CYVERSE®

Transforming Science Through Data-Driven Discovery

CyVerse Visual Interactive Computing Environment

Jason Williams
Cold Spring Harbor Laboratory, DNA Learning Center;
CyVerse EOT Lead
williams@cshl.edu
@JasonWilliamsNY

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CYVERSE®

Why use VICE?

How (most) applications in the Discovery Environment work

```
[root@localhost ~]# ping -q fa.wikipedia.org
PING text.pmtpa.wikimedia.org (208.80.152.2) 56(84) bytes of data.
^C
--- text.pmtpa.wikimedia.org ping statistics ---
1 packets transmitted, 1 received, 0% packet loss, time 0ms
rtt min/avg/max/mdev = 540.528/540.528/540.528/0.000 ms
[root@localhost ~]# pwd
/root
[root@localhost ~]# cd /var
[root@localhost var]# ls -la
total 72
drwxr-xr-x. 18 root root 4096 Jul 30 22:43 .
drwxr-xr-x. 23 root root 4096 Sep 14 20:42 ..
drwxr-xr-x.  2 root root 4096 May 14 00:15 account
drwxr-xr-x. 11 root root 4096 Jul 31 22:26 cache
drwxr-xr-x.  3 root root 4096 May 18 16:03 db
drwxr-xr-x.  3 root root 4096 May 18 16:03 empty
drwxr-xr-x.  2 root root 4096 May 18 16:03 games
drwxrwx--T.  2 root gdm  4096 Jun  2 18:39 gdm
drwxr-xr-x. 38 root root 4096 May 18 16:03 lib
drwxr-xr-x.  2 root root 4096 May 18 16:03 local
lrwxrwxrwx.  1 root root   11 May 14 00:12 lock -> ../run/lock
drwxr-xr-x. 14 root root 4096 Sep 14 20:42 log
lrwxrwxrwx.  1 root root   10 Jul 30 22:43 mail -> spool/mail
drwxr-xr-x.  2 root root 4096 May 18 16:03 nis
drwxr-xr-x.  2 root root 4096 May 18 16:03 opt
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drwxrwxrwt.  4 root root 4096 Sep 12 23:50 tmp
drwxr-xr-x.  2 root root 4096 May 18 16:03 yp
[root@localhost var]# yum search wiki
Loaded plugins: langpacks, presto, refresh-packagekit, remove-with-leaves
rpmfusion-free-updates                                          | 2.7 kB     00:00
rpmfusion-free-updates/primary_db                               | 206 kB     00:04
rpmfusion-nonfree-updates                                       | 2.7 kB     00:00
updates/metalink                                                | 5.9 kB     00:00
updates                                                         | 4.7 kB     00:00
updates/primary_db                      73% [=================       ]  62 kB/s | 2.6 MB     00:15 ETA
```

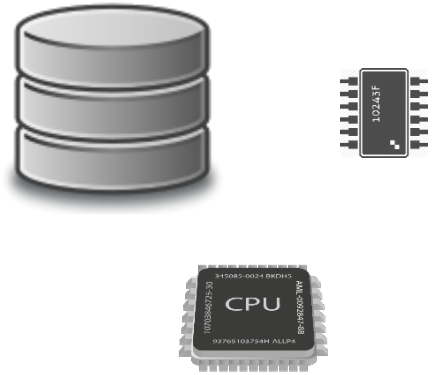

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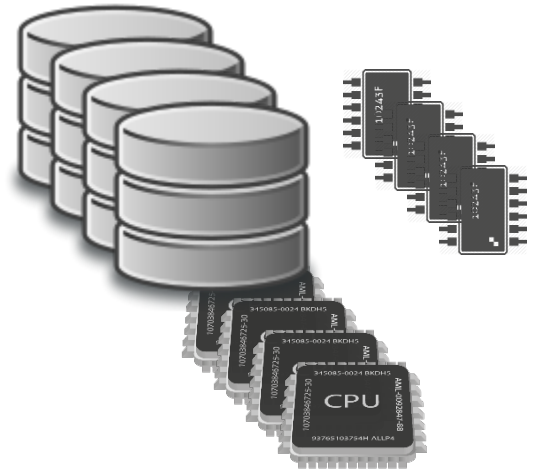

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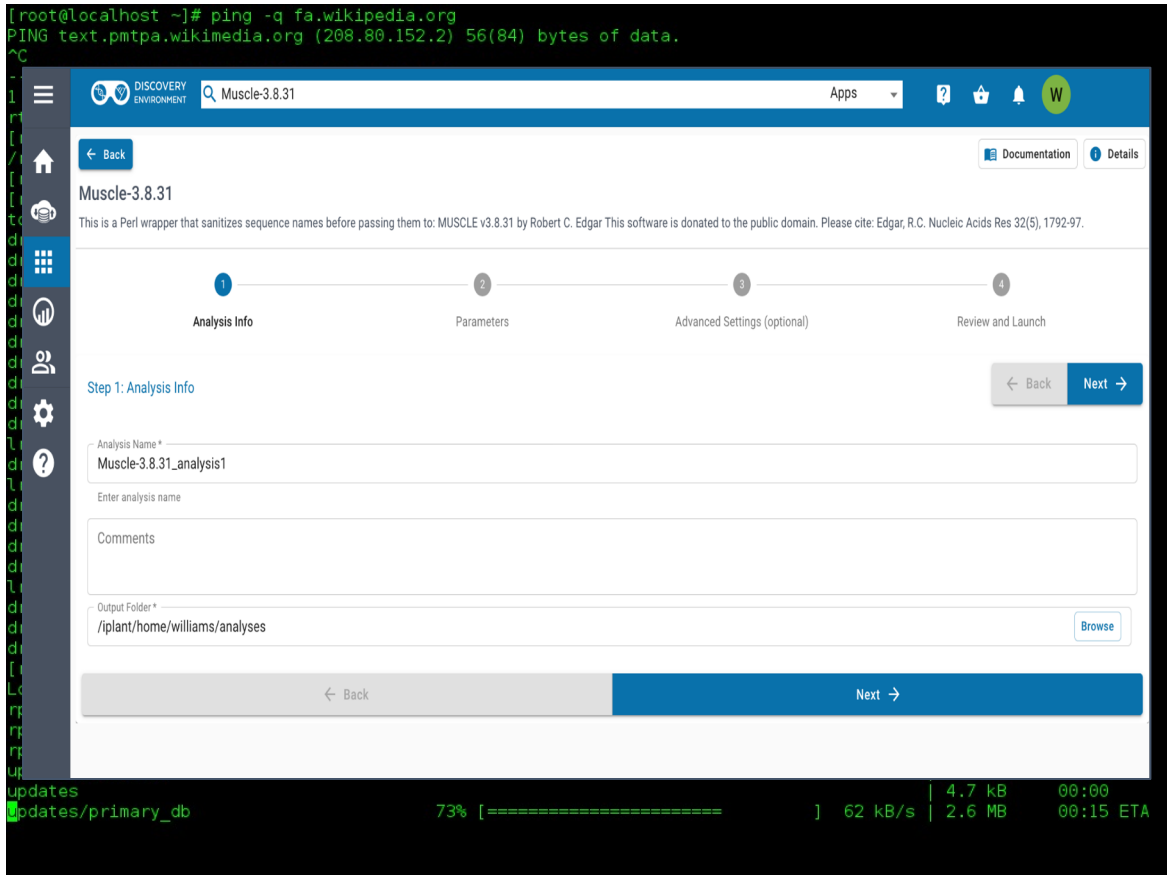

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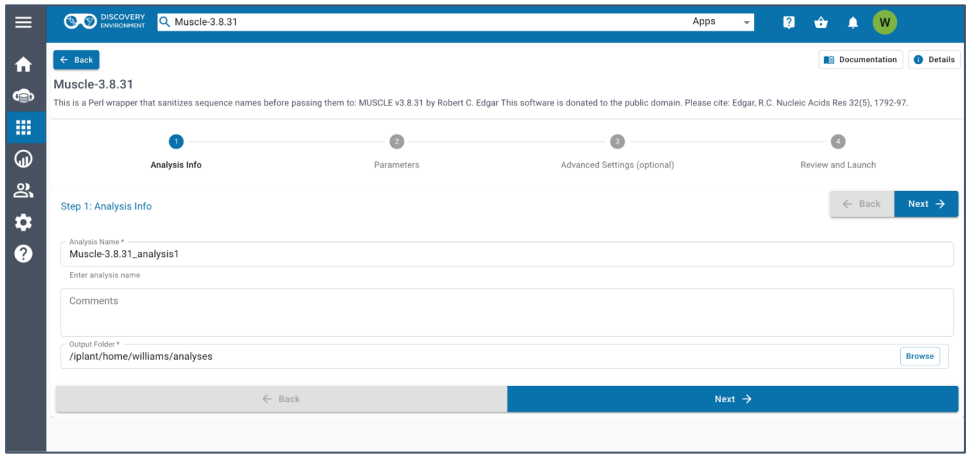
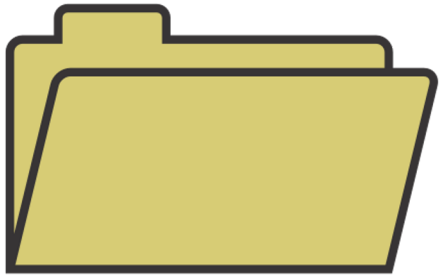


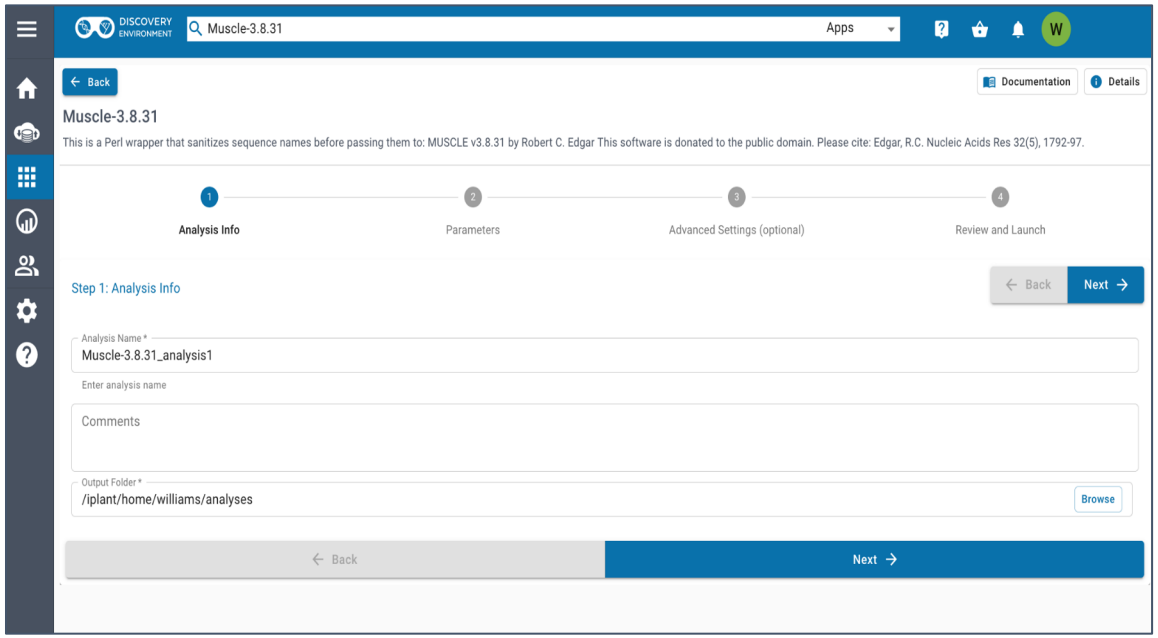


(non-interactive)

What if you want to…

- See and adjust intermediate steps in an analysis
- Use an application that has a graphical user interface (GUI)
- Make data visualization easy for you and your collaborators\students

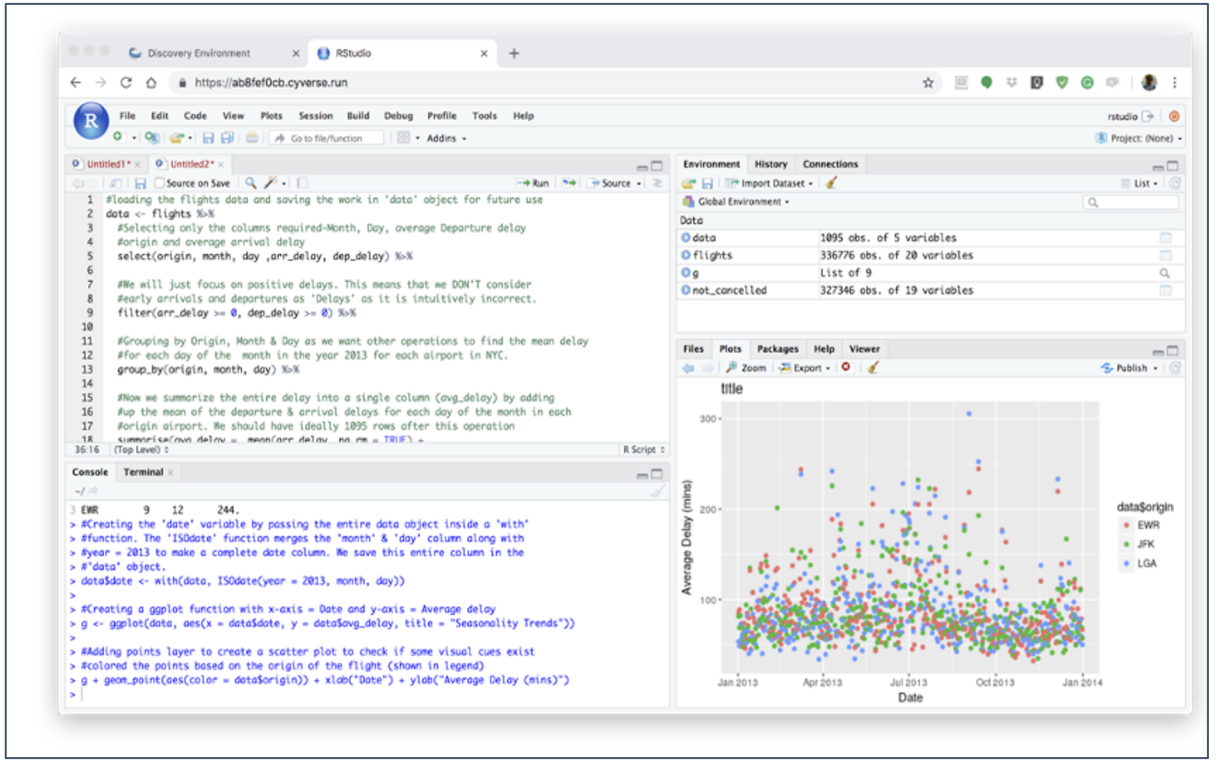
What VICE application enable



(Interactive)

Visual Interactive Computing Environment (VICE)

- Interactively manipulate analyses and visualize data



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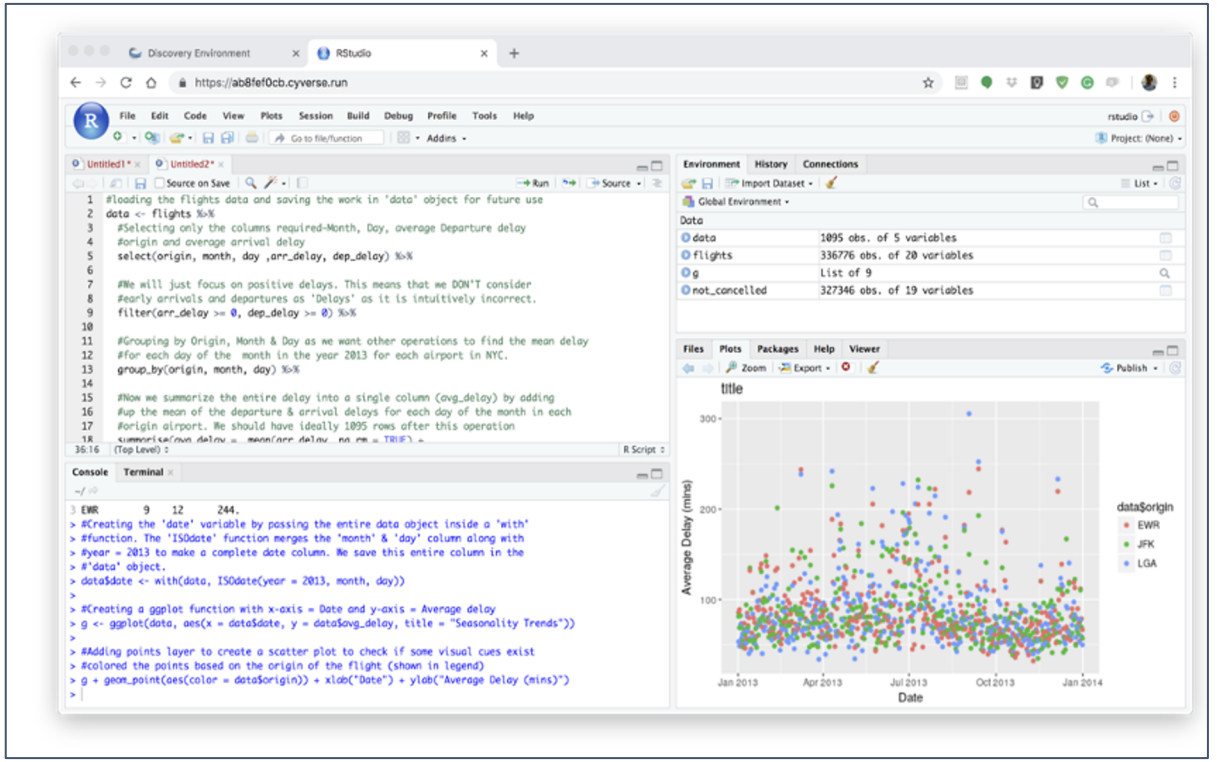
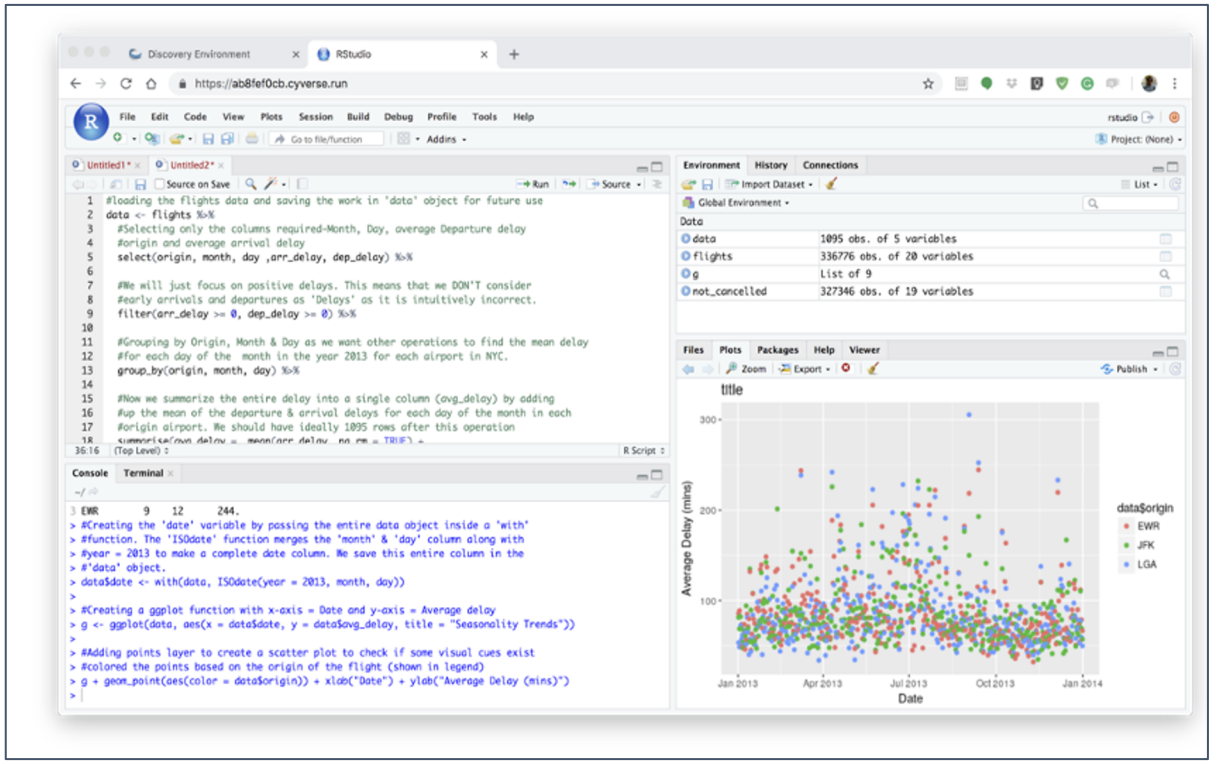


Visual Interactive Computing Environment (VICE)

- Interactively manipulate analyses and visualize data
- Run popular applications such as Jupyter, RStudio, RShiny, Linux shell and more
- Allows users to launch web applications packaged into the DE (Docker)

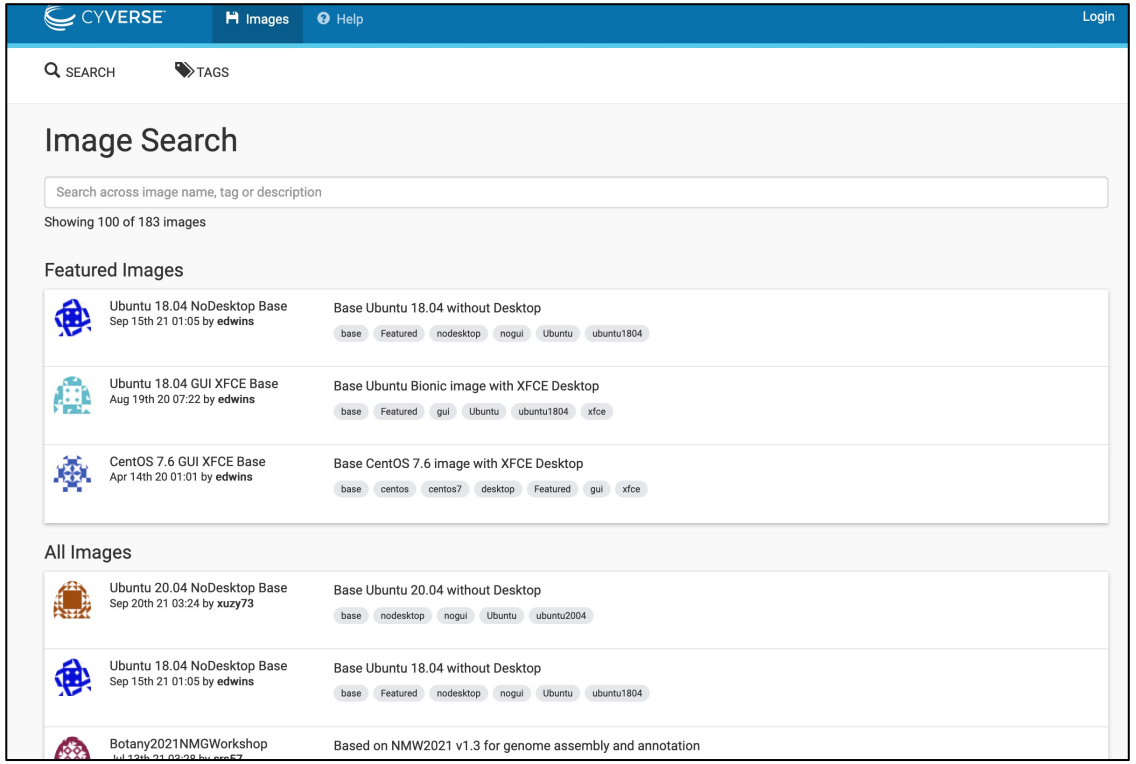


VICE advantages

- No restriction on data limits
- Secure environment
- User can select/create custom computing environments
- Longer run times
- Highly scalable
- Share both apps and analyses

Focusing the Atmosphere use case

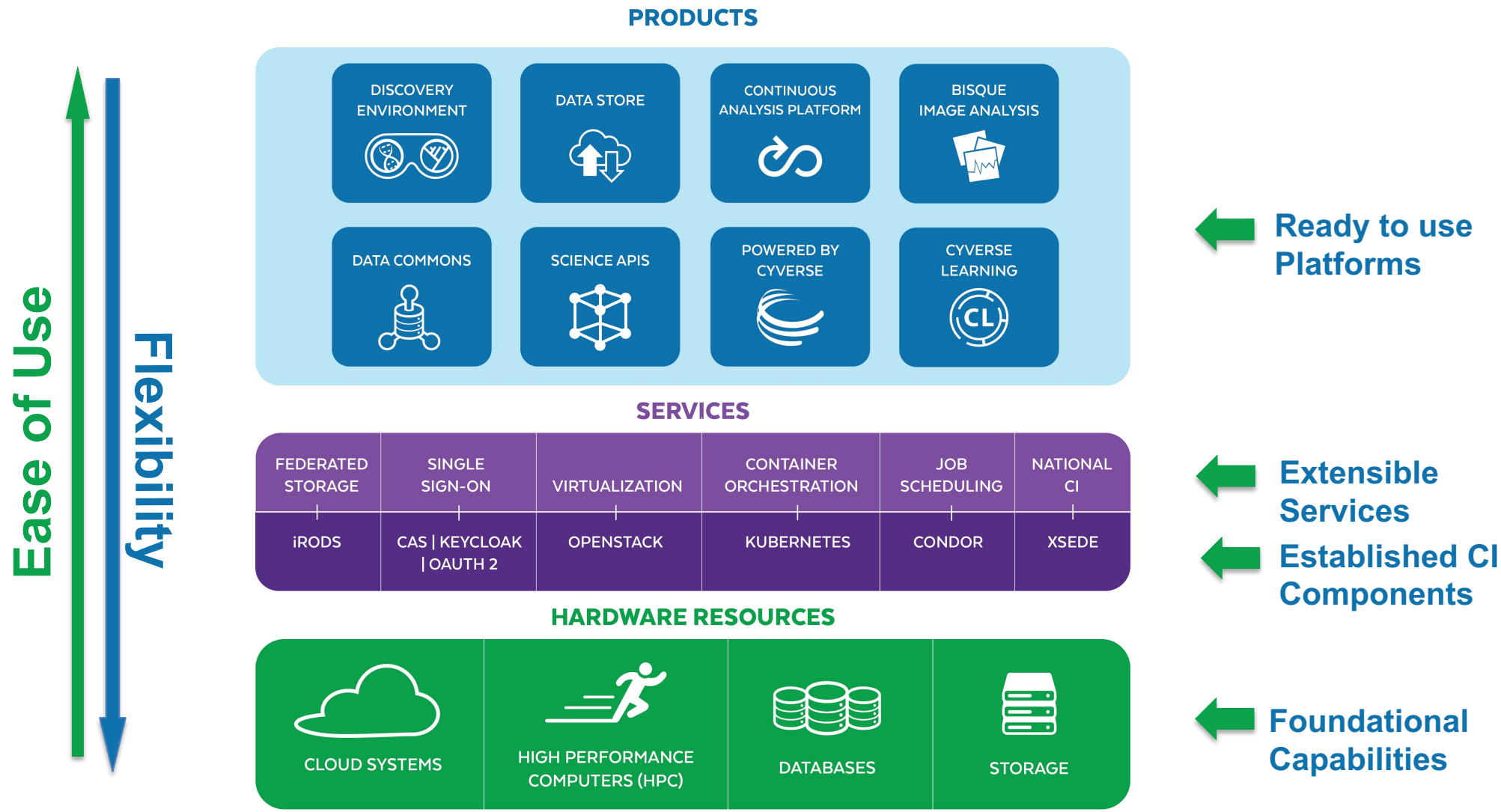
- Users who need to work with a GUI
- Using one or a few apps (again often involving visualization)
- Atmosphere still available for development purposes; JetStream for general purpose use



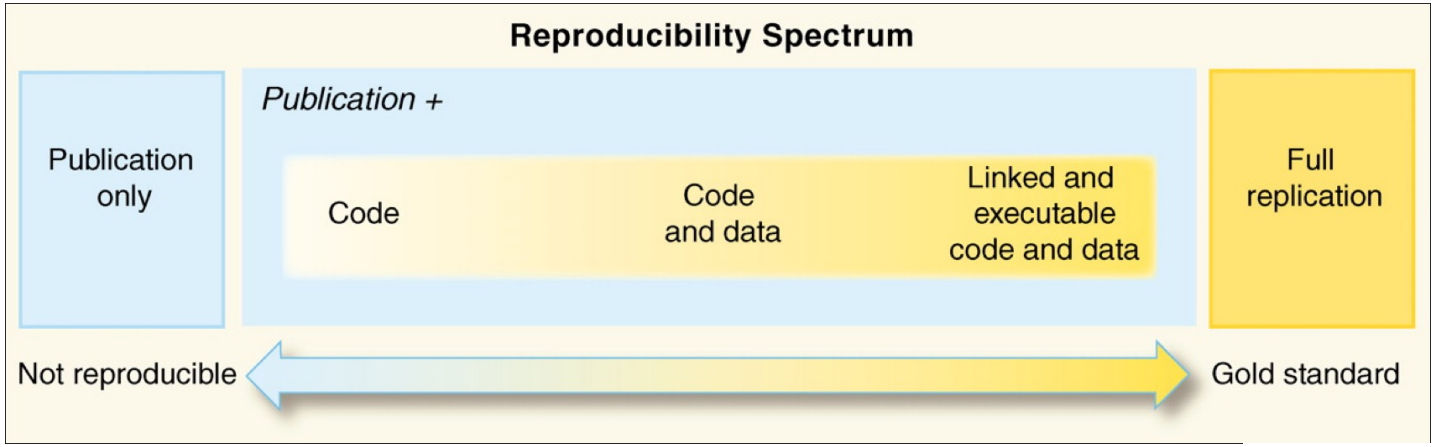
VICE reminders

- Available on the US (cyverse.org) DE
- Authorization required to use (user.cyverse.org)
- Runtimes are for 48 hours by default
- Data transfer and mounting

VICE reminders



VICE reminders



Peng, 2011 Science DOI: 10.1126/science.1213847

3rd party technologies

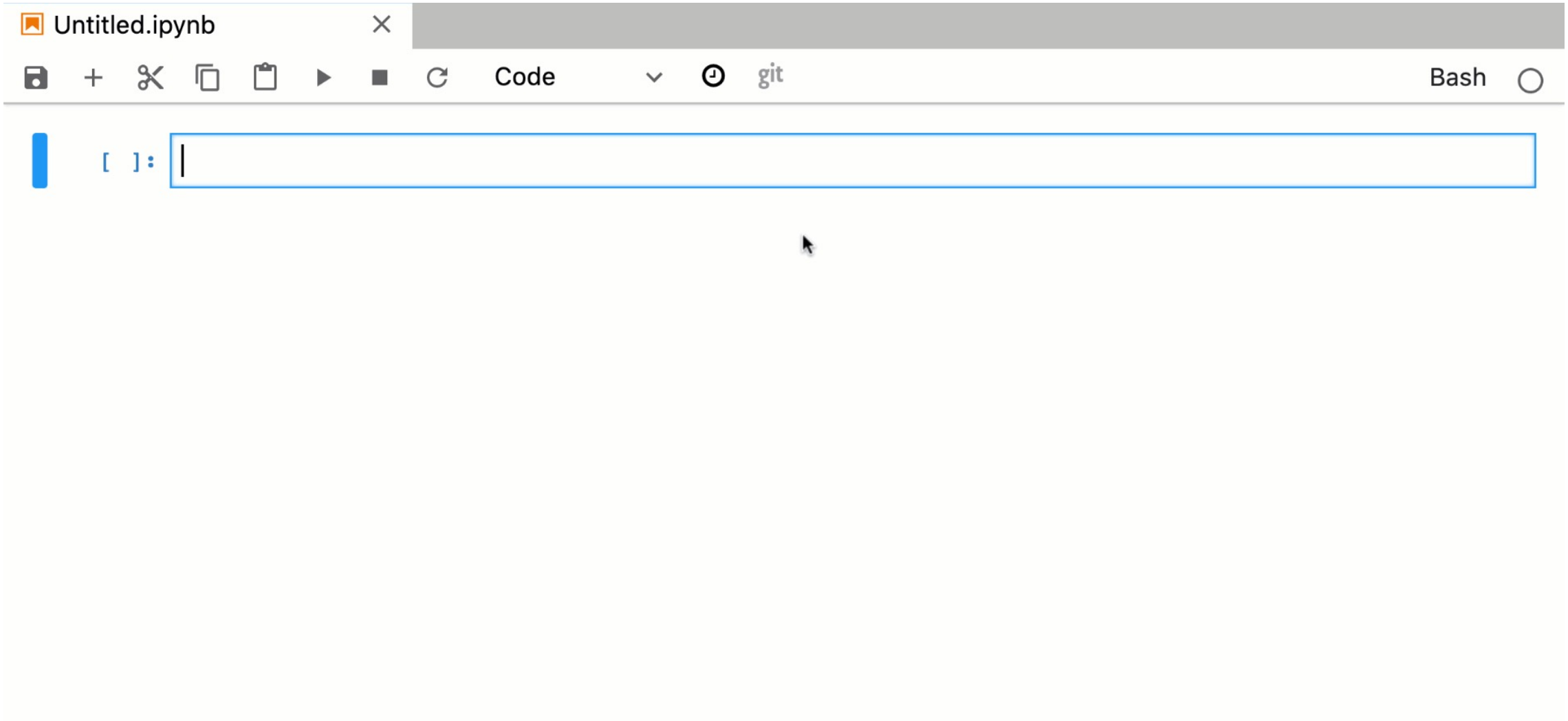
CyVerse CI Platforms

External Repositories and Compute

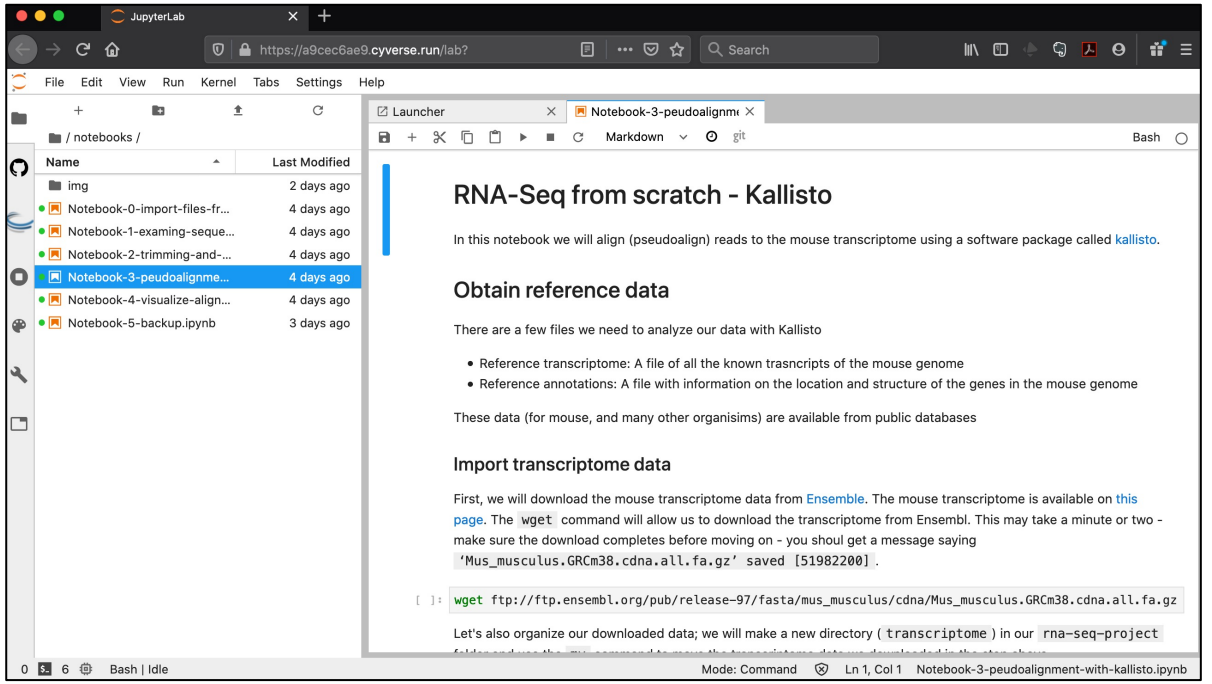
VICE example use case

Project Jupyter exists to develop open-source software, open-standards, and services for interactive computing across dozens of programming languages.

VICE example use case



VICE example use case: RNA-Seq w/Jupyter



0 - Import from SRA

1 - Sequence QC

2 - Sequencing Trimming

3 - Read Pseudoalignment

4 - Read Visualization

5 - Data Backup

VICE example use case: RNA-Seq w/Jupyter

Import transcriptome data

First, we will download the mouse transcriptome data from Ensemble. The mouse transcriptome is available on this page. The `wget` command will allow us to download the transcriptome from Ensembl. This may take a minute or two - make sure the download completes before moving on - you shoul get a message saying `'Mus_musculus.GRCm38.cdna.all.fa.gz' saved [51982200]`.

```
[ ]: wget ftp://ftp.ensembl.org/pub/release-97/fasta/mus_musculus/cdna/Mus_musculus.GRCm38.cdna.all.fa.gz
```

Let's also organize our downloaded data; we will make a new directory (`transcriptome`) in our `rna-seq-project` folder and use the `mv` command to move the transcriptome data we downloaded in the step above.

```
[ ]: mkdir -p /home/gea_user/rna-seq-project/transcriptome && mv Mus_musculus.GRCm38.cdna.all.fa.gz /home/
```

Index transcriptome

We will now use Kallisto's indexing function to prepare the transcriptome for analysis. The "Index" is a lookup table for the transcriptome that allows it to be more easily searched by Kallisto. First let's organize our files by creating a new directory to hold our kallisto work.

```
[ ]: mkdir -p /home/gea_user/rna-seq-project/kallisto
```

Code is there when you need it

VICE example use case: RNA-Seq w/Jupyter

2. Complete the code below to trim your reads. Make sure that you change `INPUT` and `OUTPUT` to reflect your file(s). If you are working with more than one file, see the bonus exercise.

- INPUT - should be the name of your file
- OUTPUT - should be changed so that the prefix of the file (e.g. SRR5017XXX) is followed by `_trimmed.fastq.gz`

```
[ ]: trimmomatic SE INPUT OUTPUT -threads 8 SLIDINGWINDOW:4:20 MINLEN:75
```

3. Move your trimmed files to our previously created output folder (no need to change this code)

```
[ ]: mv *_trimmed.fastq.gz /home/gea_user/rna-seq-project/trimmed-reads
```

4. Complete the cells below to change directories into the trimmed-reads folder and run `fastqc`

```
[ ]: cd
```

```
[ ]: fastqc
```

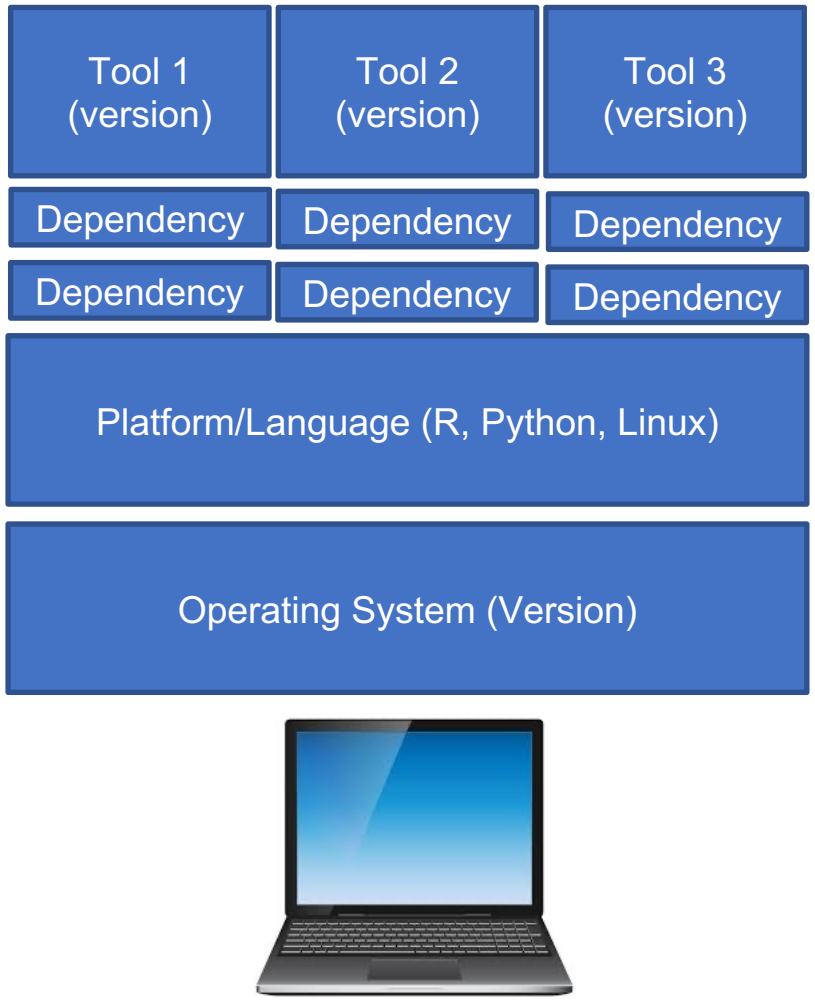
Using the Jupyter Labs files browser you can navigate to the `trimmed-reads` folder in `rna-seq-project` to view your fastqc results

Teaching code/command line with faded examples

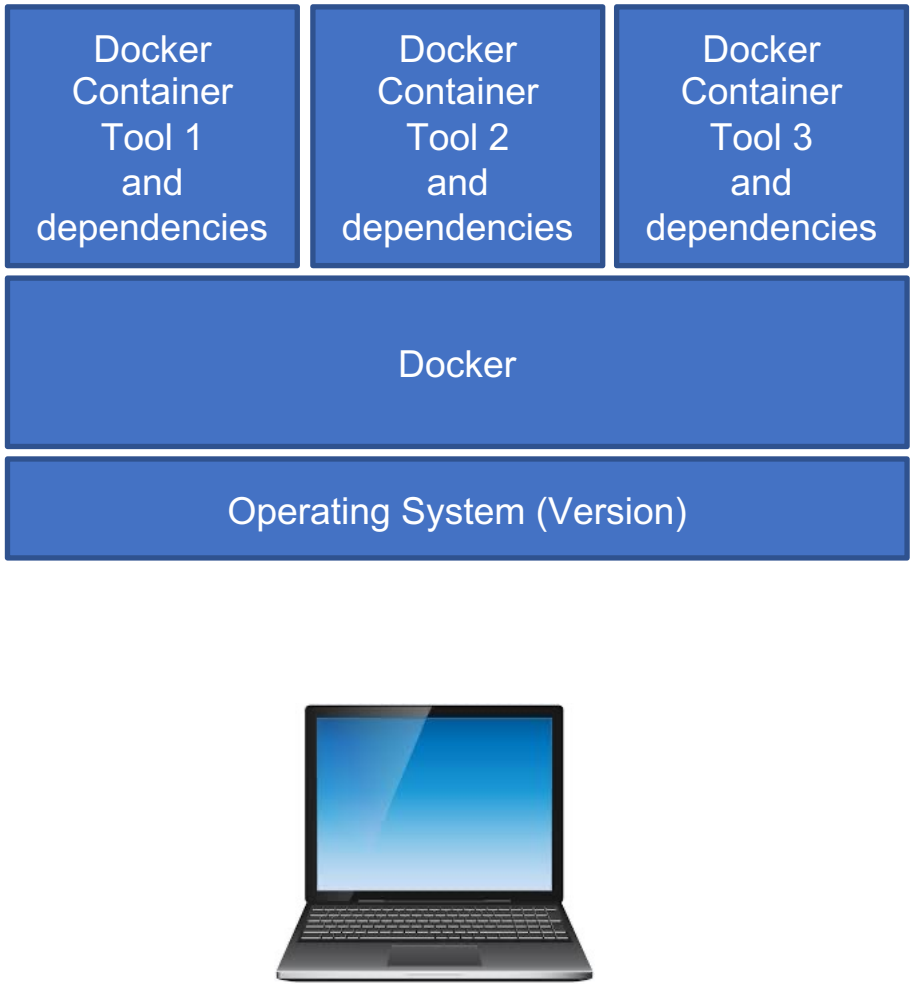
Advanced – Customizing VICE

Advanced – Customizing VICE

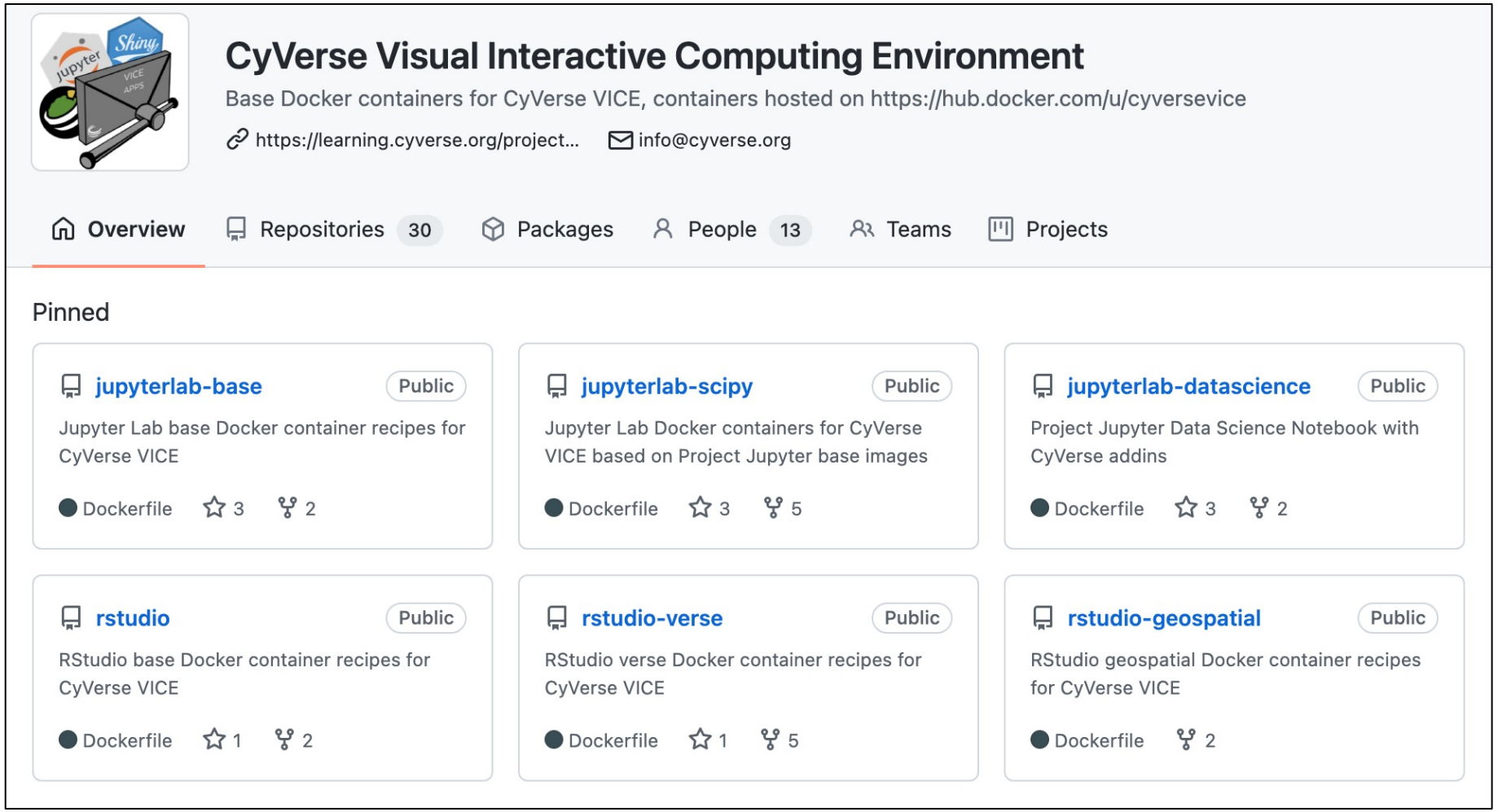
Tools and dependencies separate



Tools and dependencies bundled



Advanced – Customizing VICE



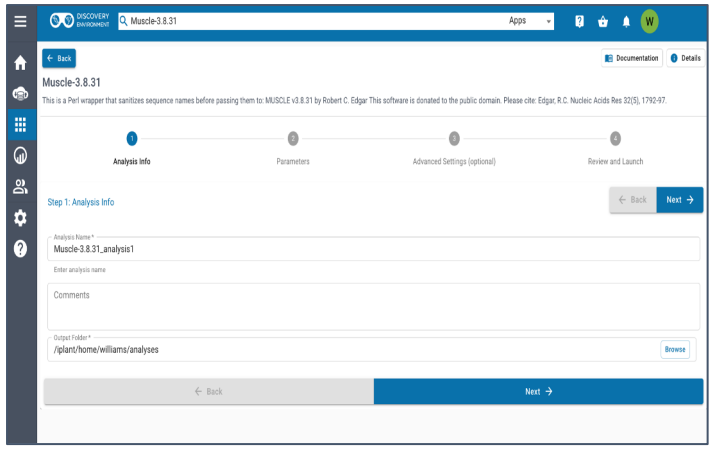
Advanced – Customizing VICE

1. Write a Dockerfile

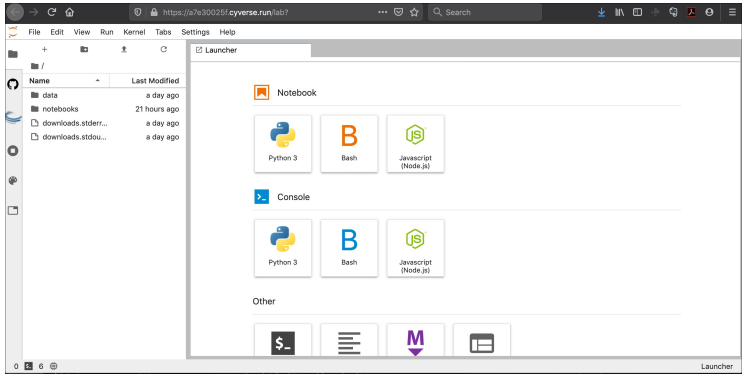
```
# Install bioconda packages
RUN /opt/conda/bin/conda install -y -q fastqc=0.11.7=5
RUN /opt/conda/bin/conda install -y -q trimmomatic=0.38=0
RUN /opt/conda/bin/conda install -y -q sra-tools=2.9.6=hf484d3e_0
RUN /opt/conda/bin/conda install -y -q parallel-fastq-dump=0.6.5=py_0
RUN /opt/conda/bin/conda install -y -q kallisto=0.46.0=hb6a4e58_0
RUN /opt/conda/bin/conda install -y -q fastp=0.20.0=hdbcaa40_0
#
```

2. Push container to CyVerse

3. Create an interface and get button



4. Use your tools



Learning.cyverse.org