Vital-IT
High Performance Computing Center

@HPCevent_171018

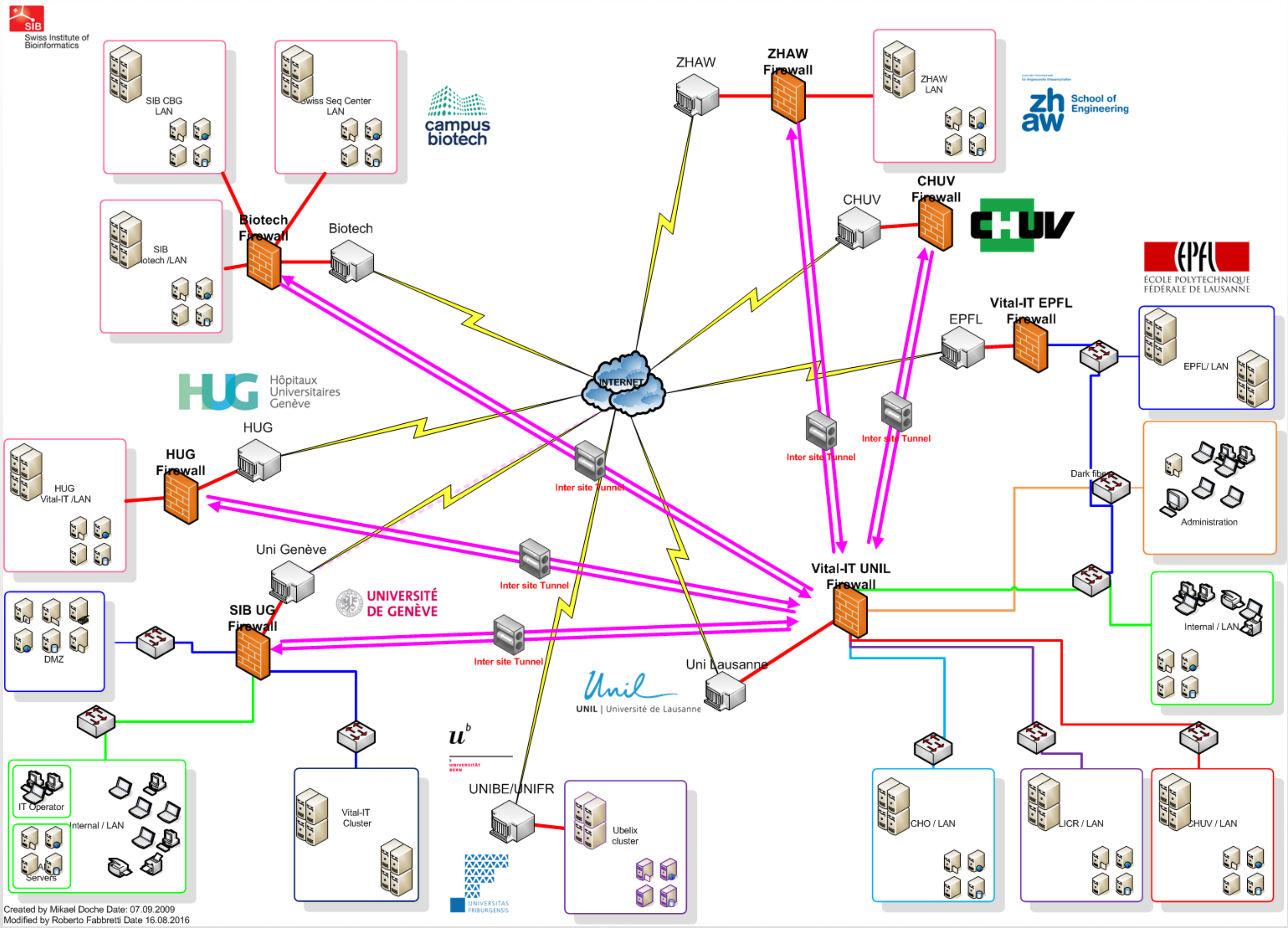
A Data Science's Perspective of the Use of Containers.

Bioinformatics x Digital humanities

martial.sankar@sib.swiss

Vital-IT, lead by **I. Xenarios**, Competency Centre in Bioinformatics and Computational Biology that provides **infrastructure**, **support and technological R&D** for life science and clinical research.

Vital-IT Embassies



Created by Mikael Doche Date: 07.09.2009
Modified by Roberto Fabbretti Date 16.08.2016

Vital-IT Key Numbers

77 scientists

12 seniors

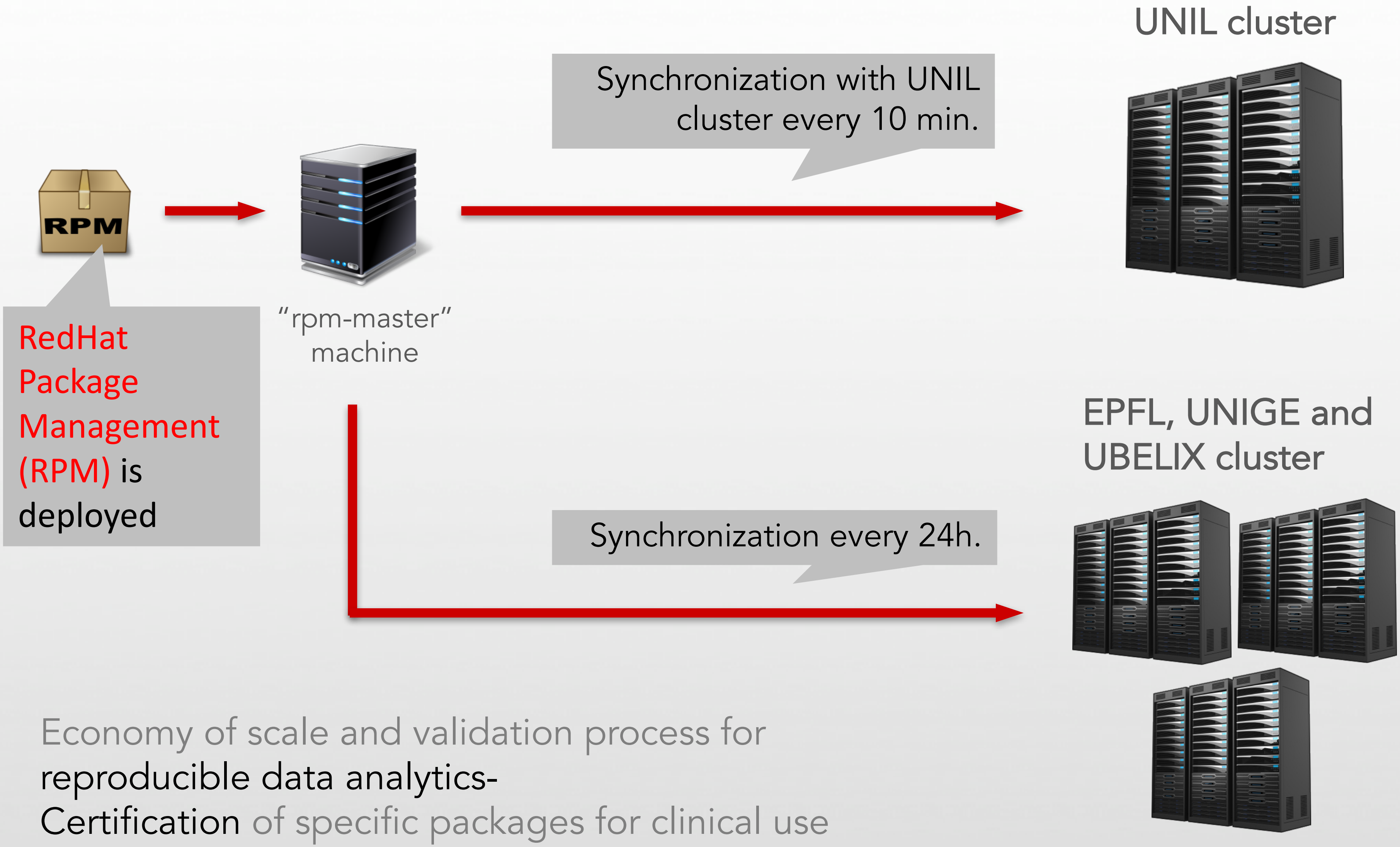
1 COO

14 Life-Science tech. platforms and “core” facilities entrust Vital-IT with their data

2’500 packaged and verified/certified softwares maintained as RPM release

Maintaining and deploying “Fedora-like” Scientific packages

Enabling reproducible science



RedHat Package Management (RPM) is deployed

“rpm-master” machine

Synchronization with UNIL cluster every 10 min.

UNIL cluster

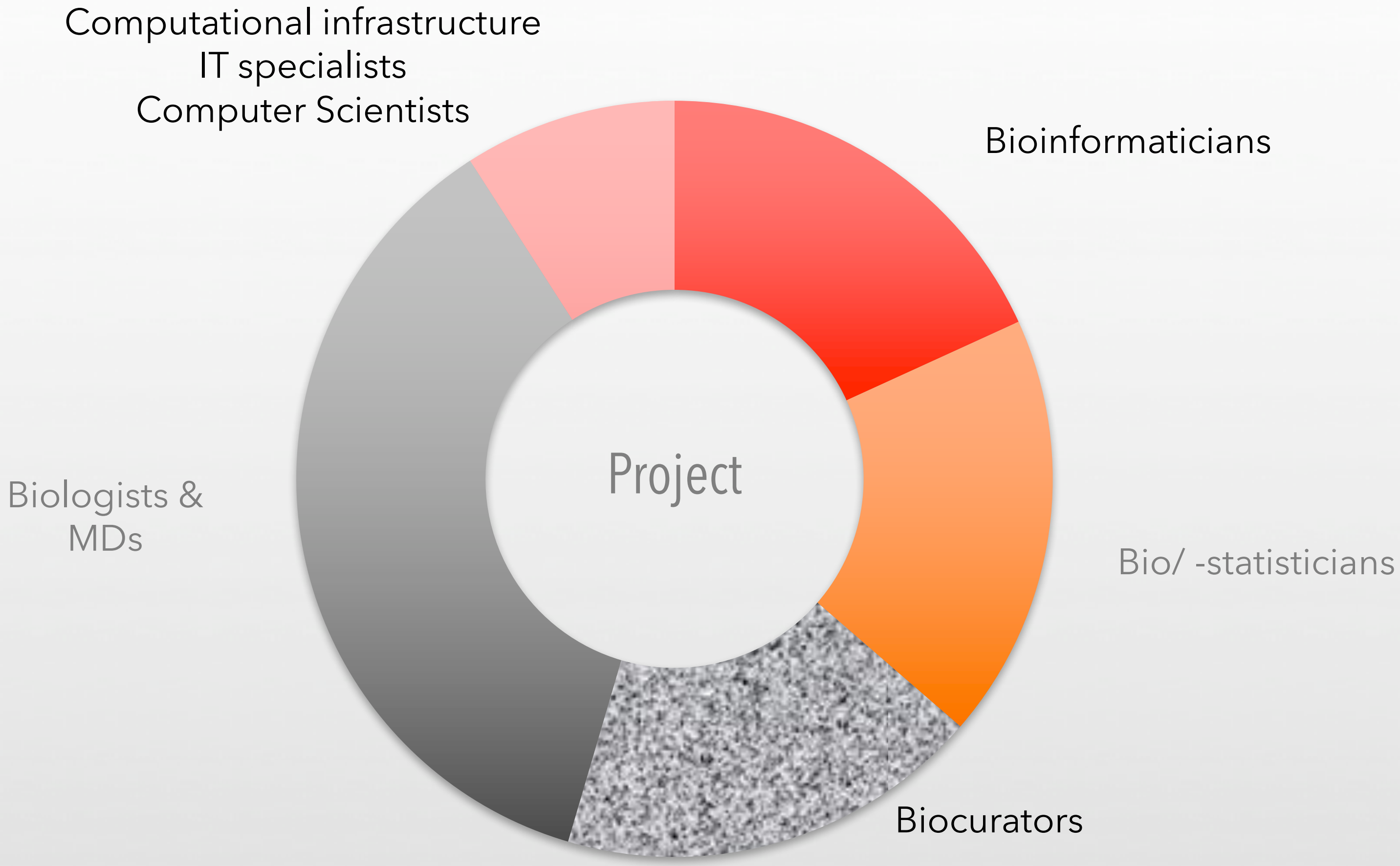
Synchronization every 24h.

EPFL, UNIGE and UBELIX cluster

Economy of scale and validation process for reproducible data analytics-

Certification of specific packages for clinical use

Industry-like approach to research projects



Various projects – diversity of competencies

Wide range of Issues

Solving collaborators/customers Issues

Portability of pipeline/tools with/wo complex setup

, Reproducibility

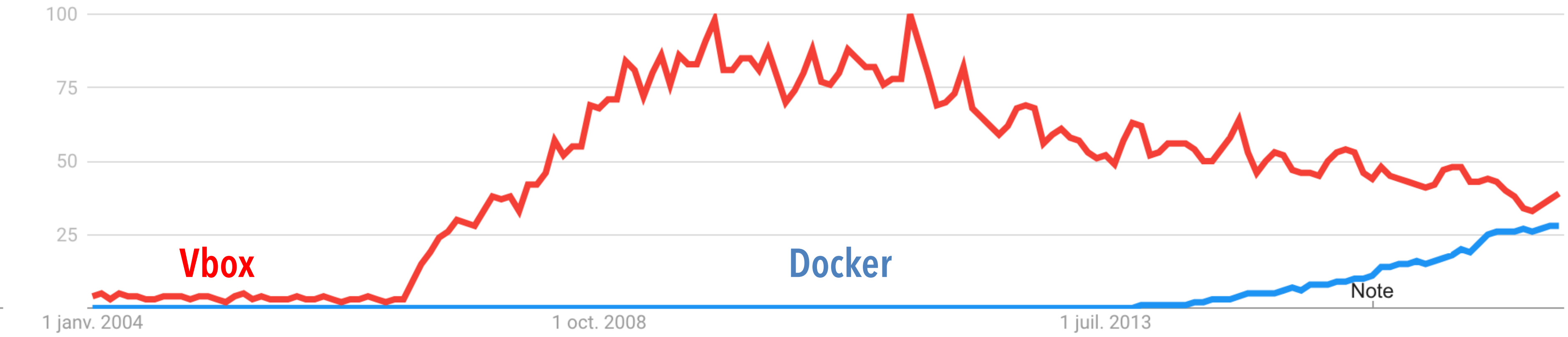
, Interoperability and Safety

& Others.

> “ PACKAGE THE APPLICATION INTO A **STANDARDIZED UNIT** FOR SOFTWARE DEVELOPMENT

Source : https://www.docker.com/what-docker

Docker trends

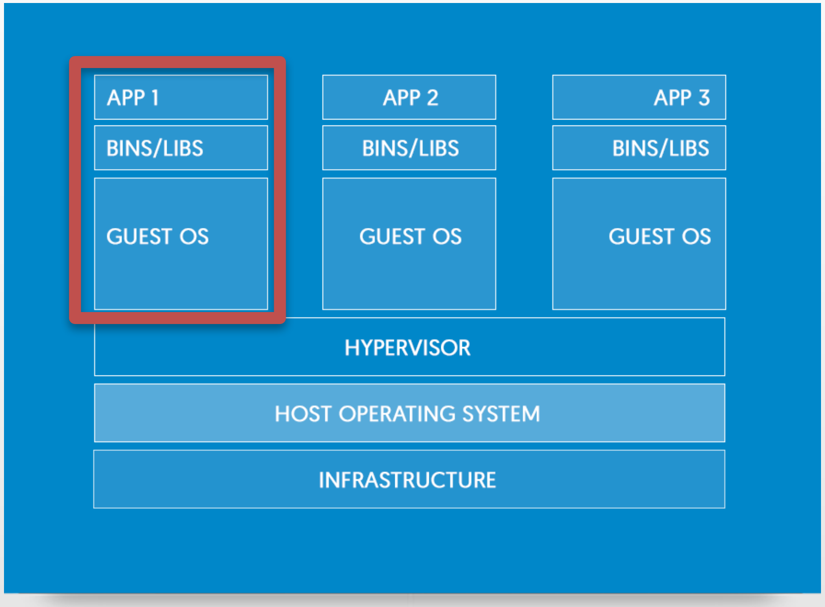


Source : google trends

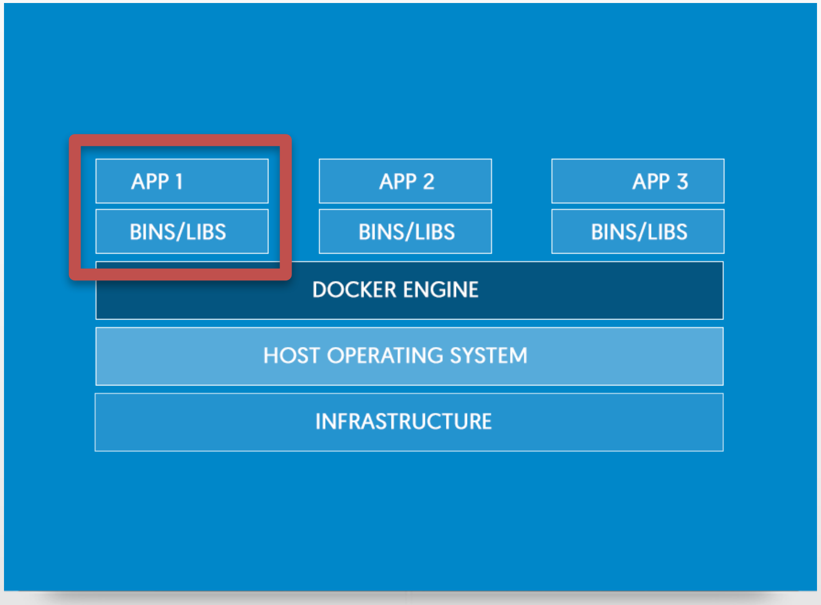
Focus on Application

Docker vs classic Vbox

Virtual machine



Docker Container



Source : https://www.docker.com/what-docker

Key advantages

Lightweight

,Versatile

~~, & “Secure by default”.~~

Drawbacks

Security breach

, MPI not supported

& HPC is not the target segment.

Singularity

Solving collaborators/customers Issues

Portability of pipeline/tools with/wo complex setup

, Reproducibility

, Interoperability and Safety

& Others.

Portability

Center of Experimental Pathology

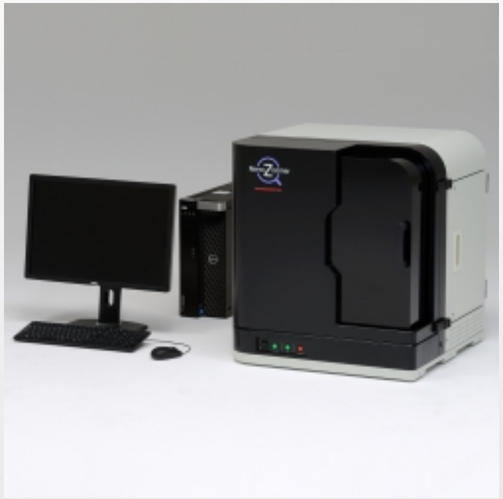
Collaboration

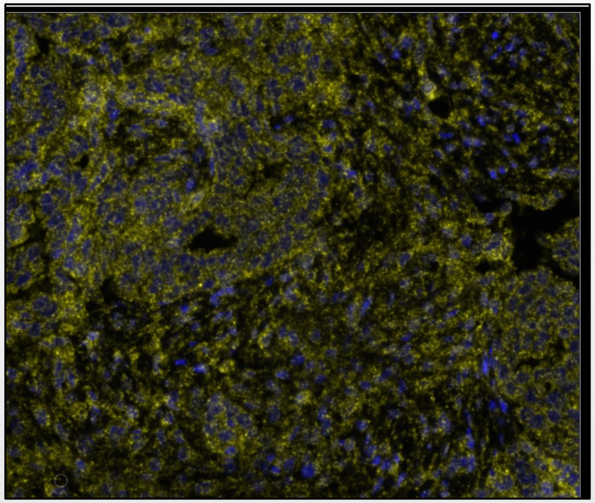
With O. Martin, R. Engler & N. Guex

Collaboration : Rusakiewicz S.(CHUV) & Danenberg E. (CHUV)

NDP.READ

SDK used to access image data in proprietary format (produced by the Hamamatsu NanoZoomer digital slide scanner).

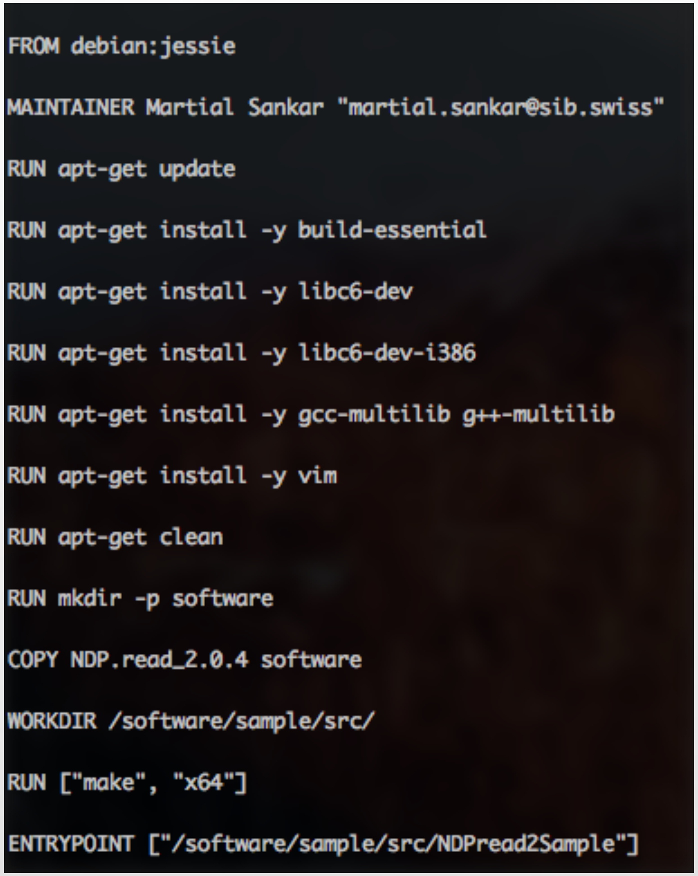




Issue : NDP.Read SDK only for specific Windows version and Linux.

NDP.READ

Dockerfile



```
FROM debian:jessie

MAINTAINER Martial Sankar "martial.sankar@sib.swiss"

RUN apt-get update

RUN apt-get install -y build-essential

RUN apt-get install -y libc6-dev

RUN apt-get install -y libc6-dev-i386

RUN apt-get install -y gcc-multilib g++-multilib

RUN apt-get install -y vim

RUN apt-get clean

RUN mkdir -p software

COPY NDP.read_2.0.4 software

WORKDIR /software/sample/src/

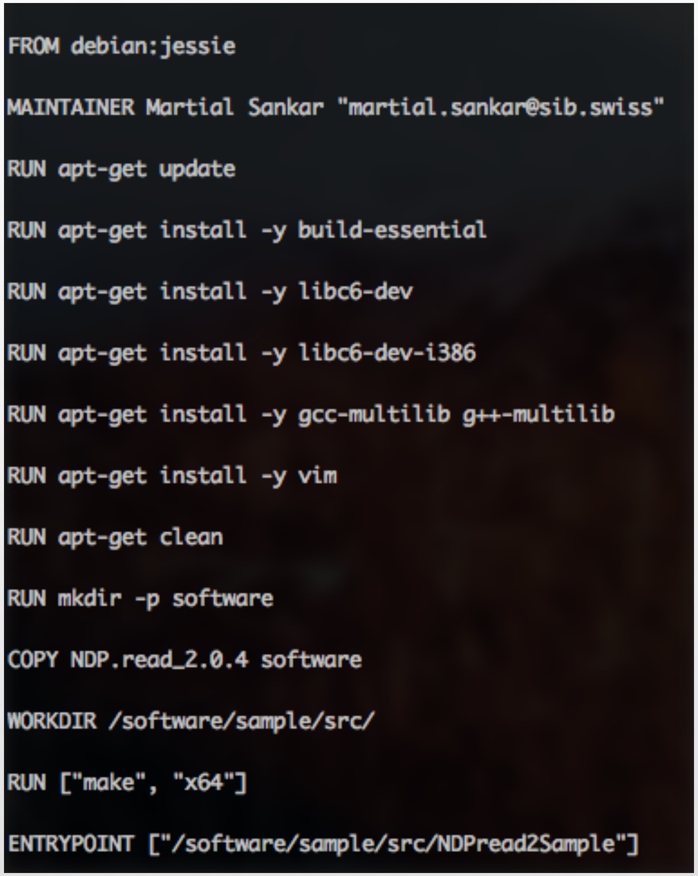
RUN ["make", "x64"]

ENTRYPOINT ["/software/sample/src/NDPread2Sample"]
```

```
$ docker run -it raw/ndpreadraw
```

NDP.READ

Dockerfile



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```

```
$ docker run -it raw/ndpreadraw
```

Cross-platform,

Bypassing installation procedure.

SourceData

Making Figures Discoverable

With A. Chasapi, J. Delafontaine, L. Gotz, I. Crespo, I. Xenarios & R. Liechti

Collaboration : T. Lemberger (EMBO), E. B. Garagorri (EMBO), N. George (EMBO), S. El-Gebali (EMBO), E. Boutet (Swiss-Prot), N. Nouspikel (Swiss-Prot)

EMBO excellence in life sciences

Robert Bosch Stiftung

Collaborative effort

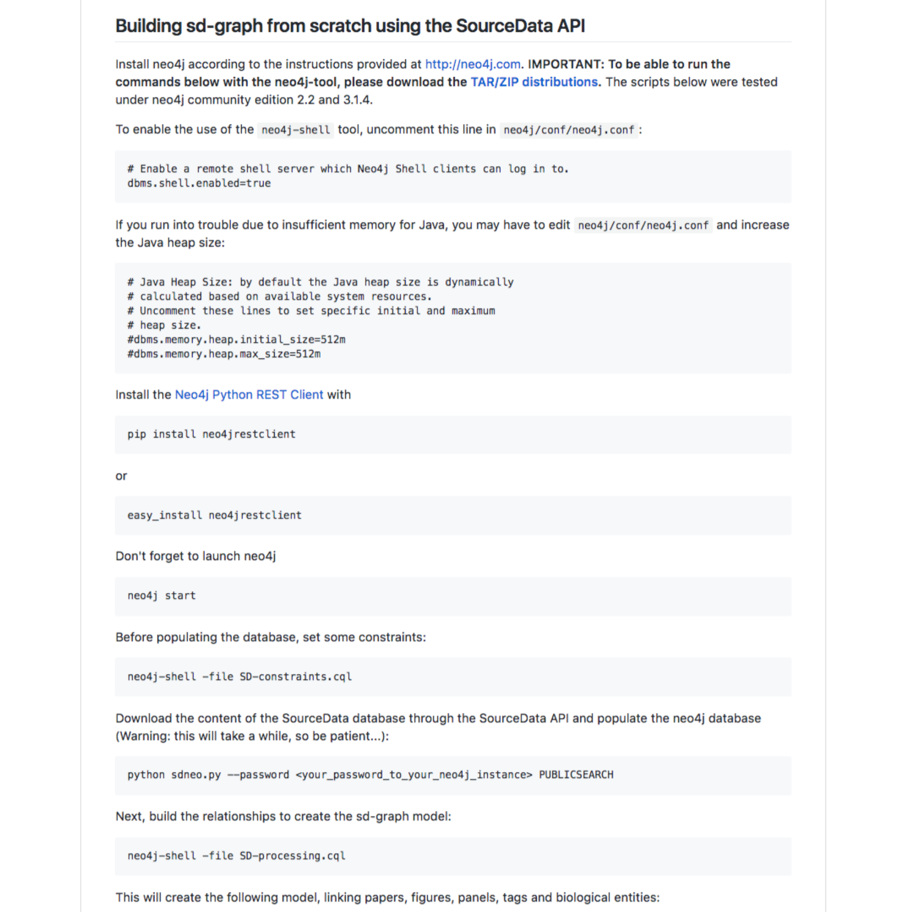
nature publishing group npg HighWire WILEY EMBOpress

Figure centered- data curation

Curation by experts & validation by authors

Data are stored in semantic graph using neo4j.

Mining the source data graph database



Building sd-graph from scratch using the SourceData API

Install neo4j according to the instructions provided at http://neo4j.com. **IMPORTANT: To be able to run the commands below with the neo4j-tool, please download the TAR/ZIP distributions.** The scripts below were tested under neo4j community edition 2.2 and 3.1.4.

To enable the use of the `neo4j-shell` tool, uncomment this line in `neo4j/conf/neo4j.conf` :

```
# Enable a remote shell server which Neo4j Shell clients can log in to.
dbms.shell.enabled=true
```

If you run into trouble due to insufficient memory for Java, you may have to edit `neo4j/conf/neo4j.conf` and increase the Java heap size:

```
# Java Heap Size: by default the Java heap size is dynamically
# calculated based on available system resources.
# Uncomment these lines to set specific initial and maximum
# heap size.
#dbms.memory.heap.initial_size=512m
#dbms.memory.heap.max_size=512m
```

Install the Neo4j Python REST Client with

```
pip install neo4jrestclient
```

or

```
easy_install neo4jrestclient
```

Don't forget to launch neo4j

```
neo4j start
```

Before populating the database, set some constraints:

```
neo4j-shell -file SD-constraints.cql
```

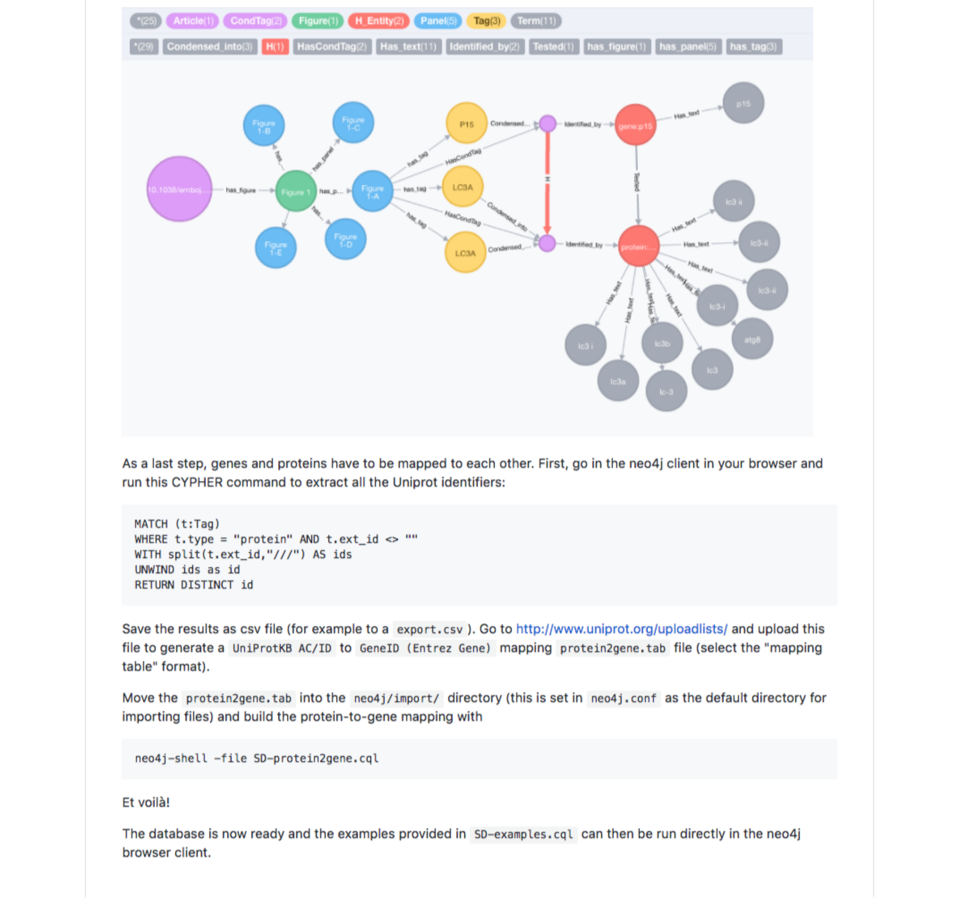
Download the content of the SourceData database through the SourceData API and populate the neo4j database (Warning: this will take a while, so be patient...):

```
python sdneo.py --password <your_password_to_your_neo4j_instance> PUBLICSEARCH
```

Next, build the relationships to create the sd-graph model:

```
neo4j-shell -file SD-processing.cql
```

This will create the following model, linking papers, figures, panels, tags and biological entities:



As a last step, genes and proteins have to be mapped to each other. First, go in the neo4j client in your browser and run this CYPHER command to extract all the Uniprot identifiers:

```
MATCH (t:Tag)
WHERE t.type = "protein" AND t.ext_id <> ""
WITH split(t.ext_id,"///") AS ids
UNWIND ids as id
RETURN DISTINCT id
```

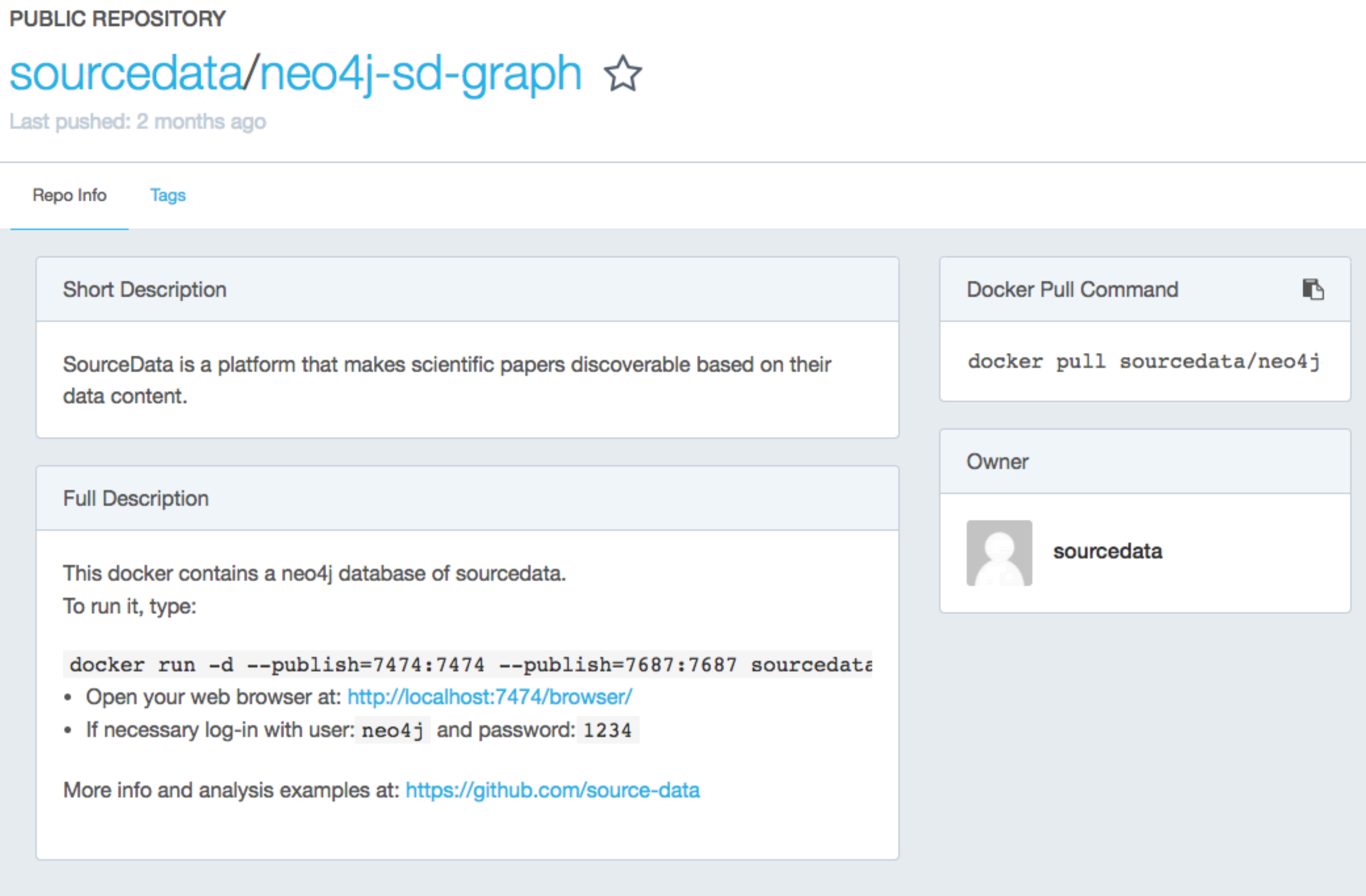
Save the results as csv file (for example to a `export.csv`). Go to http://www.uniprot.org/uploadlists/ and upload this file to generate a `UniProtKB AC/ID` to `GeneID (Entrez Gene)` mapping `protein2gene.tab` file (select the "mapping table" format).

Move the `protein2gene.tab` into the `neo4j/import/` directory (this is set in `neo4j.conf` as the default directory for importing files) and build the protein-to-gene mapping with

```
neo4j-shell -file SD-protein2gene.cql
```

Et voilà!

The database is now ready and the examples provided in `SD-examples.cql` can then be run directly in the neo4j browser client.



PUBLIC REPOSITORY

sourcedata/neo4j-sd-graph ☆

Last pushed: 2 months ago

Short Description

SourceData is a platform that makes scientific papers discoverable based on their data content.

Full Description

This docker contains a neo4j database of sourcedata.
To run it, type:

```
docker run -d --publish=7474:7474 --publish=7687:7687 sourcedata
```

- Open your web browser at: http://localhost:7474/browser/
- If necessary log-in with user: `neo4j` and password: `1234`

More info and analysis examples at: https://github.com/source-data

Docker Pull Command

```
docker pull sourcedata/neo4j
```

Owner

sourcedata

https://hub.docker.com/r/sourcedata/neo4j-sd-graph/

Reproducibility

SIGNAL INTEGRATION IN PLANTS: UV-B, SHADE AND BIOTIC STRESS

With E. Schmit

Collaboration : C. Fankhauser, E. Farmer & R. Ulm

FNSNF
FONDS NATIONAL SUISSE
SCHWEIZERISCHER NATIONALFONDS
FONDO NAZIONALE SVIZZERO
SWISS NATIONAL SCIENCE FOUNDATION

Specs

To build an interface that would allow to easily :

Mine data

,Visualize data

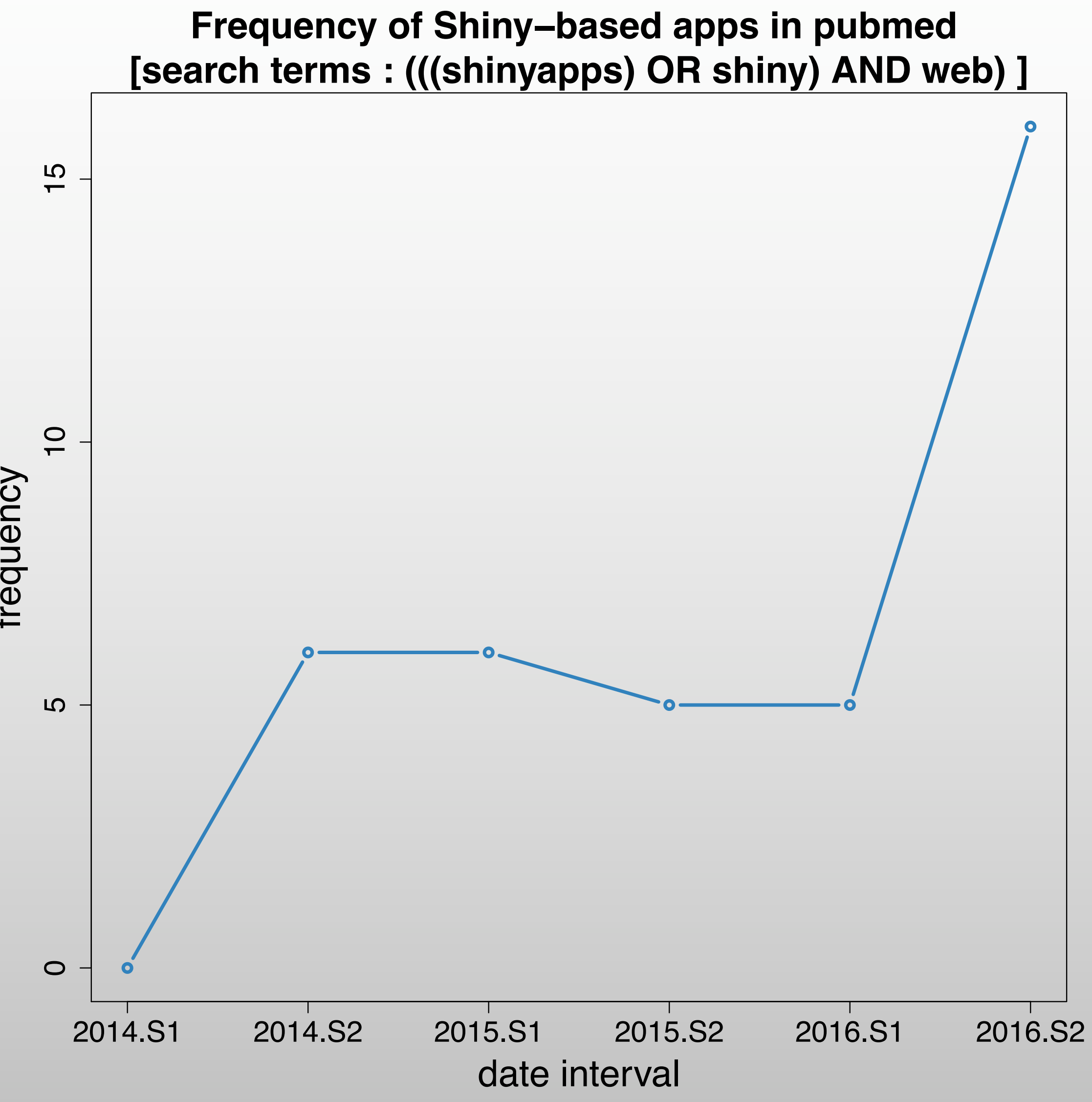
,Flexibility.

Easy web applications in R

> **Shiny** is an open source R package that provides an elegant and powerful **web framework** for building web applications **using R**. Shiny helps you turn your analyses into interactive web applications **without requiring HTML, CSS, or JavaScript knowledge**.

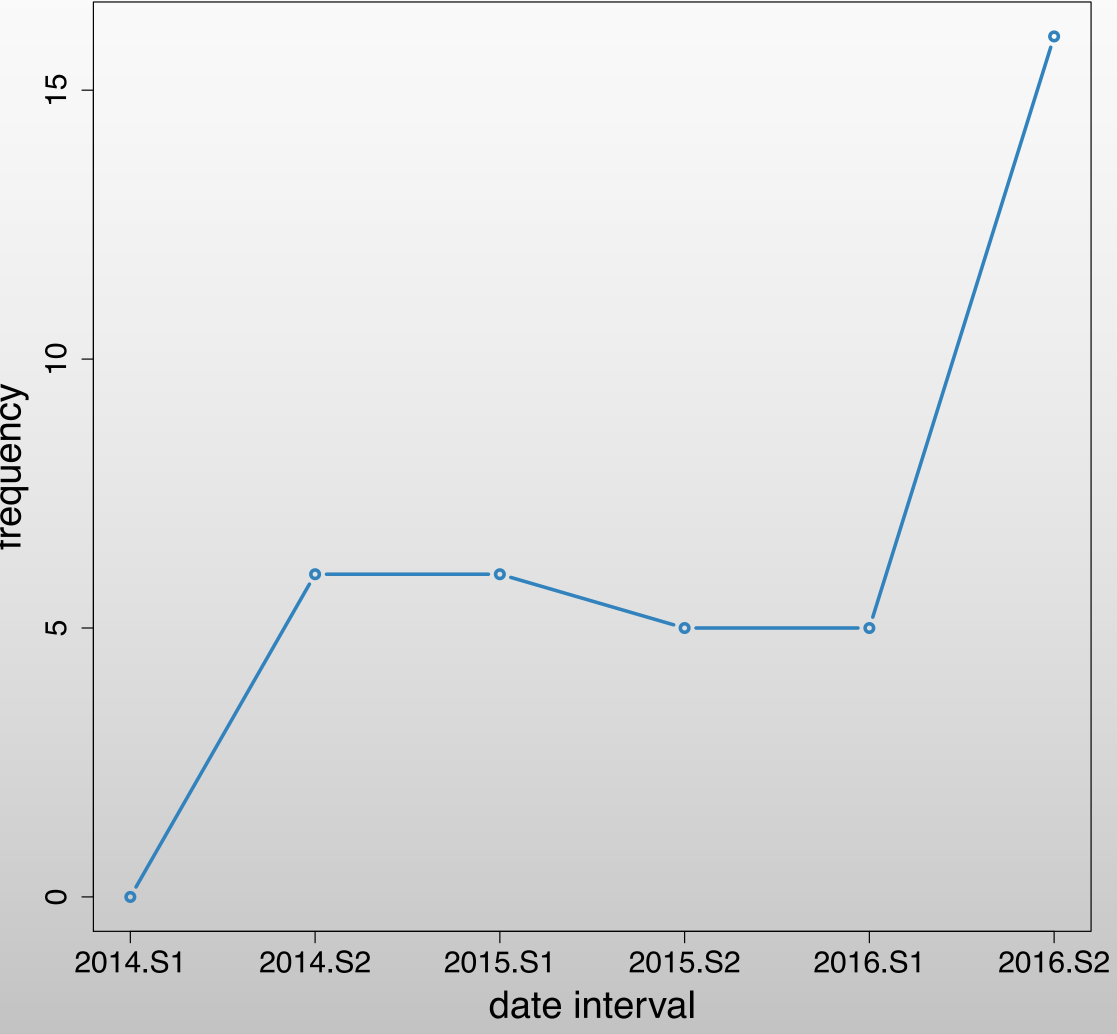
RStudio

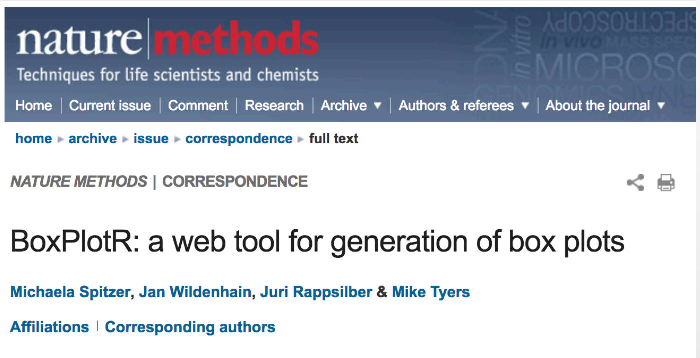
Trendy


Frequency of Shiny–based apps in pubmed
[search terms : (((shinyapps) OR shiny) AND web)]
frequency
0
5
10
15
2014.S1
2014.S2
2015.S1
2015.S2
2016.S1
2016.S2
date interval

Trendy

Frequency of Shiny–based apps in pubmed
[search terms : (((shinyapps) OR shiny) AND web)]

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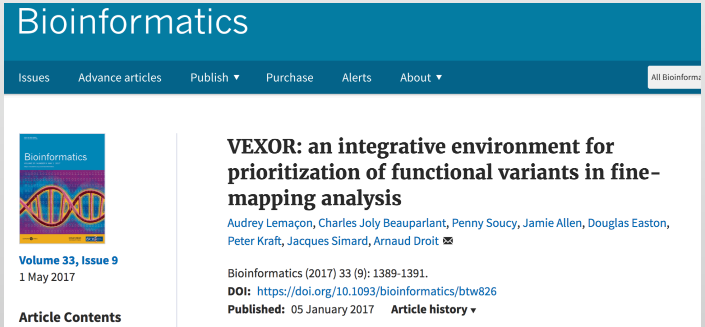
NATURE METHODS | CORRESPONDENCE

BoxPlotR: a web tool for generation of box plots

Michaela Spitzer, Jan Wildenhain, Juri Rappsilber & Mike Tyers



Volume 33, Issue 9
1 May 2017

VEXOR: an integrative environment for prioritization of functional variants in fine-mapping analysis

Audrey Lemaçon, Charles Joly Beauparlant, Penny Soucy, Jamie Allen, Douglas Easton, Peter Kraft, Jacques Simard, Arnaud Droit ✉

Bioinformatics (2017) 33 (9): 1389-1391.
DOI: https://doi.org/10.1093/bioinformatics/btw826
Published: 05 January 2017

Who ?

Target Segment

Who ?

Target Segment

Data Analysis

Reporting

Who ?

Target Segment

Data Acquisition

Data Analysis

Reporting

Decision-making

Who ?

Target Segment

e.g., app to quality check

e.g., app for mining, monitoring

Data Acquisition

Data Analysis

Reporting

Decision-making

Why/when ?

Key advantages

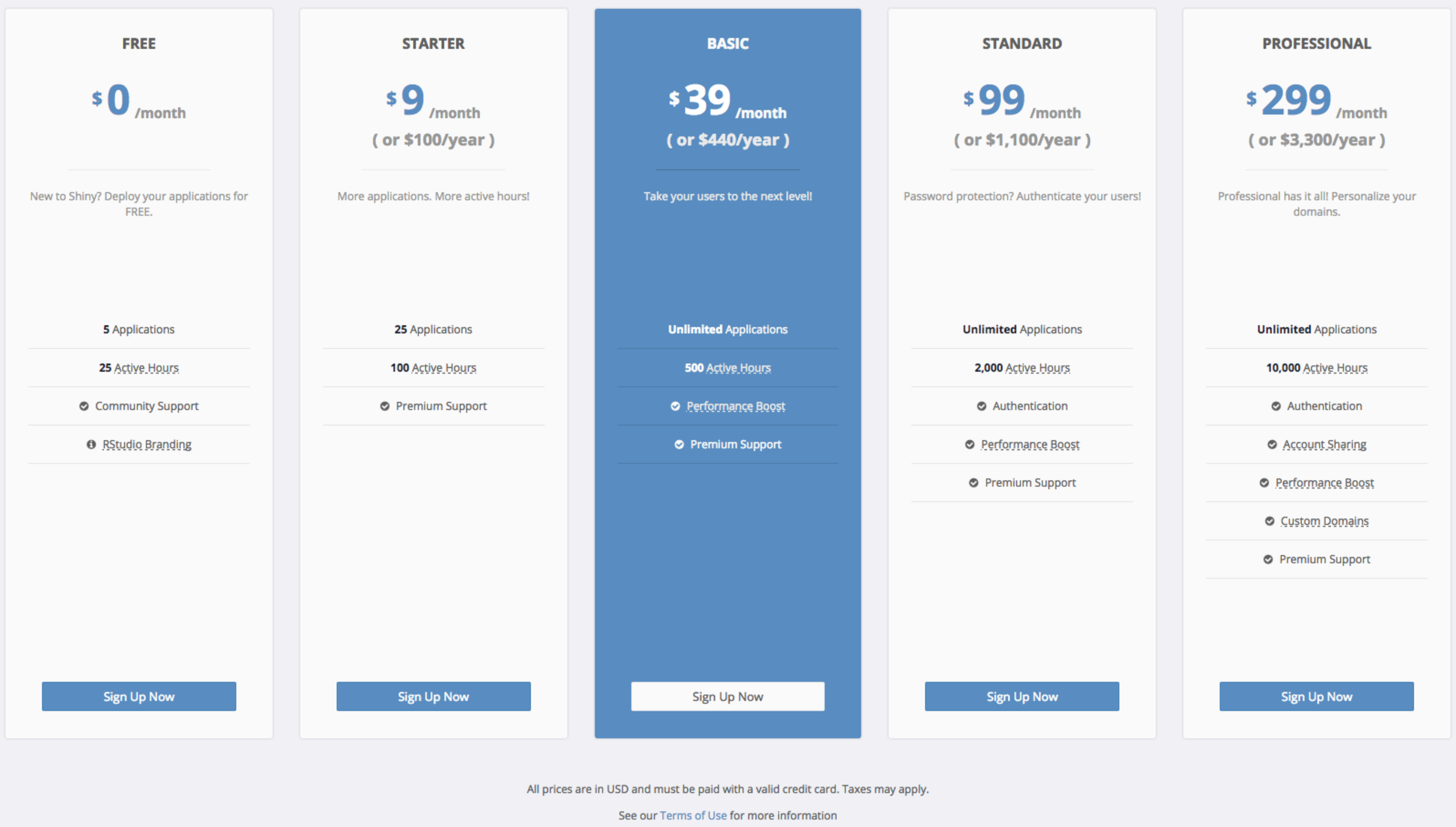
Interactive visualization

, Reporting

, Provide dashboard (e.g, QC)

, Prototyping.

Shinyapps.io pricing



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	(or $100/year)	(or $440/year)	(or $1,100/year)	(or $3,300/year)
New to Shiny? Deploy your applications for FREE.	More applications. More active hours!	Take your users to the next level!	Password protection? Authenticate your users!	Professional has it all! Personalize your domains.
5 Applications	**25** Applications	**Unlimited** Applications	**Unlimited** Applications	**Unlimited** Applications
25 Active Hours	**100** Active Hours	**500** Active Hours	**2,000** Active Hours	**10,000** Active Hours
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ⓘ RStudio Branding		✓ Premium Support	✓ Performance Boost	✓ Account Sharing
			✓ Premium Support	✓ Performance Boost
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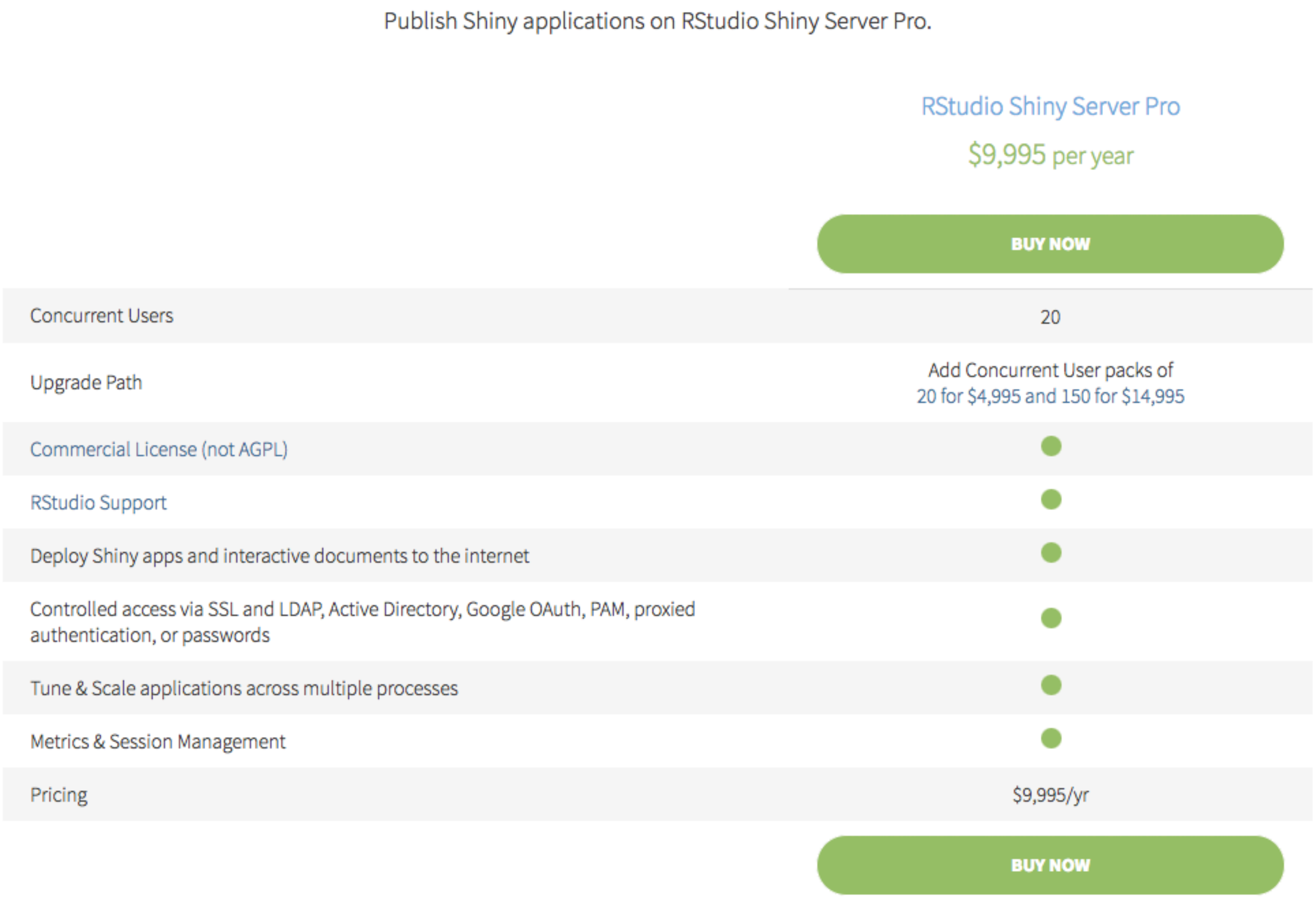


Publish Shiny applications on RStudio Shiny Server Pro.

RStudio Shiny Server Pro

$9,995 per year

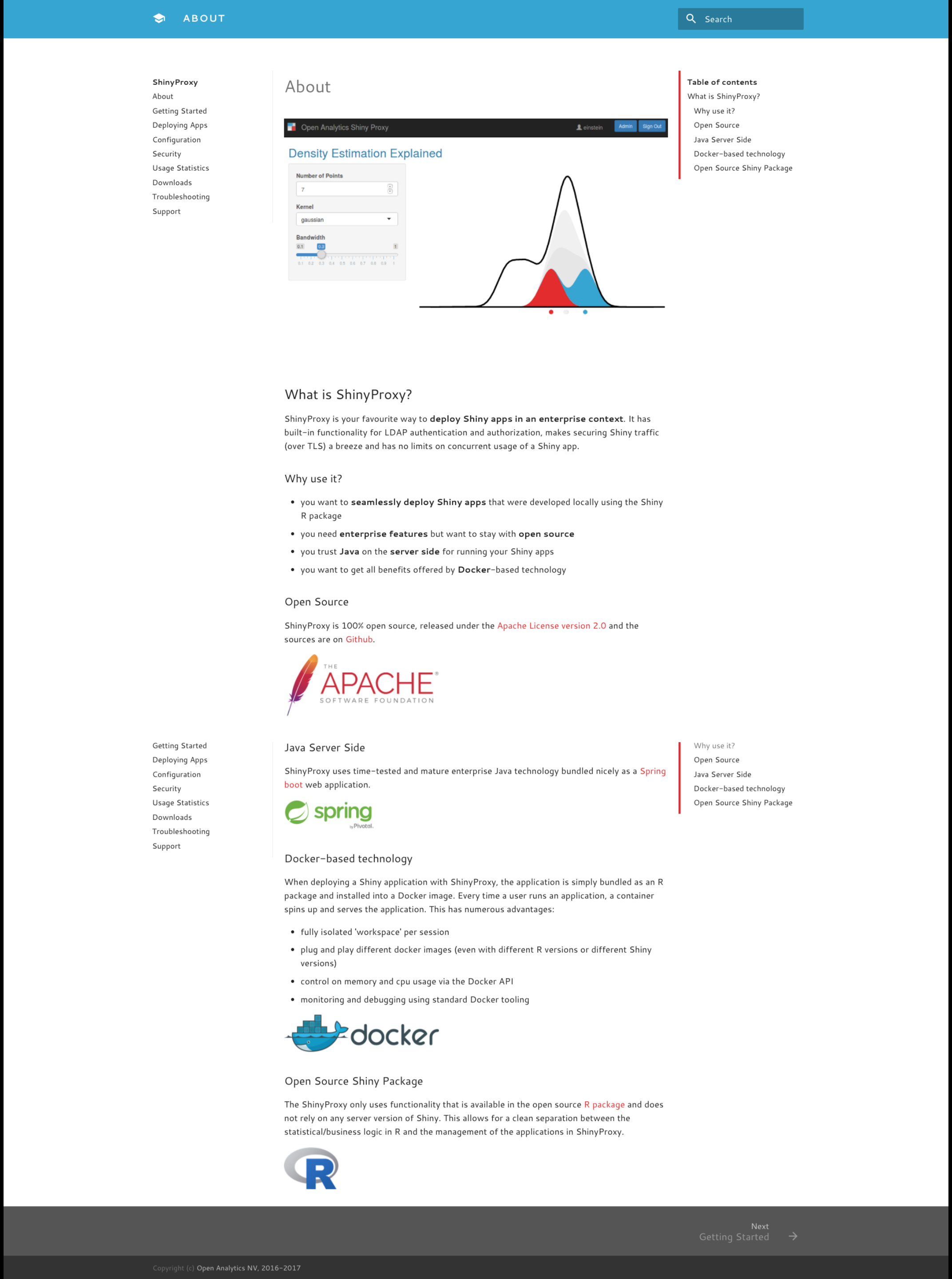
BUY NOW

Concurrent Users	20
Upgrade Path	Add Concurrent User packs of 20 for $4,995 and 150 for $14,995
Commercial License (not AGPL)	●
RStudio Support	●
Deploy Shiny apps and interactive documents to the internet	●
Controlled access via SSL and LDAP, Active Directory, Google OAuth, PAM, proxied authentication, or passwords	●
Tune & Scale applications across multiple processes	●
Metrics & Session Management	●
Pricing	$9,995/yr

BUY NOW

ShinyProxy

https://www.shinyproxy.io/



ShinyProxy
About
Getting Started
Deploying Apps
Configuration
Security
Usage Statistics
Downloads
Troubleshooting
Support

About

What is ShinyProxy?

ShinyProxy is your favourite way to **deploy Shiny apps in an enterprise context**. It has built-in functionality for LDAP authentication and authorization, makes securing Shiny traffic (over TLS) a breeze and has no limits on concurrent usage of a Shiny app.

Why use it?

- you want to **seamlessly deploy Shiny apps** that were developed locally using the Shiny R package
- you need **enterprise features** but want to stay with **open source**
- you trust **Java** on the **server side** for running your Shiny apps
- you want to get all benefits offered by **Docker**-based technology

Open Source

ShinyProxy is 100% open source, released under the Apache License version 2.0 and the sources are on Github.

Getting Started
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Support

Why use it?
Open Source
Java Server Side
Docker-based technology
Open Source Shiny Package

Java Server Side

ShinyProxy uses time-tested and mature enterprise Java technology bundled nicely as a Spring boot web application.

Docker-based technology

When deploying a Shiny application with ShinyProxy, the application is simply bundled as an R package and installed into a Docker image. Every time a user runs an application, a container spins up and serves the application. This has numerous advantages:

- fully isolated 'workspace' per session
- plug and play different docker images (even with different R versions or different Shiny versions)
- control on memory and cpu usage via the Docker API
- monitoring and debugging using standard Docker tooling

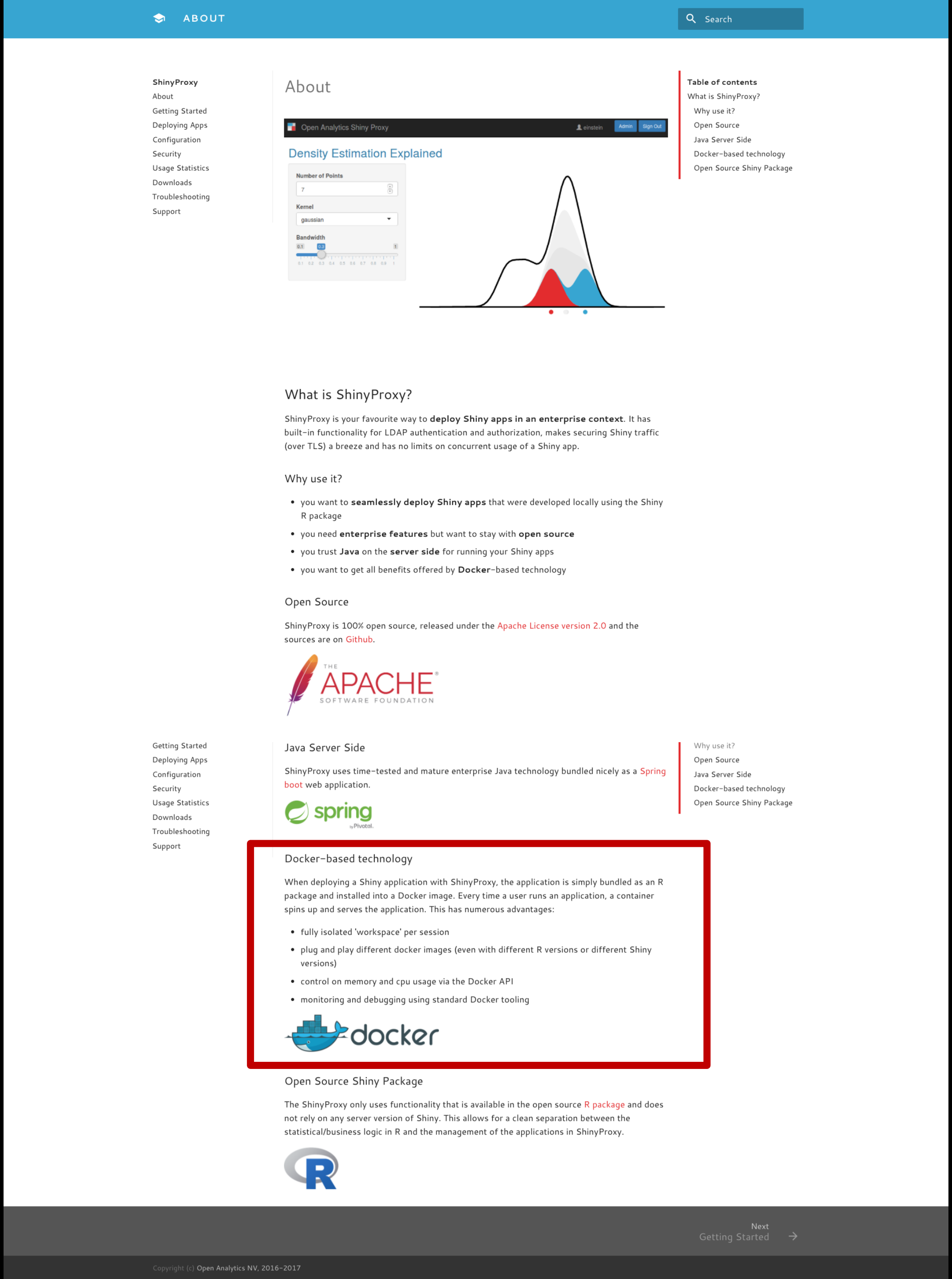
Open Source Shiny Package

The ShinyProxy only uses functionality that is available in the open source R package and does not rely on any server version of Shiny. This allows for a clean separation between the statistical/business logic in R and the management of the applications in ShinyProxy.

Next
Getting Started →

ShinyProxy

https://www.shinyproxy.io/



ShinyProxy
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Support

About

Open Analytics Shiny Proxy — einstein — Admin — Sign Out

Density Estimation Explained

Number of Points: 7

Kernel: gaussian

Bandwidth

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THE APACHE SOFTWARE FOUNDATION

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spring by Pivotal.

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docker

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Next
Getting Started →

ShinyProxy

Advantages of a container-based proxy

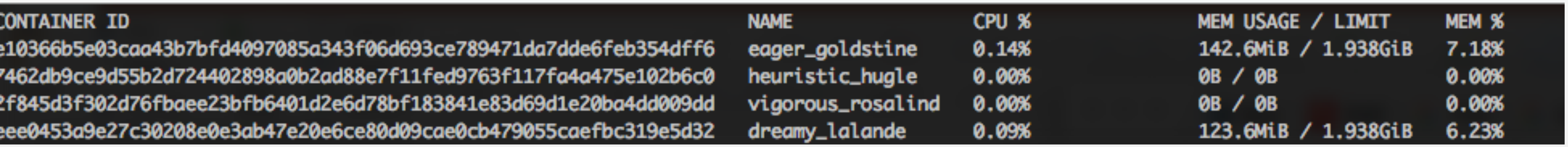
fully isolated 'workspace' per session

,plug and play different docker images (even with different R versions or different Shiny versions)

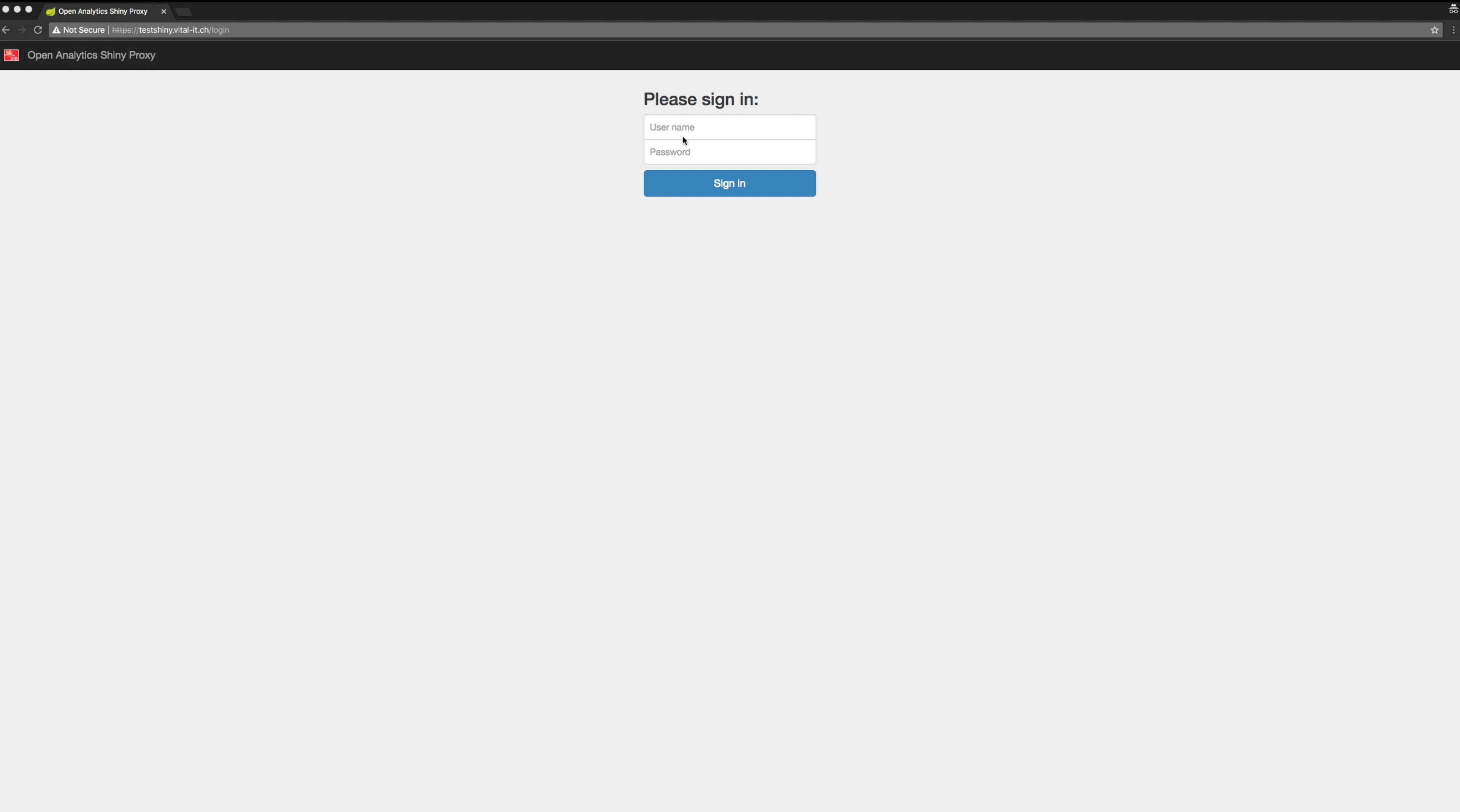
,control on memory and CPU usage via the Docker API

& monitoring and debugging using standard Docker tooling.

```
$ docker stats --all —format …
```



```
CONTAINER ID                                                       NAME                CPU %               MEM USAGE / LIMIT     MEM %
e10366b5e03caa43b7bfd4097085a343f06d693ce789471da7dde6feb354dff6   eager_goldstine     0.14%               142.6MiB / 1.938GiB   7.18%
7462db9ce9d55b2d724402898a0b2ad88e7f11fed9763f117fa4a475e102b6c0   heuristic_hugle     0.00%               0B / 0B               0.00%
2f845d3f302d76fbaee23bfb6401d2e6d78bf183841e83d69d1e20ba4dd009dd   vigorous_rosalind   0.00%               0B / 0B               0.00%
eee0453a9e27c30208e0e3ab47e20e6ce80d09cae0cb479055caefbc319e5d32   dreamy_lalande      0.09%               123.6MiB / 1.938GiB   6.23%
```



Open Analytics Shiny Proxy
Not Secure | https://testshiny.vital-it.ch/login
Open Analytics Shiny Proxy

Please sign in:

User name
Password
Sign in

Data Interoperability And **safety**

MegaClust IaaS

With R. Liechti, I. Xenarios & N.Guex

Collaboration : A. Harari[1], P. Baumgartner[1], G.Coukos[1], F. Periklis[1], E. Danenberg[1], P. Meylan[2], J. Faget[2], C. Schwärzler[3], Miguel Garcia[3], M. Moniatte[4].

1 CHUV

3 FCCF Flow Cytometry Core Facility

2 EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

4 EPFL [PCF]

Flow cytometry data analysis

The core of MegaClust implements a **high-performance unsupervised classification algorithm** allowing fast and robust prediction of cell-type population.

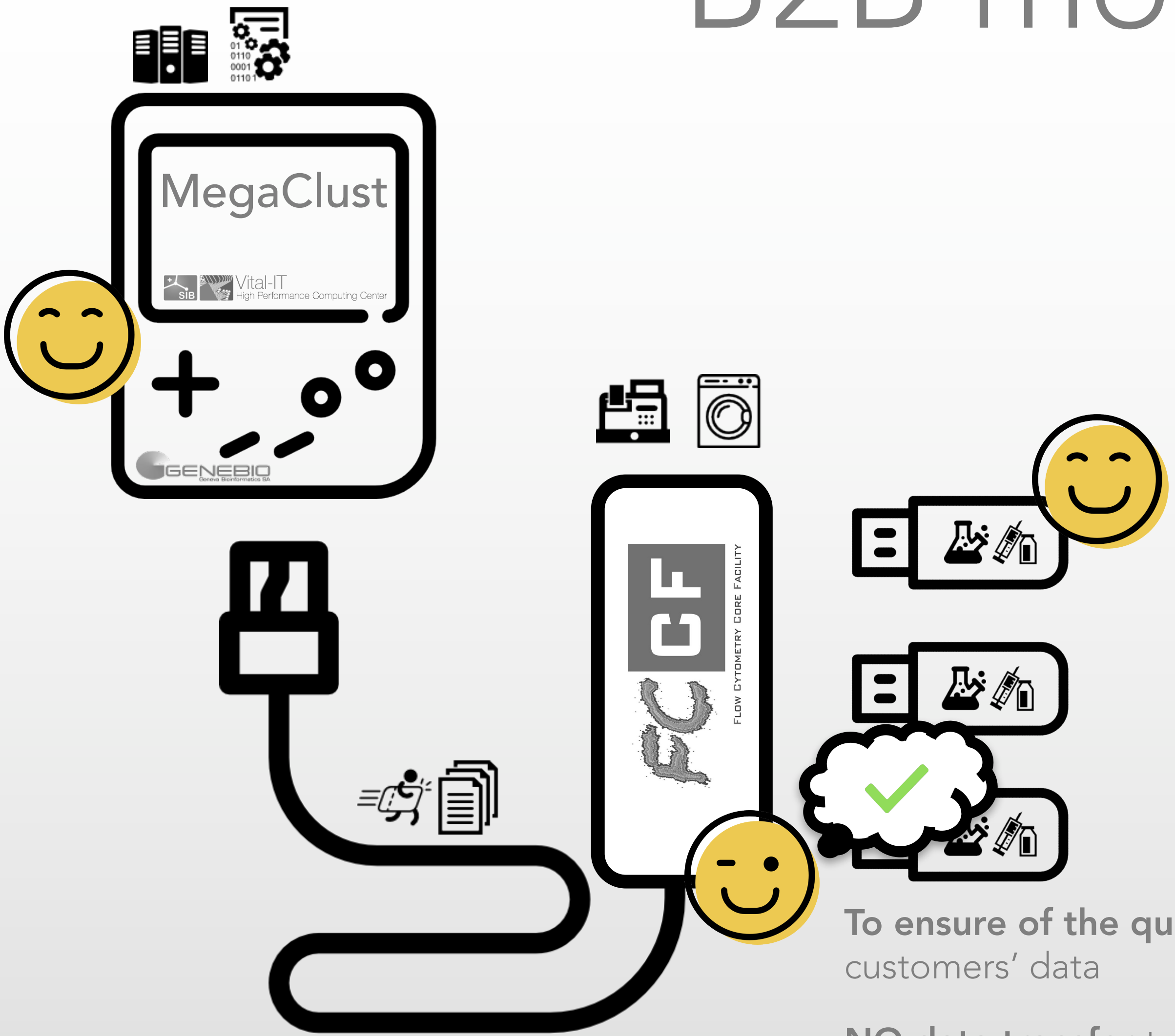
No human bias & reproducible

Designed to handle large datasets

Scale, up to 60 markers (CyTOF)

B2B model

To limit maintenance cost of the solution



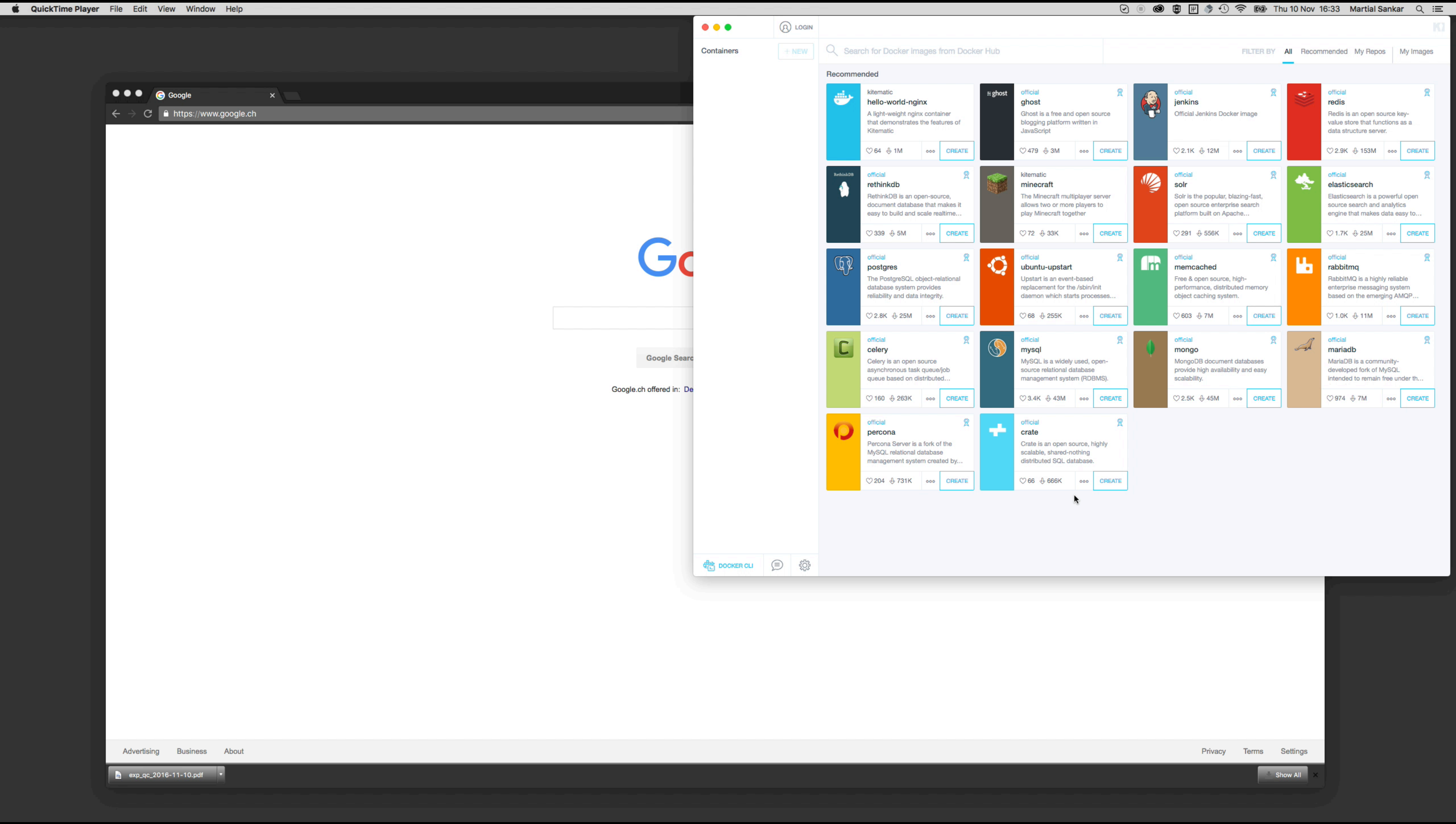
Fast release

Reproducible

To ensure of the quality of customers' data

NO data transfer to third-party server

Independent of the MegaClust clustering


QuickTime Player File Edit View Window Help
Thu 10 Nov 16:33 Martial Sankar
Google
https://www.google.ch
Google Search
Google.ch offered in: De
Advertising Business About
Privacy Terms Settings
exp_qc_2016-11-10.pdf
Show All
LOGIN
Containers
+ NEW
Search for Docker Images from Docker Hub
FILTER BY All Recommended My Repos My Images
DOCKER CLI

Recommended

kitematic
hello-world-nginx
A light-weight nginx container that demonstrates the features of Kitematic
♡ 64 ⇩ 1M CREATE

official
ghost
Ghost is a free and open source blogging platform written in JavaScript
♡ 479 ⇩ 3M CREATE

official
jenkins
Official Jenkins Docker image
♡ 2.1K ⇩ 12M CREATE

official
redis
Redis is an open source key-value store that functions as a data structure server.
♡ 2.9K ⇩ 153M CREATE

official
rethinkdb
RethinkDB is an open-source, document database that makes it easy to build and scale realtime...
♡ 339 ⇩ 5M CREATE

kitematic
minecraft
The Minecraft multiplayer server allows two or more players to play Minecraft together
♡ 72 ⇩ 33K CREATE

official
solr
Solr is the popular, blazing-fast, open source enterprise search platform built on Apache...
♡ 291 ⇩ 556K CREATE

official
elasticsearch
Elasticsearch is a powerful open source search and analytics engine that makes data easy to...
♡ 1.7K ⇩ 25M CREATE

official
postgres
The PostgreSQL object-relational database system provides reliability and data integrity.
♡ 2.8K ⇩ 25M CREATE

official
ubuntu-upstart
Upstart is an event-based replacement for the /sbin/init daemon which starts processes...
♡ 68 ⇩ 255K CREATE

official
memcached
Free & open source, high-performance, distributed memory object caching system.
♡ 603 ⇩ 7M CREATE

official
rabbitmq
RabbitMQ is a highly reliable enterprise messaging system based on the emerging AMQP...
♡ 1.0K ⇩ 11M CREATE

official
celery
Celery is an open source asynchronous task queue/job queue based on distributed...
♡ 160 ⇩ 263K CREATE

official
mysql
MySQL is a widely used, open-source relational database management system (RDBMS).
♡ 3.4K ⇩ 43M CREATE

official
mongo
MongoDB document databases provide high availability and easy scalability.
♡ 2.5K ⇩ 45M CREATE

official
mariadb
MariaDB is a community-developed fork of MySQL intended to remain free under th...
♡ 974 ⇩ 7M CREATE

official
percona
Percona Server is a fork of the MySQL relational database management system created by...
♡ 204 ⇩ 731K CREATE

official
crate
Crate is an open source, highly scalable, shared-nothing distributed SQL database.
♡ 66 ⇩ 666K CREATE

Towards a new editorial model?

Vital-DH@Vital-IT

With A.Chasapi, S. Schulthess I. Xenarios & C.Clivaz

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> “… the study of how people **process and document the human experience**.
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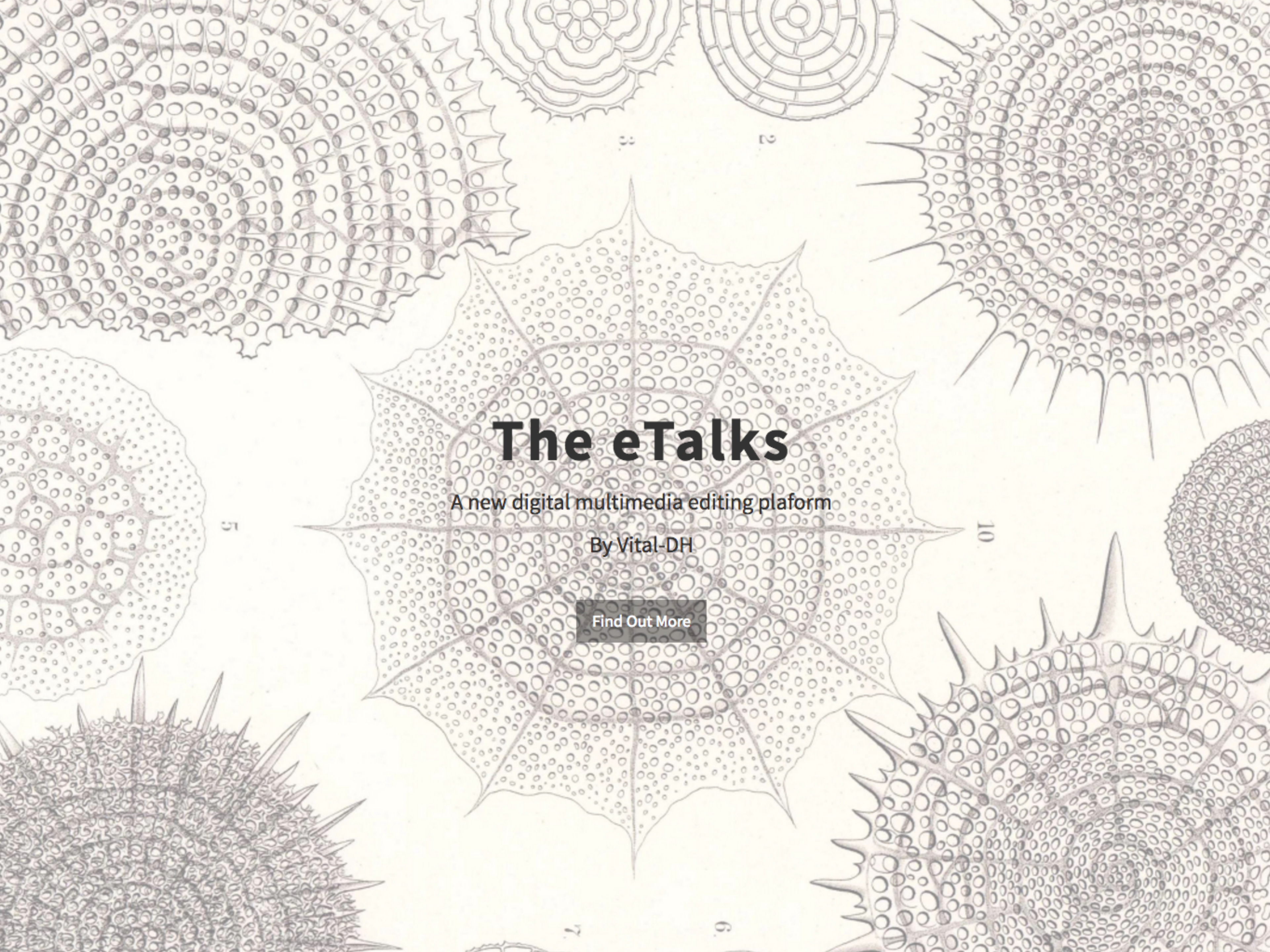


The eTalks

A new digital multimedia editing plaform

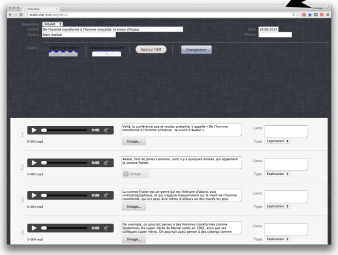
By Vital-DH

Text, image and sound together

Speech text

Speech sound records (mp3)

Image slides (e.g. *.png format)



etalk2.vital-it.ch/edit/?dir=2

Répertoire: Attalah

Intitulé: De l'homme transformé à l'homme virtualisé: la vision d'Avatar

Auteur: Marc Atallah

Date: 19.06.2014

Thème:

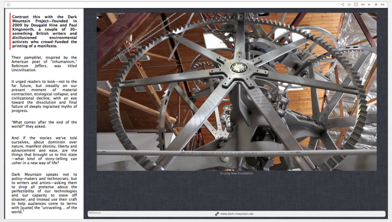
1 S-001.mp3 0:00 — Voilà, la conférence que je voulais présenter s'appelle « De l'homme transformé à l'homme virtualisé : la vision d'Avatar ». Liens: Type: Explication

2 S-002.mp3 0:00 — Avatar, film de James Cameron, sorti il y a quelques années, qui appartient la science fiction. Liens: Type: Explication

3 S-003.mp3 0:00 — La science fiction est un genre qui est littéraire d'abord, puis cinématographique, et qui s'appuie fréquemment sur le motif de l'homme transformé, qui est peut-être même d'ailleurs un des motifs les plus Liens: Type: Explication

4 S-004.mp3 0:00 — Par exemple, on pourrait penser à des hommes transformés comme Spiderman, les super-héros de Marvel sortis en 1962, ainsi que ses collègues super-héros. On pourrait aussi penser à des cyborgs comme Liens: Type: Explication

Easy-to-use **editor** interface



Contrast this with the Dark Mountain Project—founded in 2009 by Dougald Hine and Paul Kingsnorth, a couple of 30-something British writers and disillusioned environmental activists who crowd-funded the printing of a manifesto.

Their pamphlet, inspired by the American poet of "inhumanism," Robinson Jeffers, was titled Uncivilisation.

It urged readers to look—not to the far future, but steadily on our present moment of material contraction, ecological collapse, and civilizational decline, with an eye toward the dissolution and final failure of deeply ingrained myths of progress.

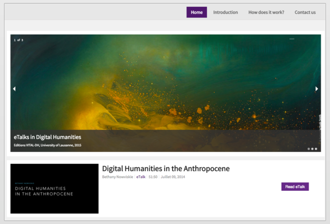
"What comes after the end of the world?" they asked.

And if the stories we've told ourselves, about dominion over nature, manifest destiny, liberty and advancement and ease, are the things that brought us to this state —what kind of story-telling can usher in a new way of life?

Dark Mountain speaks not to policy-makers and technocrats, but to writers and artists—asking them to drop all pretense about the perfectibility of our technologies and our capacity to stave off disaster, and instead use their craft to help audiences come to terms with [quote] the "unraveling... of the world."

www.dark-mountain.net

Interaction multi-media through a **viewer** interface



eTalks in Digital Humanities

Editions VITAL-DH, University of Lausanne, 2015

Digital Humanities in the Anthropocene

Bethany Nowviskie | eTalk | 51:50 | Juillet 09, 2014

DIGITAL HUMANITIES IN THE ANTHROPOCENE

Publication / Edition

4

Fully edited publication series,

21

Authors,

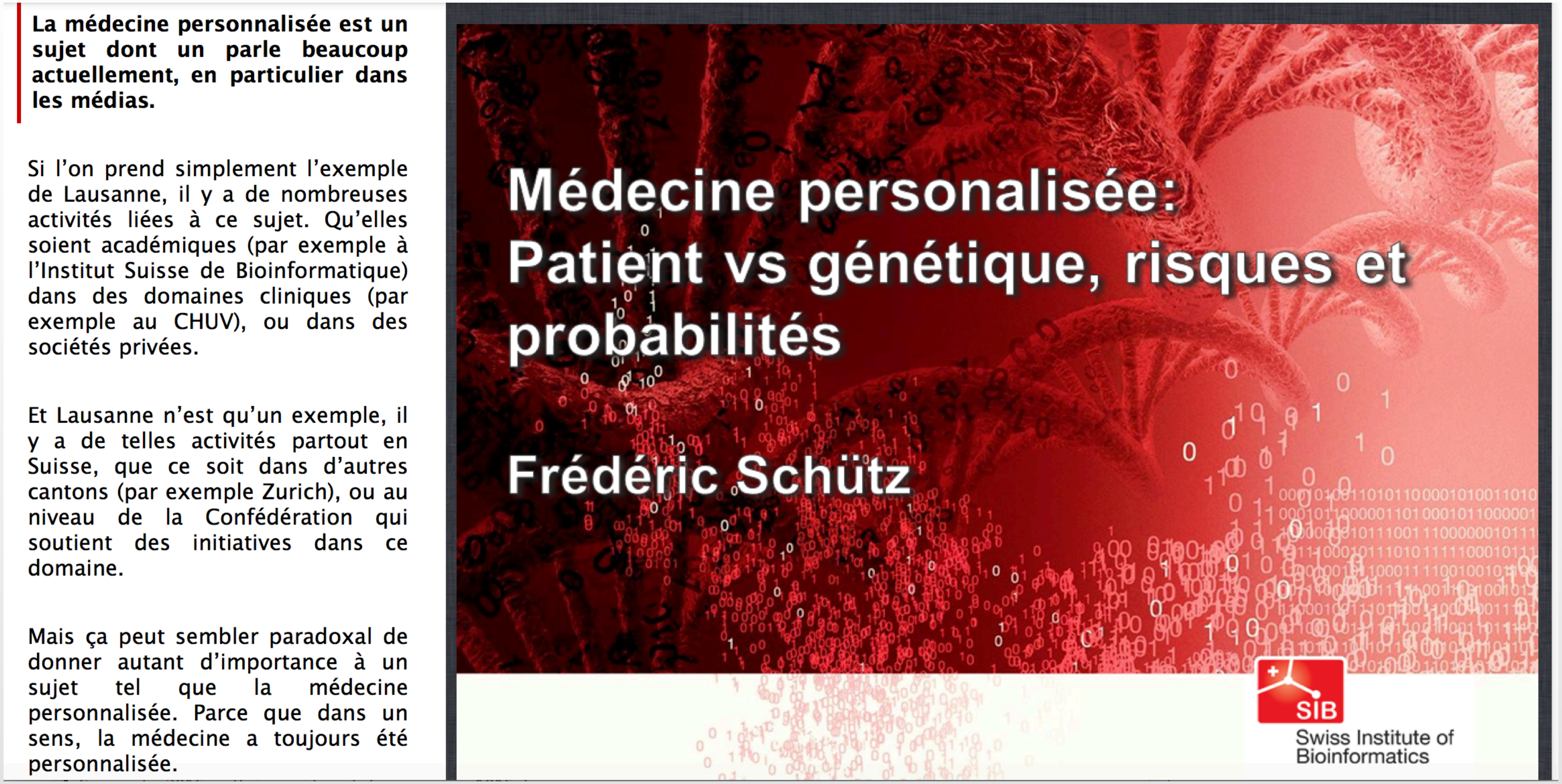
24

eTalks

767

Minutes of recorded speeches.

Personalized medicine with F. Schütz



La médecine personnalisée est un sujet dont un parle beaucoup actuellement, en particulier dans les médias.

Si l'on prend simplement l'exemple de Lausanne, il y a de nombreuses activités liées à ce sujet. Qu'elles soient académiques (par exemple à l'Institut Suisse de Bioinformatique) dans des domaines cliniques (par exemple au CHUV), ou dans des sociétés privées.

Et Lausanne n'est qu'un exemple, il y a de telles activités partout en Suisse, que ce soit dans d'autres cantons (par exemple Zurich), ou au niveau de la Confédération qui soutient des initiatives dans ce domaine.

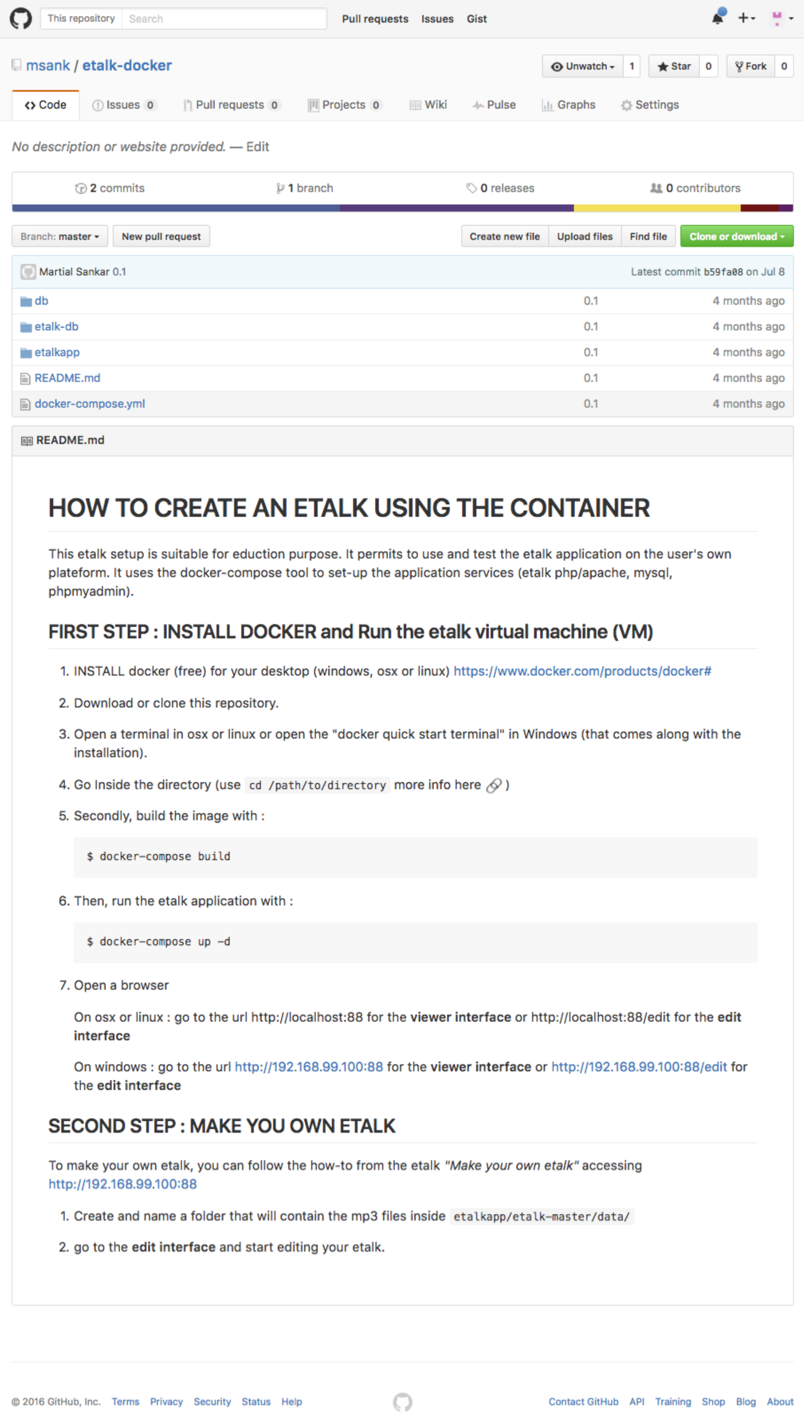
Mais ça peut sembler paradoxal de donner autant d'importance à un sujet tel que la médecine personnalisée. Parce que dans un sens, la médecine a toujours été personnalisée.

Médecine personalisée:
Patient vs génétique, risques et probabilités

Frédéric Schütz

SIB
Swiss Institute of Bioinformatics

https://github.com/msank/etalk-docker



HOW TO CREATE AN ETALK USING THE CONTAINER

This etalk setup is suitable for eduction purpose. It permits to use and test the etalk application on the user's own plateform. It uses the docker-compose tool to set-up the application services (etalk php/apache, mysql, phpmyadmin).

FIRST STEP : INSTALL DOCKER and Run the etalk virtual machine (VM)

1. INSTALL docker (free) for your desktop (windows, osx or linux) https://www.docker.com/products/docker#
2. Download or clone this repository.
3. Open a terminal in osx or linux or open the "docker quick start terminal" in Windows (that comes along with the installation).
4. Go Inside the directory (use `cd /path/to/directory` more info here 🔗)
5. Secondly, build the image with :

```
$ docker-compose build
```

6. Then, run the etalk application with :

```
$ docker-compose up -d
```

7. Open a browser

   On osx or linux : go to the url http://localhost:88 for the **viewer interface** or http://localhost:88/edit for the **edit interface**

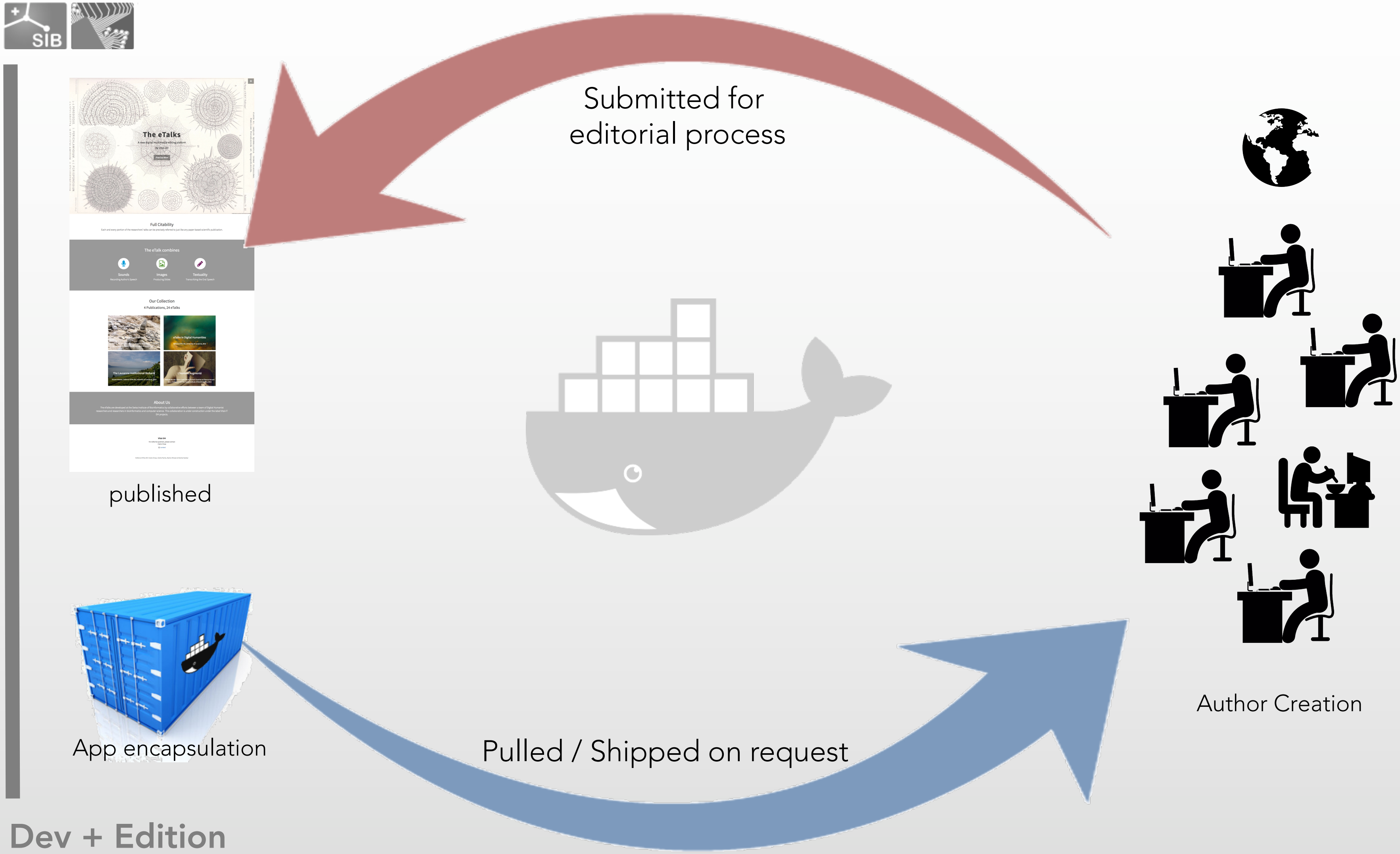
   On windows : go to the url http://192.168.99.100:88 for the **viewer interface** or http://192.168.99.100:88/edit for the **edit interface**

SECOND STEP : MAKE YOU OWN ETALK

To make your own etalk, you can follow the how-to from the etalk *"Make your own etalk"* accessing http://192.168.99.100:88

1. Create and name a folder that will contain the mp3 files inside `etalkapp/etalk-master/data/`
2. go to the **edit interface** and start editing your etalk.

Towards a Docker-based editorial process (?)



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By Vital-DH

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About Us

The eTalks are developed at the Swiss Institute of Bioinformatics by collaborative efforts between a team of Digital Humanist researchers and researchers in bioinformatics and computer science. This collaboration is under construction under the label Vital-IT DH projects.

Vital-DH

For editorial questions, please contact
Claire Clivaz

contact

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editorial process

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Pulled / Shipped on request

Author Creation

Dev + Edition

Summary

Revolution, Evolution …

Or ...