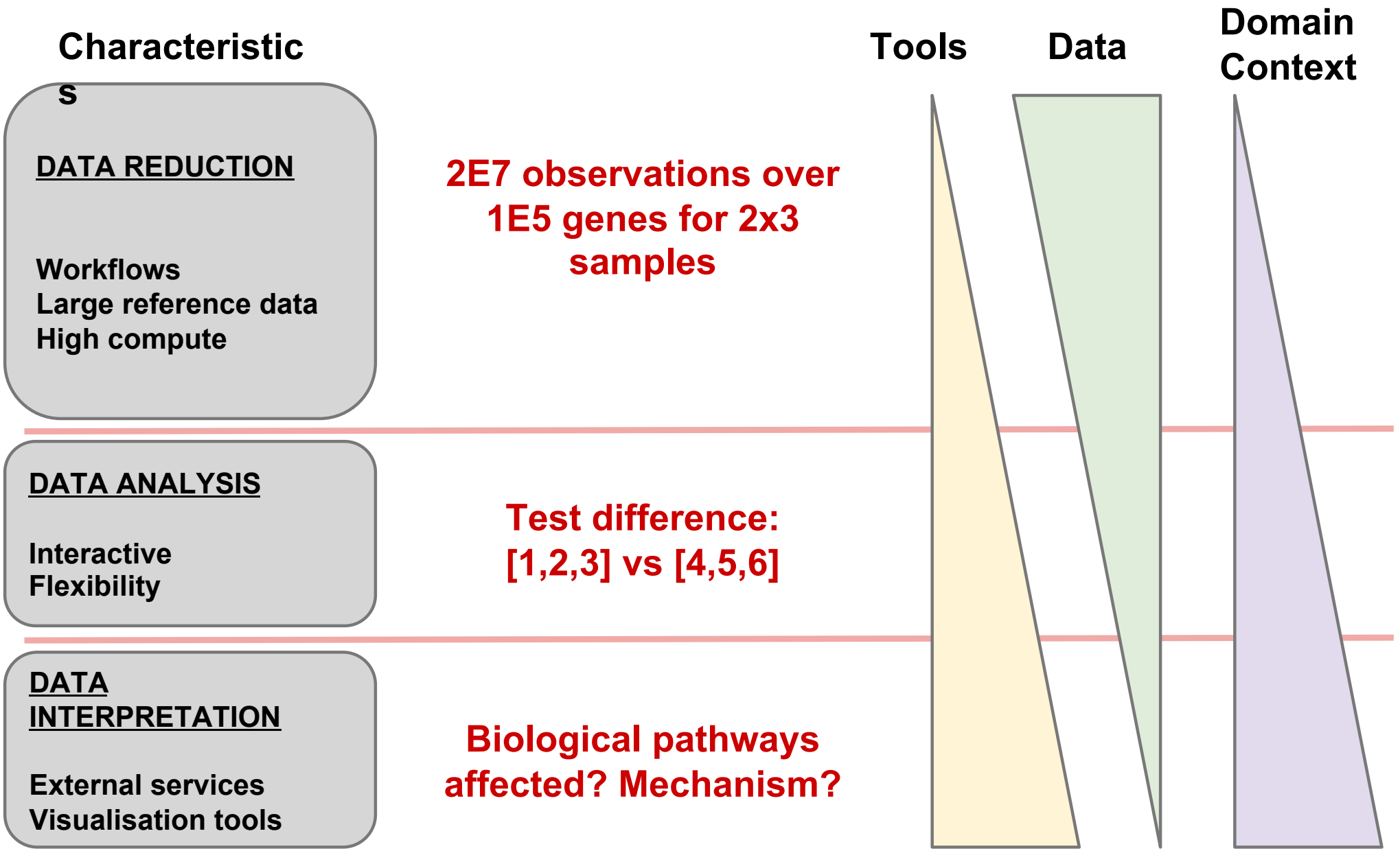
External services
Visualisation tools

Biological pathways affected? Mechanism?



Pathway knowledge

Differential Gene Expression



What characterises genomics?

- Very large experimental datasets per user/ group
- I/O intensive high compute initial analysis
  - ‘data reduction’: raw data to sample summaries
- Large suite of data analysis tools, interactive
  - a bit subjective
- Complex context for interpretation, external tools
  - more subjective, domain knowledge
- Little modelling/simulation

GVL Workbench: Requirements

A web-based *per-user* workbench providing:

- **access to multiple tools**
- **on a scalable back end compute cluster**
- **with fast access to large reference data,**
- **user administrable and configurable**
- **with multiple modes of interaction**
- **and a mechanism for reproducible workflows**

all highly available and accessible
i.e. with a minimal cost of entry to the user

Why per-user?

Managed service: objective

A short time later…

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Managed service: objective

A short time later…

GVL: Philosophical assertion

>

GET a GVL

http://genome.edu.au → GET

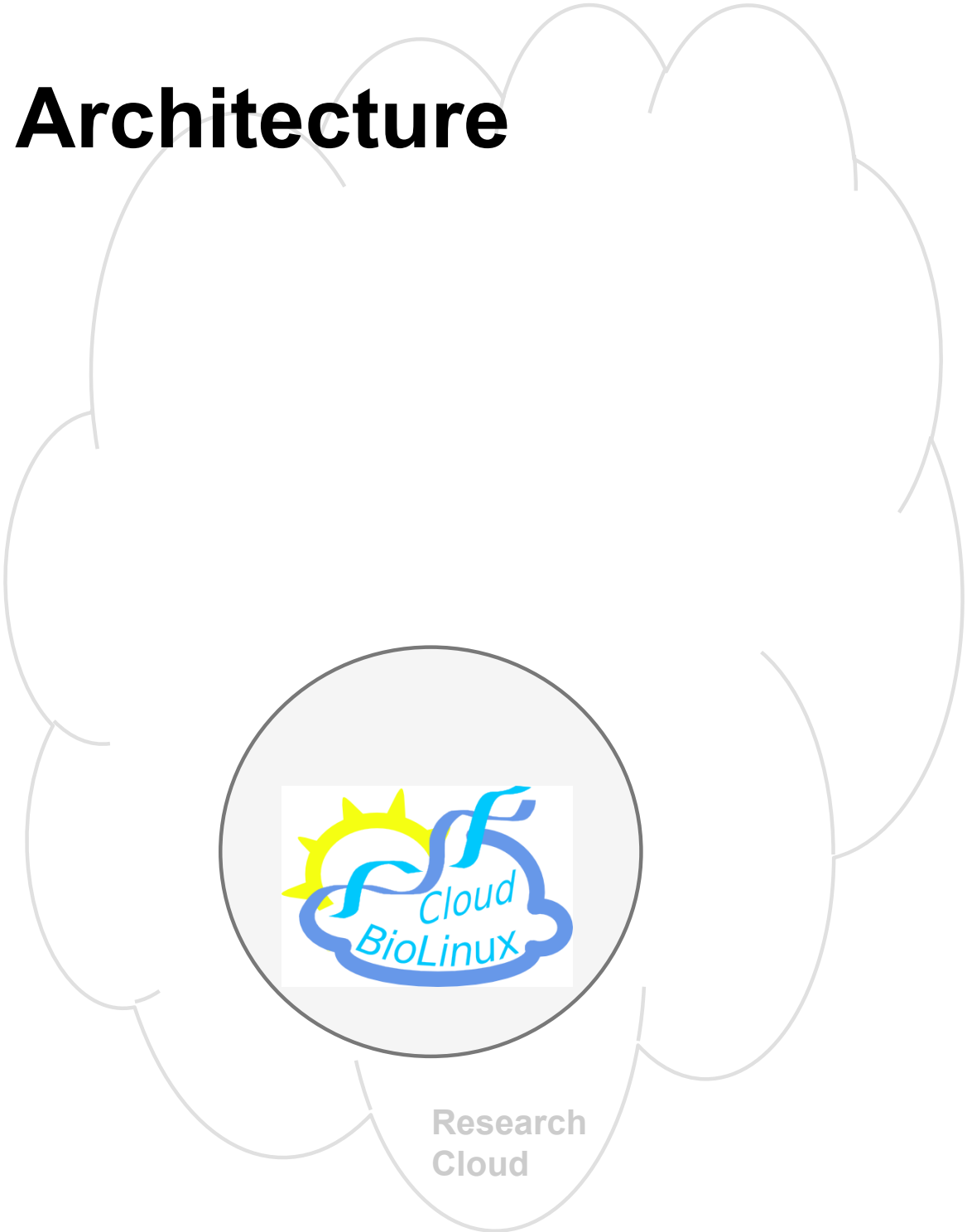
Building (deploying and running) a GVL instance:

1. *Create a CloudBioLinux server VM*
2. *Download and install a preconfigured Galaxy*
3. *Attach pre-populated indexed genomes data*
4. *Start Galaxy*
5. *Add extra compute nodes as required*

GVL Workbench: Architecture

GVL Workbench

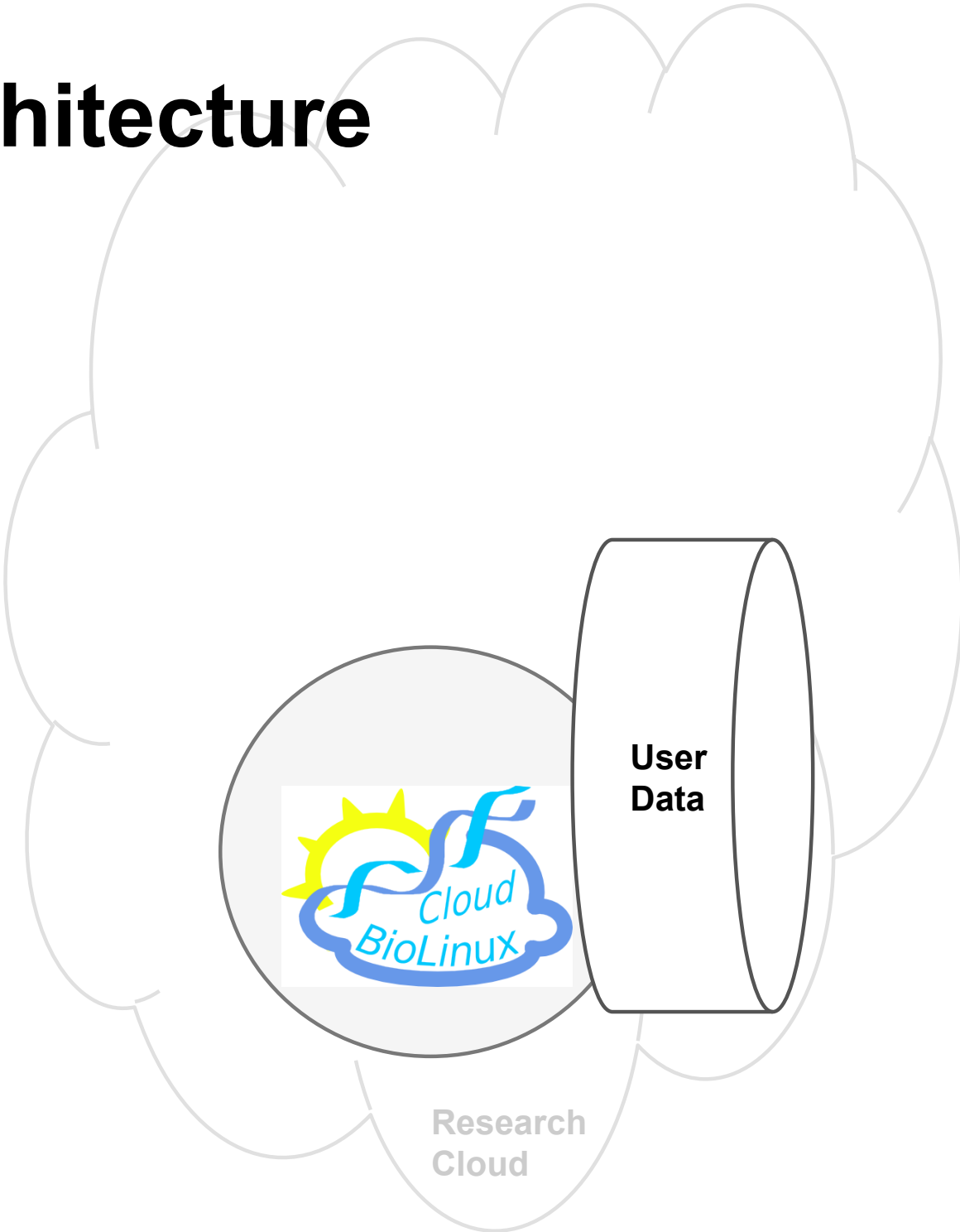
Workflow & analysis platforms



Workbench: Architecture

GVL Workbench

Workflow & analysis platforms



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GVL Workbench

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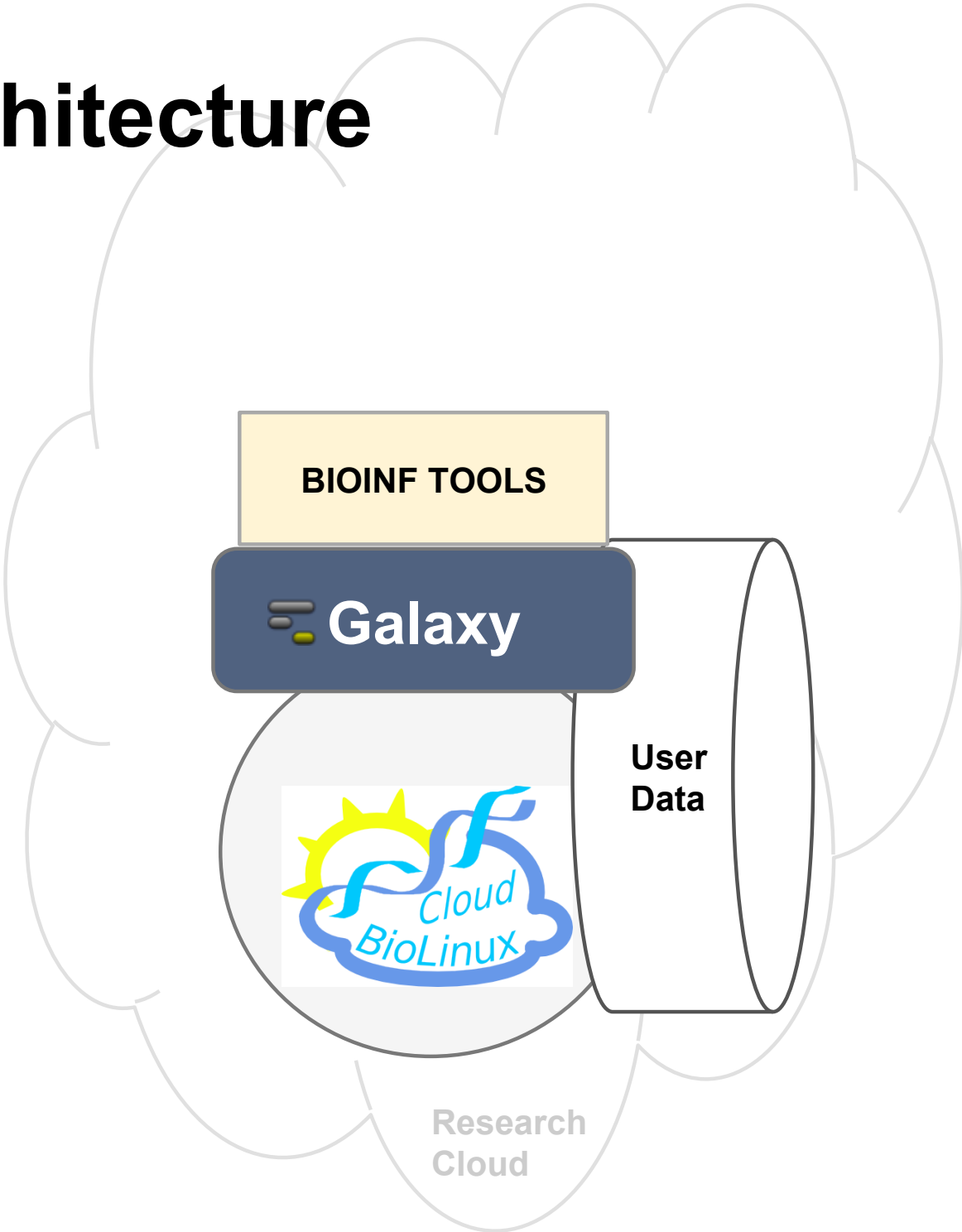
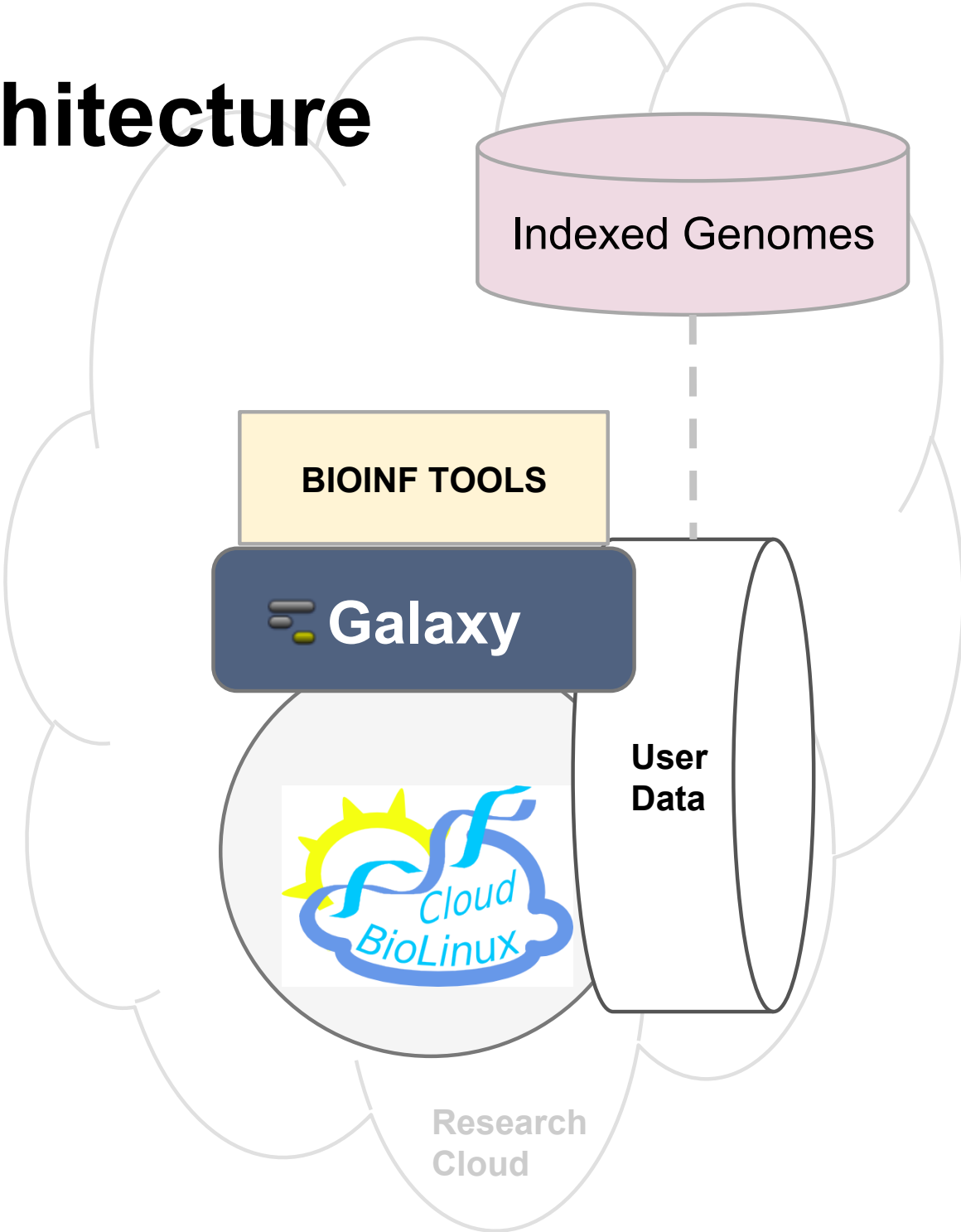


Workbench: Architecture

GVL Workbench

Workflow & analysis platforms

Fast reference data



Workbench: Architecture

GVL Workbench

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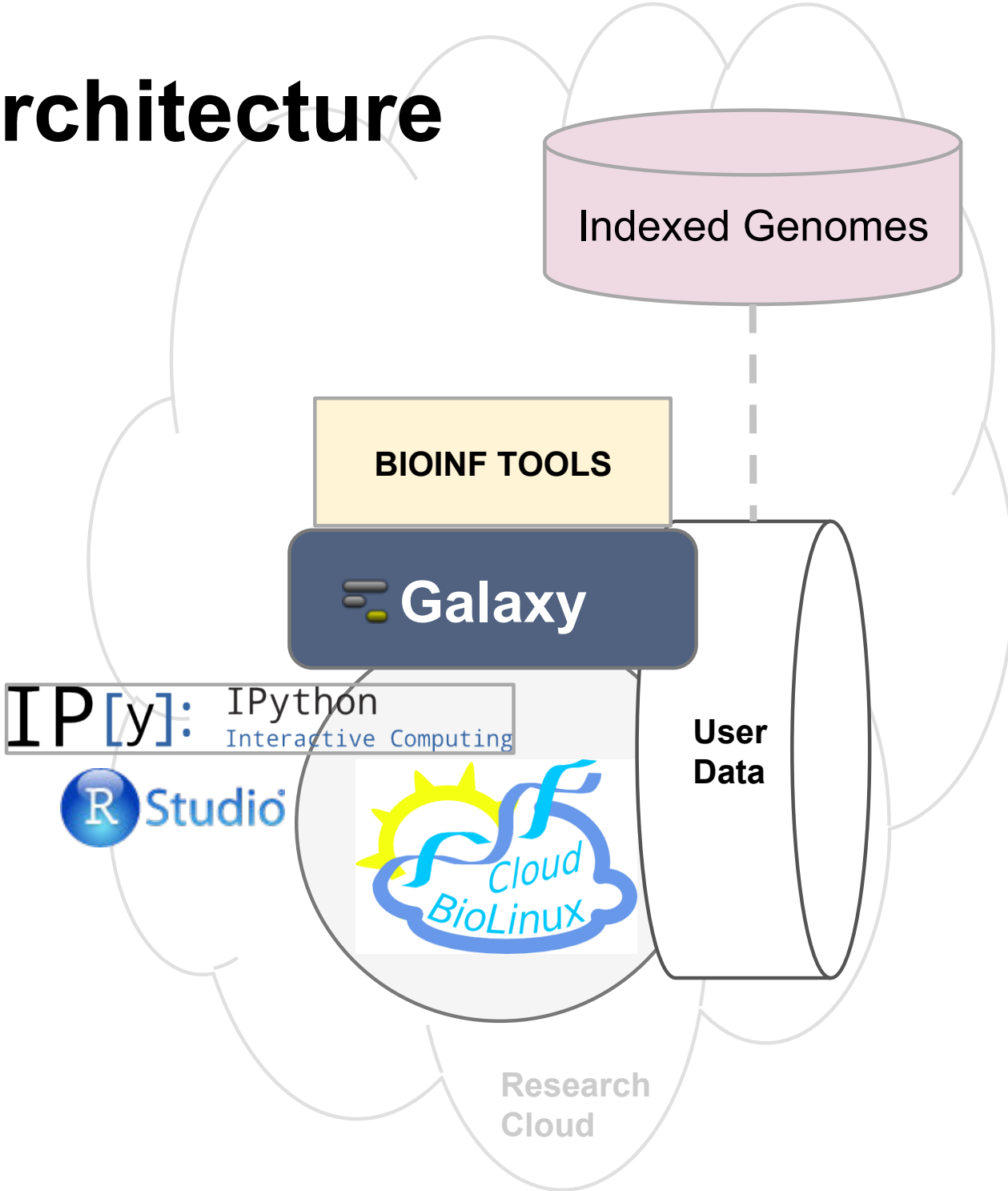


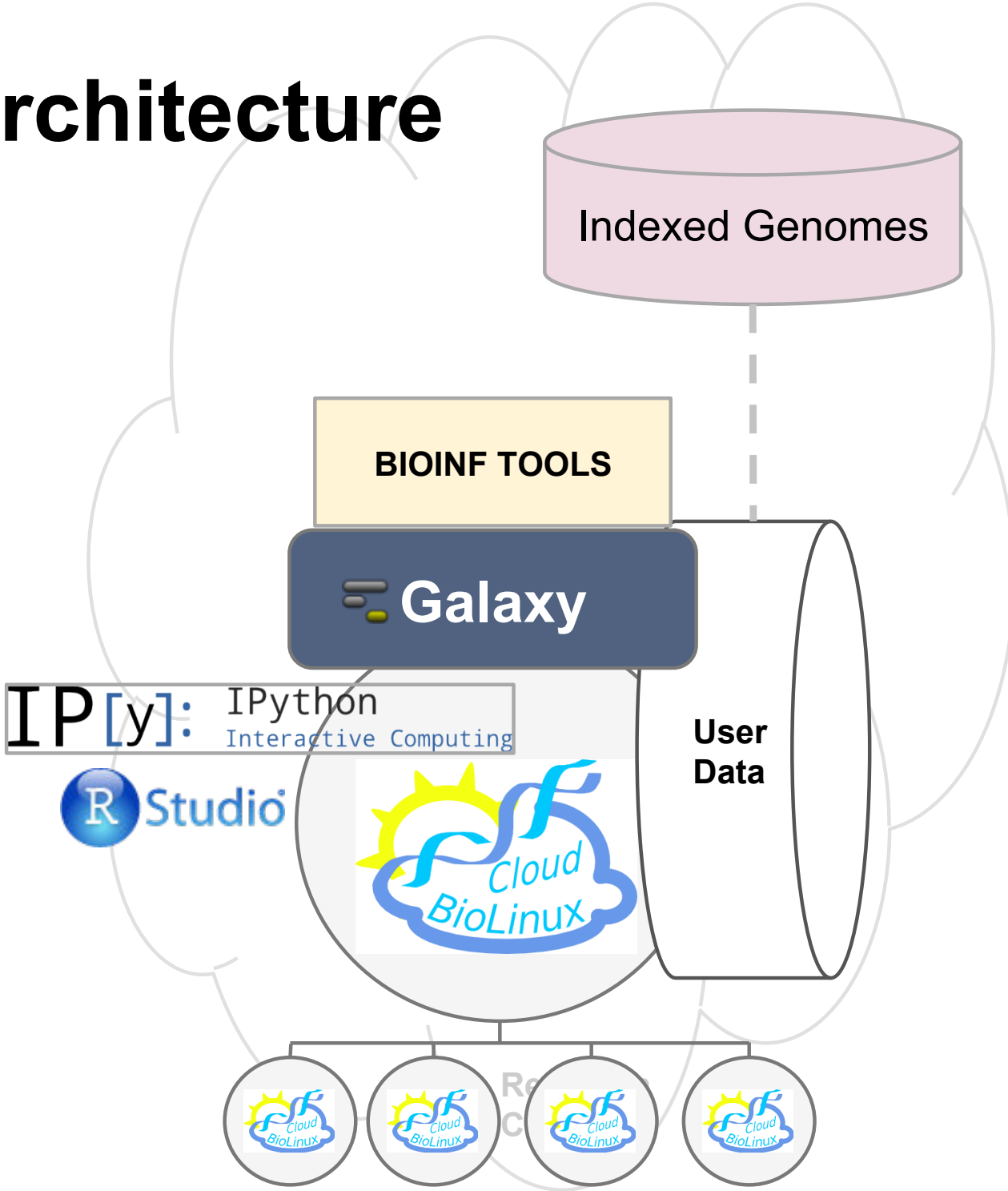
Workbench: Architecture

GVL Workbench

Workflow & analysis platforms

Fast reference data

Scalable compute



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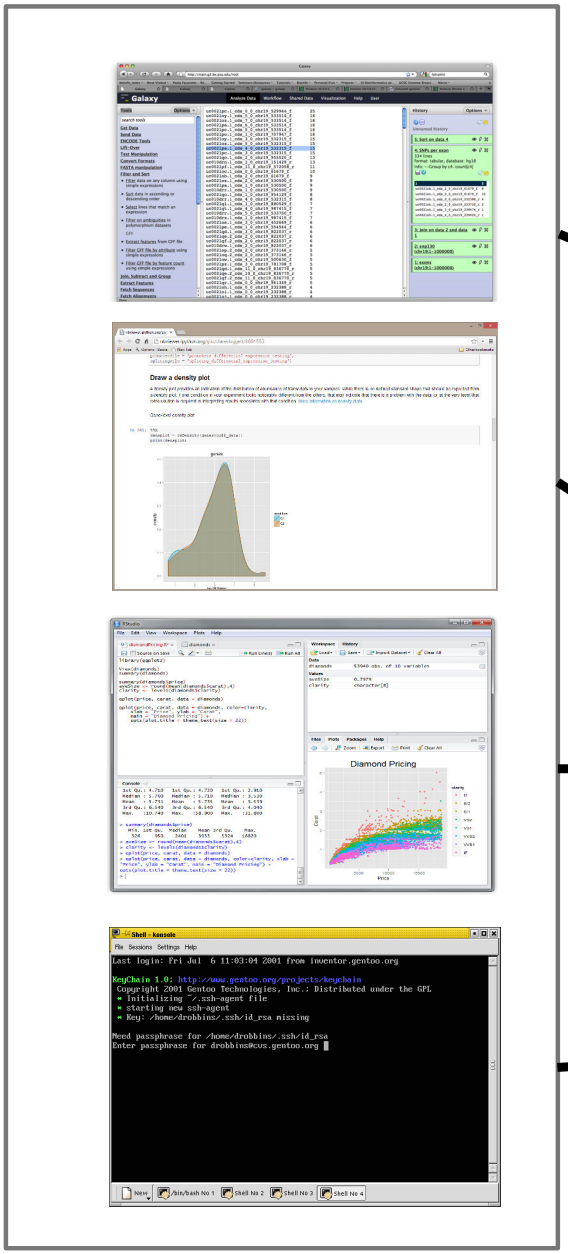


Indexed Genomes

BIOINF TOOLS

Galaxy

IP[y]: IPython Interactive Computing

RStudio

User Data

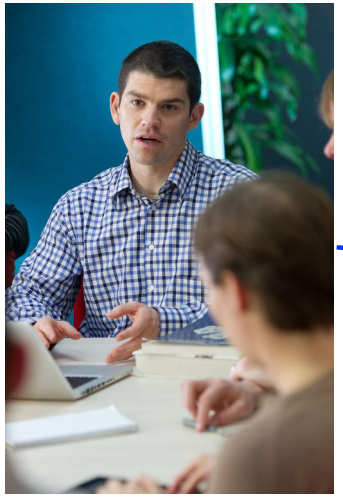
Cloud BioLinux

Engineering:
Deploying and running a GVL

http://launch.genome.edu.au

Cloudman = Middleware for building, distributing and managing cloud-based platforms, especially Galaxy

CloudMan



Afgan *et al. BMC Bioinformatics* 2012, **13**:315
http://www.biomedcentral.com/1471-2105/13/315

BMC Bioinformatics

SOFTWARE Open Access

CloudMan as a platform for tool, data, and analysis distribution

Enis Afgan[1,3,4] Brad Chapman[2] and James Taylor[3,4]

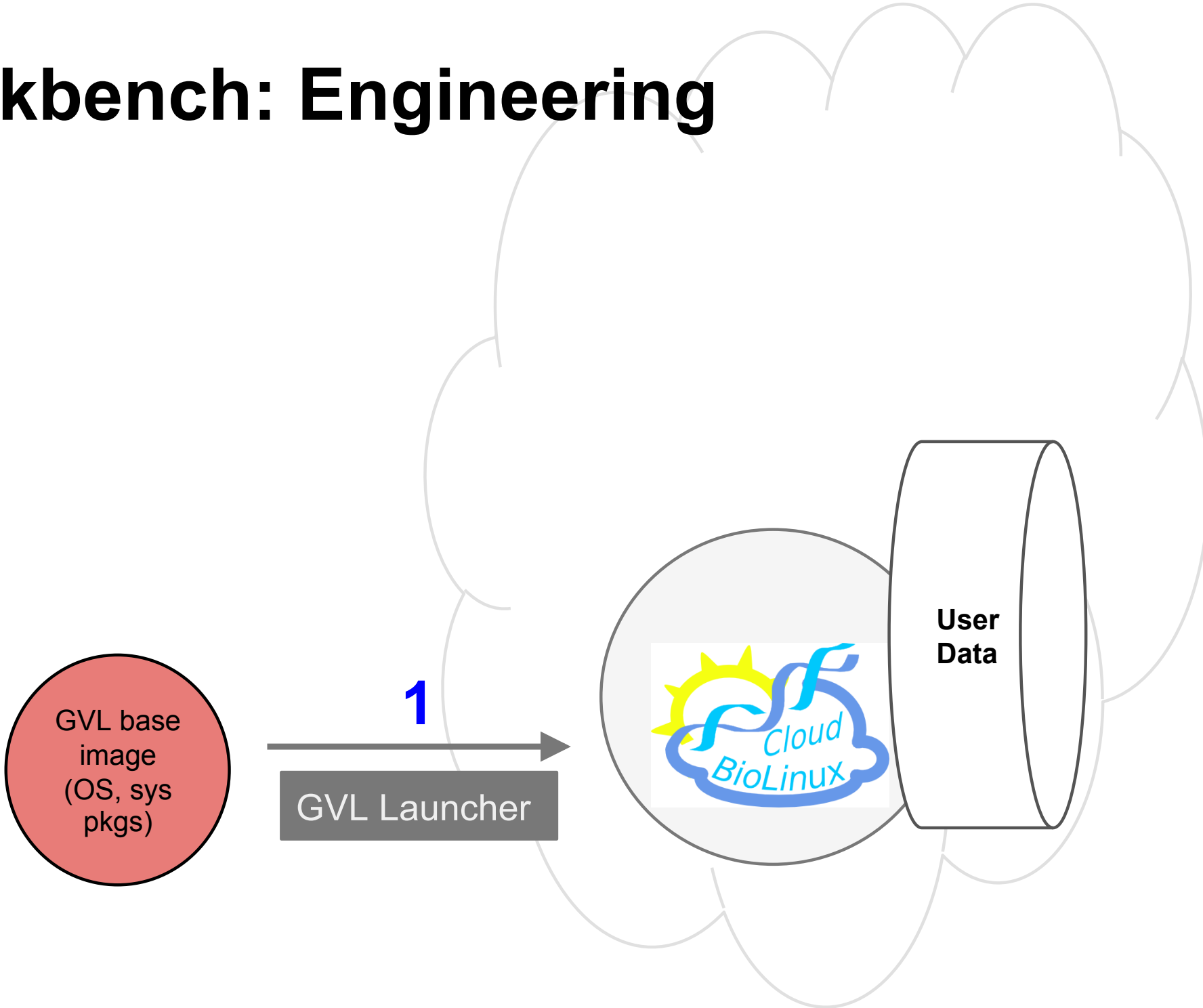
Abstract

Background: Cloud computing provides an infrastructure that facilitates large scale computational analysis in a scalable, democratized fashion, However, in this context it is difficult to ensure sharing of an analysis environment and associated data in a scalable and precisely reproducible way.

Results: CloudMan (usecloudman.org) enables individual researchers to easily deploy, customize, and share their entire cloud analysis environment, including data, tools, and configurations.

Conclusions: With the enabled customization and sharing of instances, CloudMan can be used as a platform for collaboration. The presented solution improves accessibility of cloud resources, tools, and data to the level of an

Workbench: Engineering



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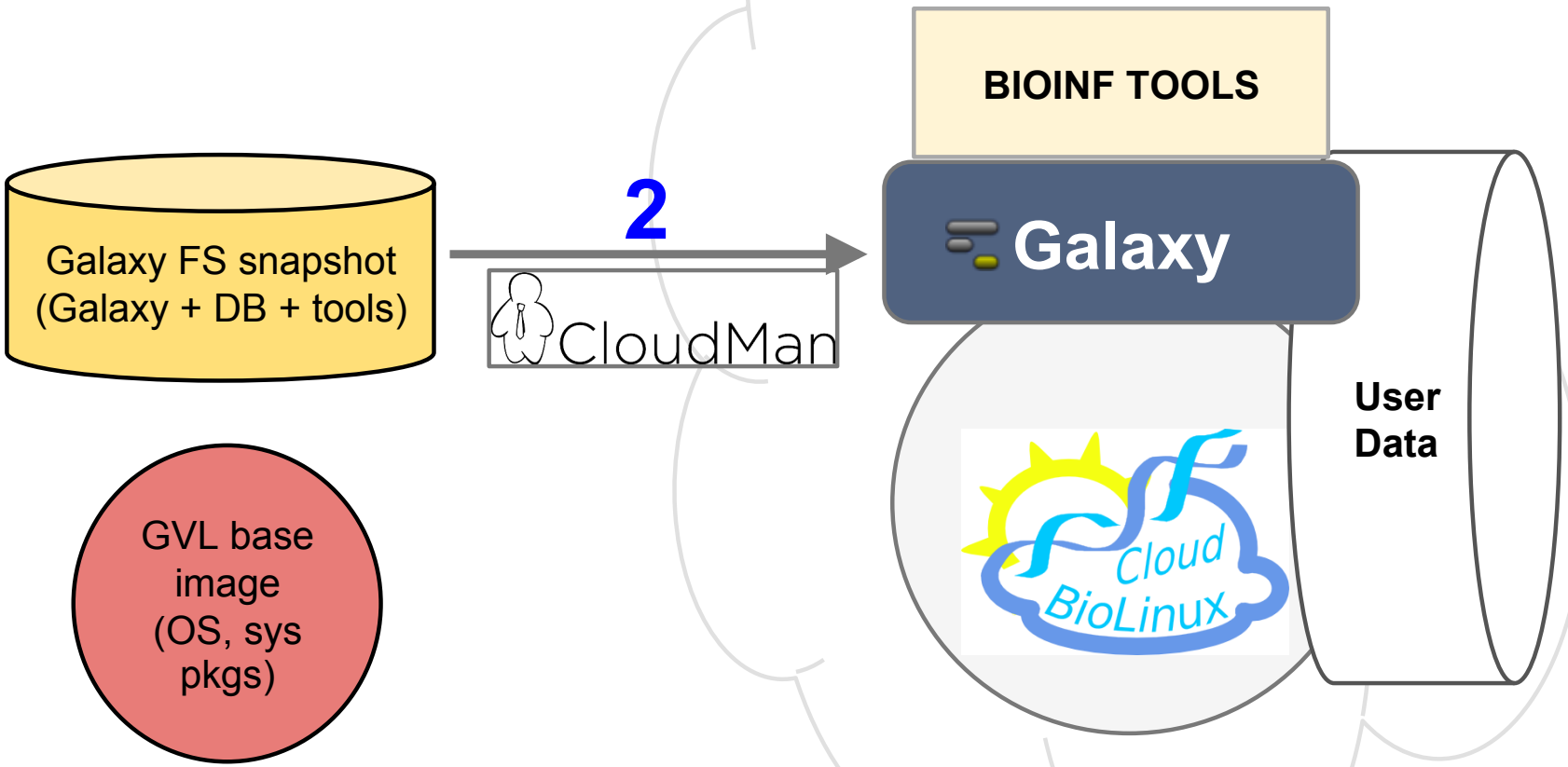

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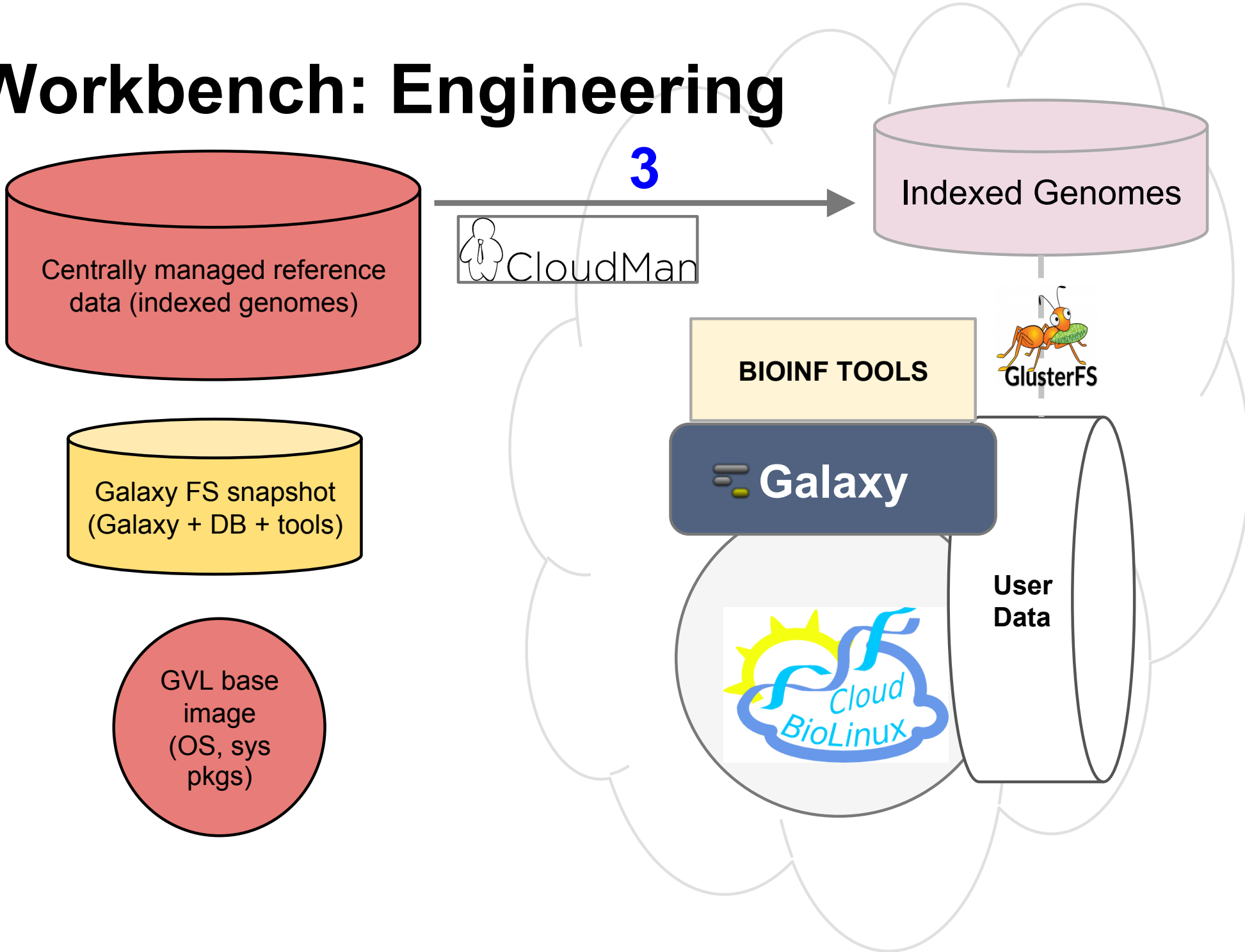
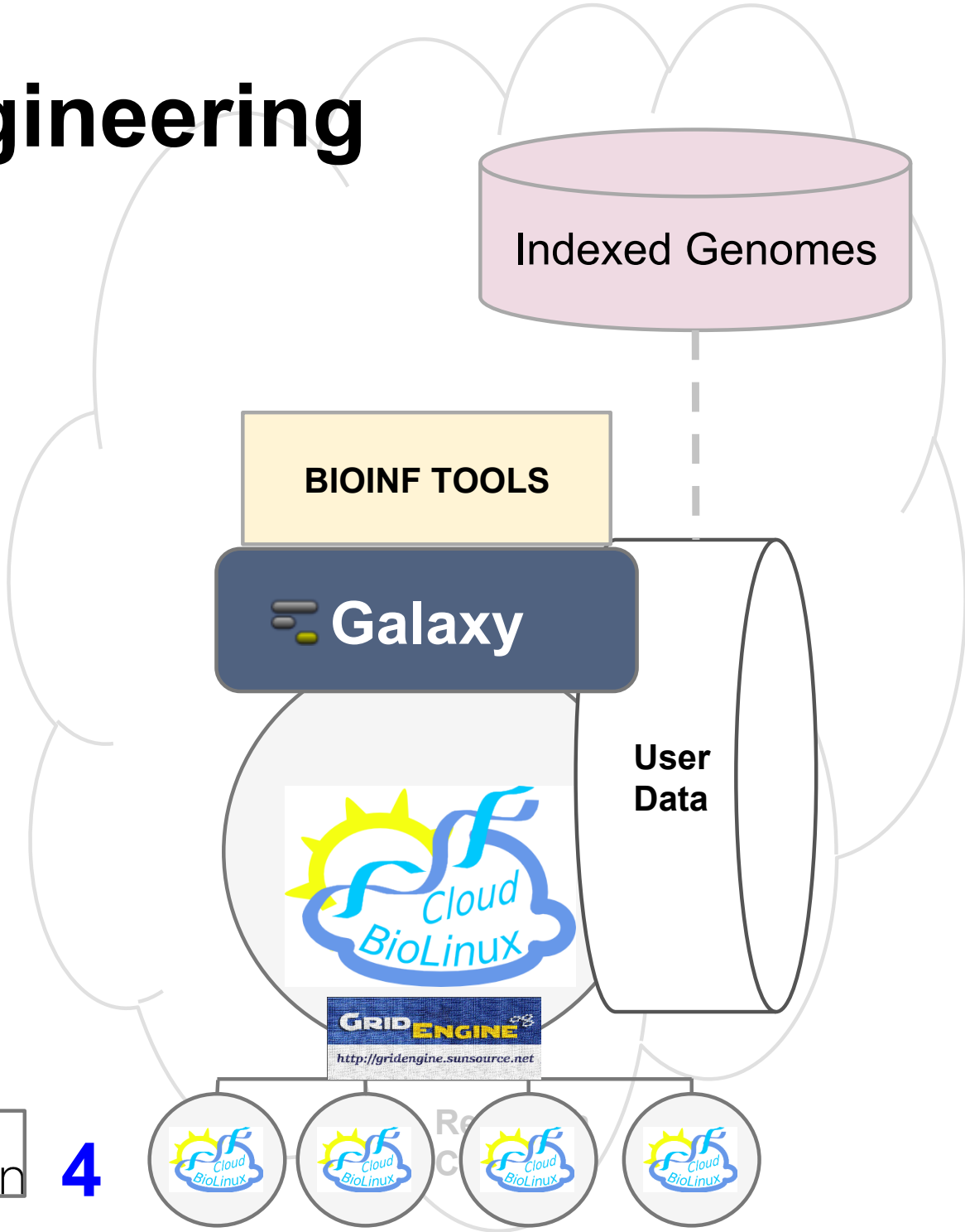


Workbench: Engineering

Centrally managed reference data (indexed genomes)

Galaxy FS snapshot (Galaxy + DB + tools)

GVL base image (OS, sys pkgs)



CloudMan

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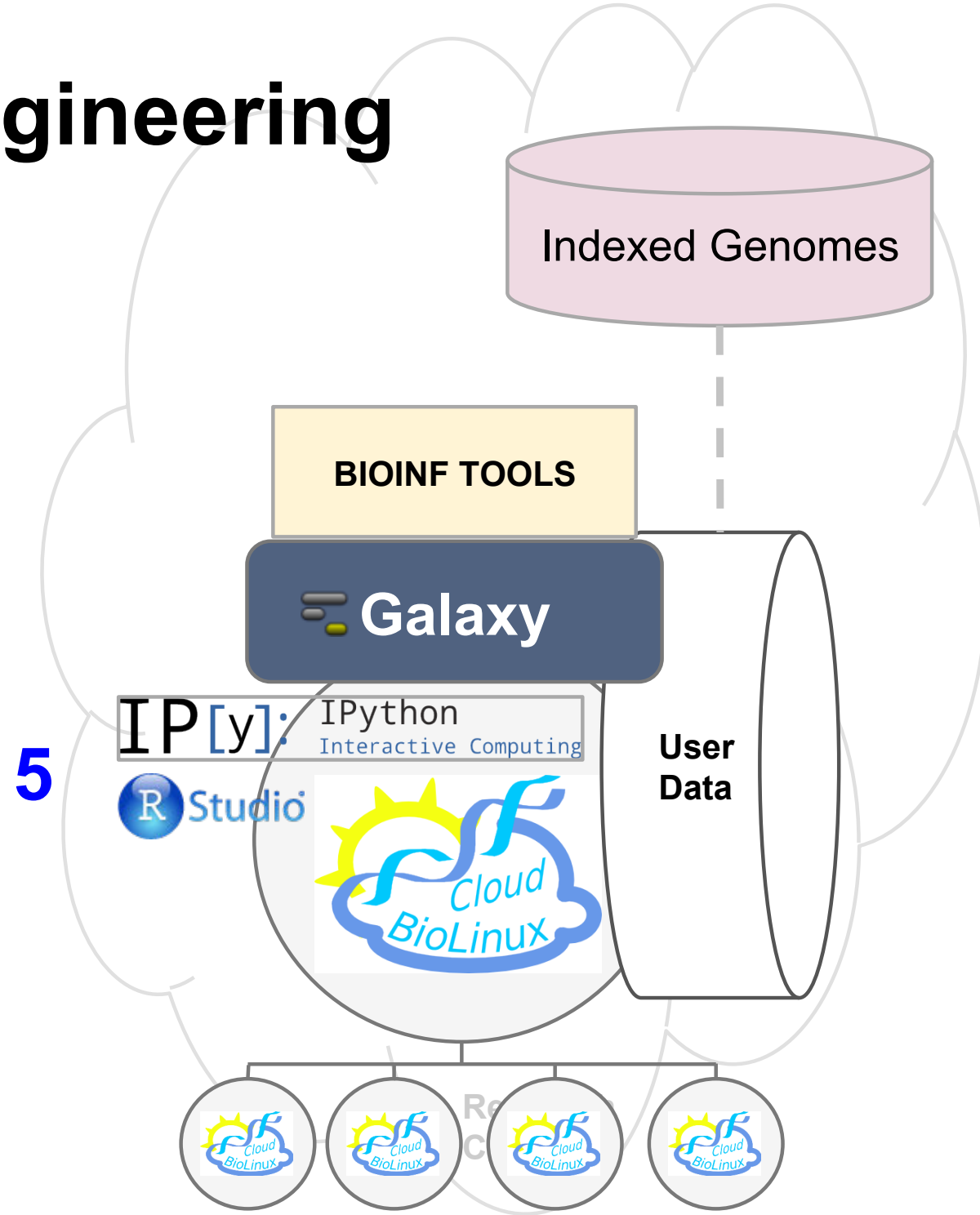

Workbench: All components

Management layer

CloudMan

GVL Launcher

Application layer

Galaxy

RStudio

IPython Interactive Computing

System layer

CloudBioLinux

GridEngine http://gridengine.sunsource.net

GlusterFS

Cloud layer

openstack CLOUD SOFTWARE

amazon web services™

Component build layer

Base

Galaxy FS

Ref data

GVL: Does it work?

Technically?

Practically?

http://genome.edu.au → GET

	Personal GVL	Server GVL	Cluster GVL
Suitable for	**Single user**	Single user Small group/lab	Large groups Institutions
Storage	**60GB**	100-5000GB	TBs
Compute	**2 cores**	8-64* cores	>50 cores
Requires	**NeCTAR account**	NeCTAR allocation: Compute and Volume storage	Large NeCTAR allocation of compute + user-provided fast storage
Runs on	**Any Research Cloud node**	RC nodes with volumes	RC nodes co-located with fast file system
Setup	**Automatic via website**	**Automatic via website**	Collaboration with GVL team
Configuration	**No configuration required**	Some configuration to tune analyses	Dedicated management

Lessons?

Defining and maintaining a set of tools is challenging

Providing per-user performance is challenging

The cloud is only so scalable!

Not all cloud nodes are equal

Geography matters

Lessons?

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Geography matters

Resourcing is key!

What's next for GVL?

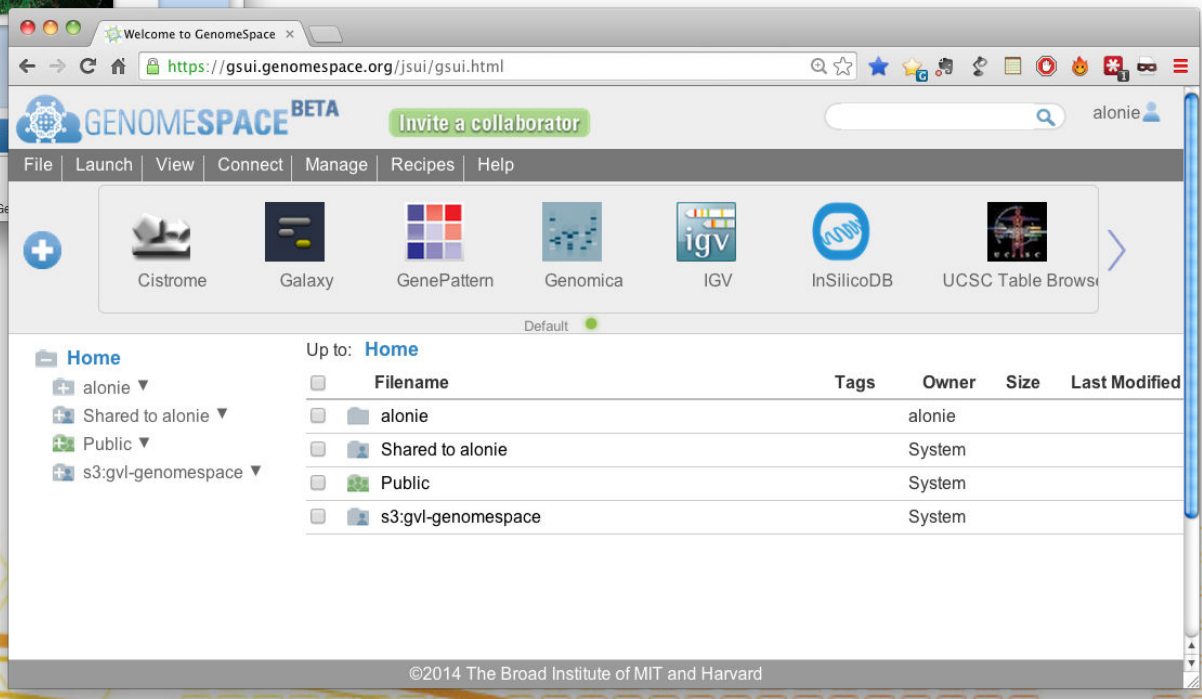
http://genome.edu.au

Moving data around is a problem

Whole genomes: 300GB raw data

We need to remove the desktop and USB sticks from the process!

Genomics lifecycle on the cloud: GenomeSpace



Making the GVL possible

Go8 Universities

- The University of Queensland
- The University of Melbourne
- Monash University
- The University of Sydney
- The University of Western Australia

Medical Research Institutes

- The Garvan Institute of Medical Research
- Victor Chang Cardiac Research Institute
- Baker IDI Heart and Diabetes Institute
- Peter MacCallum Cancer Centre

eResearch Agencies

- Queensland Facility for Advanced Bioinformatics (QFAB)
- Queensland Cyber Infrastructure Foundation (QCIF)
- Life Sciences Computation Centre (LSCC) at the VLSCI
- Victorian eResearch Strategic Initiative (VeRSI)

National Agencies

- NeCTAR, DIISRTE
- CSIRO
- EMBL Australia
- Bioplatforms Australia (BPA)
- Australian Genome Research Facility (AGRF)
- Australian National Data Service (ANDS)