



CyVerse UK @ Warwick

15 September 2016



WARWICK
THE UNIVERSITY OF WARWICK



Part 1: Infrastructures

Part 2: Applications

About CyVerse UK



software driven



Prof. David Wild



software driven



Prof. Anthony Hall



hardware driven



Dr. Rob Davey



software driven



Prof. Tony Pridmore

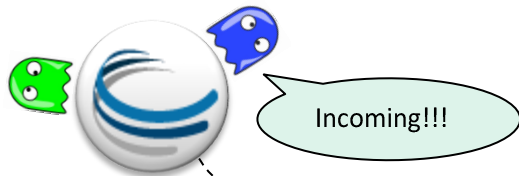


Warwick Team and Hardware



CPU/Memory/OS:
64 Cores/1T/CentOS7
External Storage:
101T(iRODS)/101T

Objective: App Integration



Analysis of Plant Promoter-Linked Elements (APPLES)



How does this
work?



How to get
onto CyVerse?



Learning CyVerse: The beginning

In chronological order



- Atmosphere



- iCommands



- Agave



- Ask iPlant



dooley

501 ● 1 ● 6



bogao

231 ● 3 ● 5 ● 13



- CoGe



- Docker & Docker on CyVerse



- Discovery Environment



Learning CyVerse: Docker and Discovery Environment

Docker

- Docker and Docker on CentOS
 - devicemapper (loop-lvm > direct-lvm)
 - Docker restart

Front End

- Configure de, de-db, terrain, CyVerse CAS, JWT (de-terrain), nginx-ssl, GPG (terrain-agave), user-preference, data-info...

iRODS

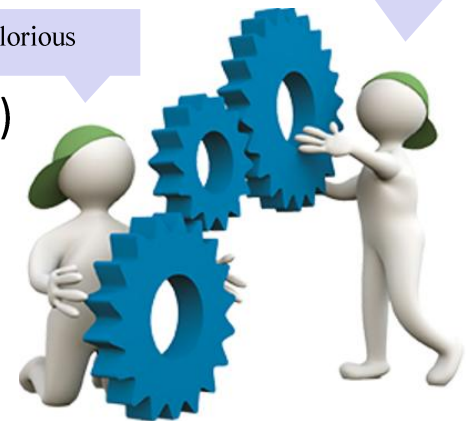
- Dockerise(compose) iRODS(need admin user)
 - RabbitMQ (AMQP)
 - IES (apply cyVerse patches, patch the patch)
 - iCommand client

terrain

- Still can't bootstrap

Glorious

Docker, Docker everywhere...



Learning CyVerse: Docker and Discovery Environment (cont.)

Authentication

DE

DE

DE

iRODS

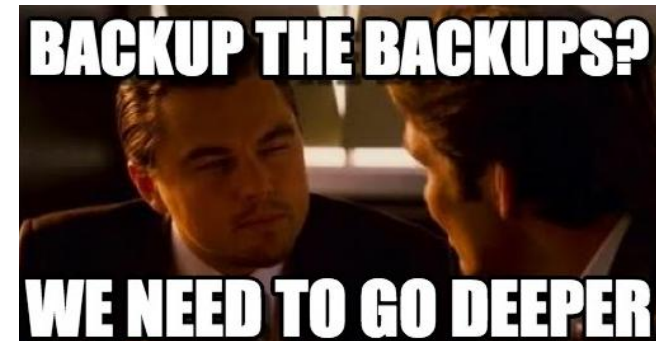
- CAS, LDAP, iplant-groups, grouper, grouper-db (sharkbait > de-db)
- Docker Compose (fill in grouper, RabbitMQ, IES)
- Service Configurations with Ansible
- Docker Compose Networking
- data-info, (also dewey) complaints
 - Zone configuration
 - More patch
(irods-3.3.1-cyverse/iRODS/server/icat/patches/patch3.3to3.3)
 - Shared folder permission
 - Missing UUID on home/shared/trash

```
imeta add -c /cyverseZone/home/bogao ipc_UUID "${uuidgen | tr '[:upper:]' '[:lower:]'}
```



Learning CyVerse: Docker and Discovery Environment (cont.)

- https • 301 Error, nginx SSL Certificate
- DE • Belphegor 😂
- jobs • JEX, Job Status (iplant-email)
- DE • Community Folder config
- DE • InfoText
 - update parameter_types set deprecated = false where name = 'Info'
- iRODS • Open iRODS patching iCAT
- DE • Workflow Bug



Learning CyVerse: Credit to the DE team



Dennis Roberts

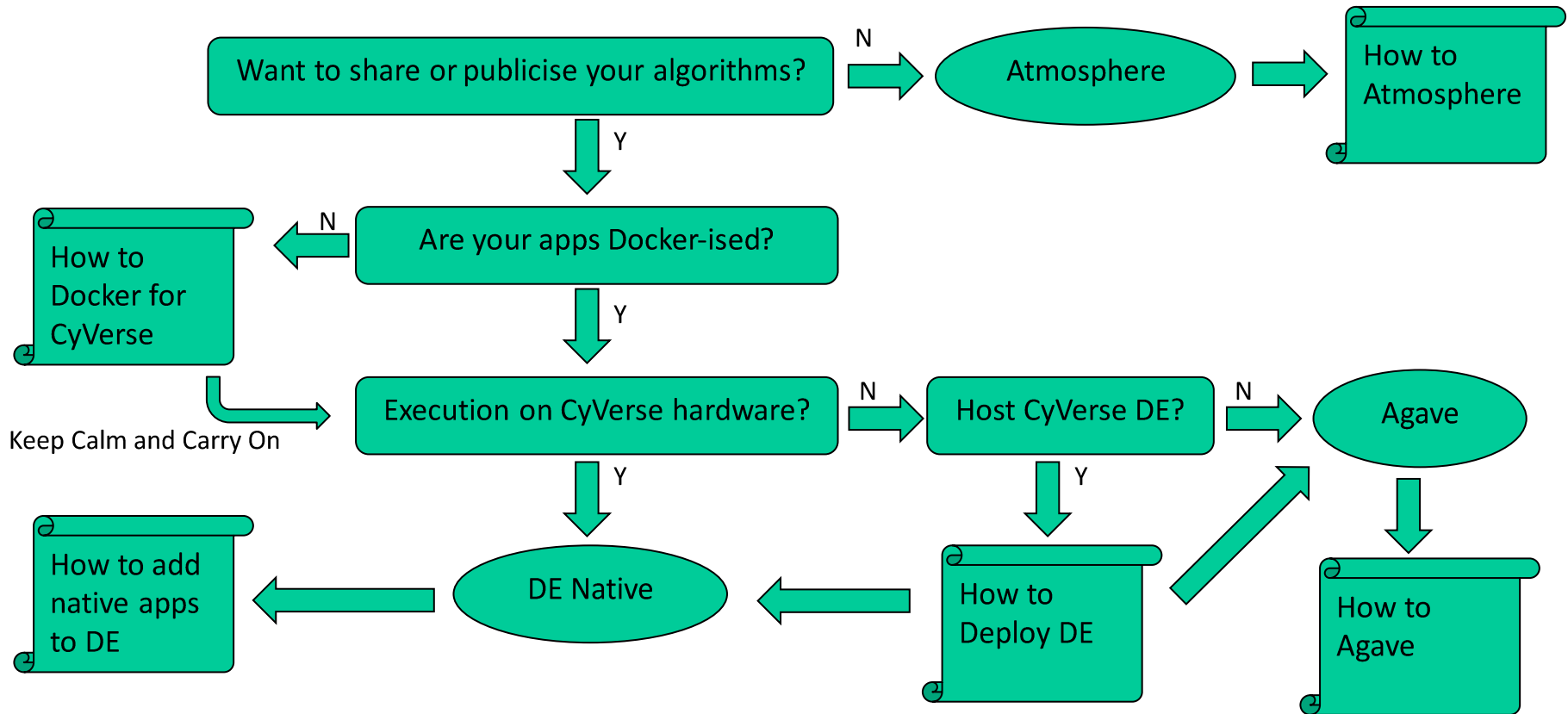
Paul Sarando, Tony Edgin, John Wreggle, ...

Learning CyVerse: Takeaway and Feedback: Packaging DE

Towards a (relatively) portable DE

- Geographically constrained data
- Ease of deployment

Learning CyVerse: Takeaway and Feedback: Navigate CyVerse Assets



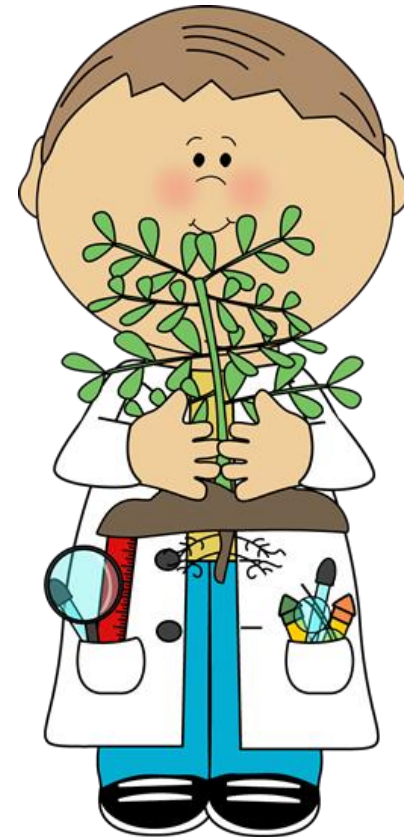
Learning CyVerse: Takeaway and Feedback: Misc

- User Share between DE sites
- Multiple Condor to DE (ClassAds)
- Documentation on DE deployment
- Embedded http link in app UI
- Link to specific app from outside DE
- Output viewer



App CyVerse-isation Pipeline

Be Biologist-Friendly

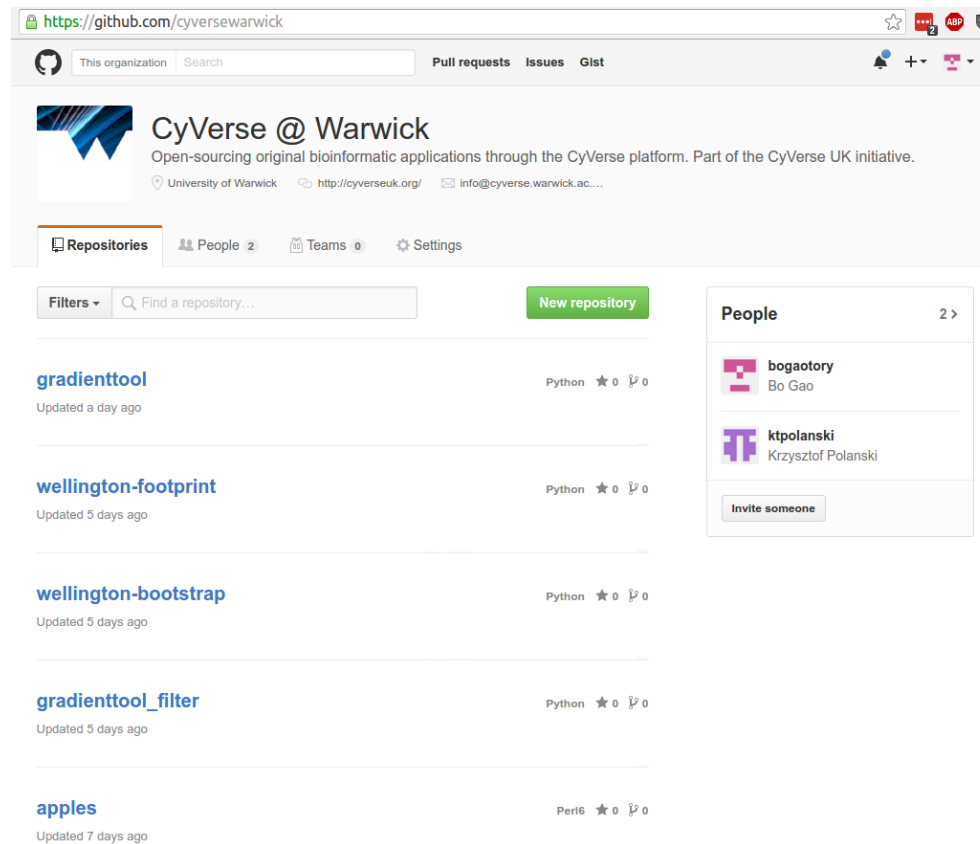


App CyVerse-isation Pipeline (cont.)

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github.com/
cyversewarwick

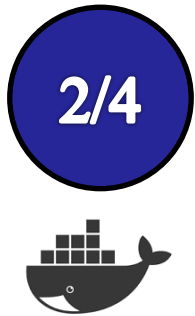


The screenshot shows the GitHub organization page for 'CyVerse @ Warwick'. The page header includes the organization name, a description ('Open-sourcing original bioinformatic applications through the CyVerse platform. Part of the CyVerse UK initiative.'), and contact information. Below the header, there are tabs for 'Repositories', 'People', 'Teams', and 'Settings'. The 'Repositories' tab is active, showing a list of repositories with columns for repository name, language, stars, forks, and updates. The 'People' tab shows a list of members with their avatars, usernames, and names.

Repository	Language	Stars	Forks	Updated
gradienttool	Python	0	0	Updated a day ago
wellington-footprint	Python	0	0	Updated 5 days ago
wellington-bootstrap	Python	0	0	Updated 5 days ago
gradienttool_filter	Python	0	0	Updated 5 days ago
apples	Perl6	0	0	Updated 7 days ago

Member	Username	Name
	bogaotory	Bo Gao
	ktpolanski	Krzysztof Polanski

App CyVerse-isation Pipeline (cont.)



hub.docker.com/
u/cyversewarwick

The screenshot shows the Docker Hub profile for the organization 'cyversewarwick'. The profile includes a header with navigation links (Dashboard, Explore, Organizations), a search bar, and a user dropdown menu. Below the header, the 'Repos' section displays a list of repositories. Each repository entry includes the repository name, its visibility (public), build status (automated build), and statistics for stars and pulls. A 'DETAILS' link is provided for each repository.

Repository	Stars	Pulls	Details
cyversewarwick/tcap	0	49	DETAILS
cyversewarwick/hmt_index	0	46	DETAILS
cyversewarwick/bhc	0	39	DETAILS
cyversewarwick/csi	0	39	DETAILS
cyversewarwick/hmt	0	35	DETAILS
cyversewarwick/gp2s	0	32	DETAILS
cyversewarwick/wigwams	0	31	DETAILS

App CyVerse-isation Pipeline (cont.)

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cyverse.warwick.ac.uk

Discovery Environment

Apps

Apps Workflow Share Search Apps

Category Public Apps (18)

- Beta (3)
- CyVerse_Warwick (15)
 - Enrichment Analysis (2)
 - Transcription Factor Binding Sites (2)
 - Genome-wide Chromatin Data (2)
 - Footprint Identification (2)
 - Sequence Conservation (1)
 - Time Series Expression Data (10)
 - Clustering/Biclustering (3)
 - Differential Expression (3)
 - Network Inference (4)
 - Temp (0)
- Workspace (24)
 - Apps under development (9)
 - Favorite Apps (1)
 - My public apps (15)
 - Shared with me (0)
 - High-Performance Computing (162)

Public Apps

Name
BHC (Bayesian Hierarchical Clustering)
CANU
CSI (Causal Structure Inference)
DE Word Count
GP2S (Gaussian Process Two-Sample test of Differen...
Gradient Tool
Gradient Tool Filter
hCSI (Hierarchical Causal Structure Inference)
hCSI_MarginalThreshold (Marginal to Cytoscape Con...
HMT (Hypergeometric Motif Test)
HMT_index (Hypergeometric Motif Test Index Creation)
MEGAHIT
oCSI (Orthologous Causal Structure Inference)
rbh-APPLES
TCAP (Temporal Clustering by Affinity Propagation)
Wellington Bootstrap
Wellington Footprint
Wigwams

App CyVerse-isation Pipeline (cont.)

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cyverseuk.org

Google Analytics Dashboard



report generated by GADWP

File Network Citation Help

Minimum Weight: 0.1

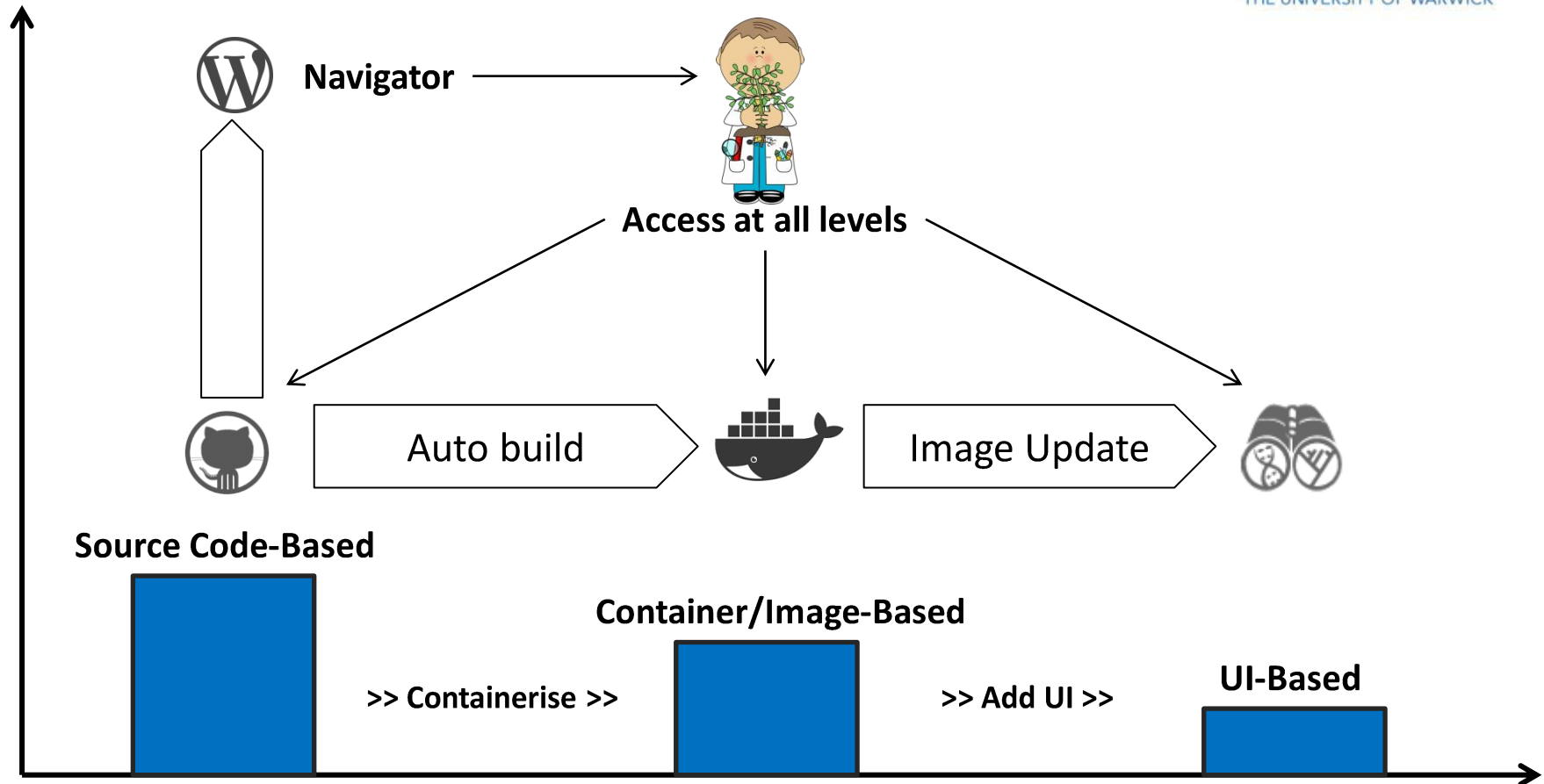
Genes	Prnt	Chld	Fit	GP-F	GP-L	GP-N
<input checked="" type="checkbox"/> G1 [+]	2	2	0.98	0.57	0.99	0.084
<input checked="" type="checkbox"/> G2 [+]	3	0	0.66	0.67	1.2	0.079
<input checked="" type="checkbox"/> G3 [+]	1	4	0.91	0.67	0.80	0.071
<input checked="" type="checkbox"/> G4 [+]	2	2	0.89	0.65	0.79	0.055
<input checked="" type="checkbox"/> G5 [+]	1	2	0.88	0.65	0.64	0.051
<input checked="" type="checkbox"/> G6 [+]	2	2	1.00	0.56	0.61	0.070
<input checked="" type="checkbox"/> G7 [+]	2	2	0.63	0.72	0.59	0.043
<input checked="" type="checkbox"/> G8 [+]	4	2	0.49	0.64	1.1	0.093
<input checked="" type="checkbox"/> G9 [+]	3	3	0.31	0.69	0.79	0.090
<input checked="" type="checkbox"/> G10 [+]	3	4	0.28	0.71	1.0	0.14

Easy High Performance Computing for UK Science
Cyverse UK provides BBSRC funded HPC hardware and pipelines for free to all scientists

Discovery Environment UK (Beta Tests)

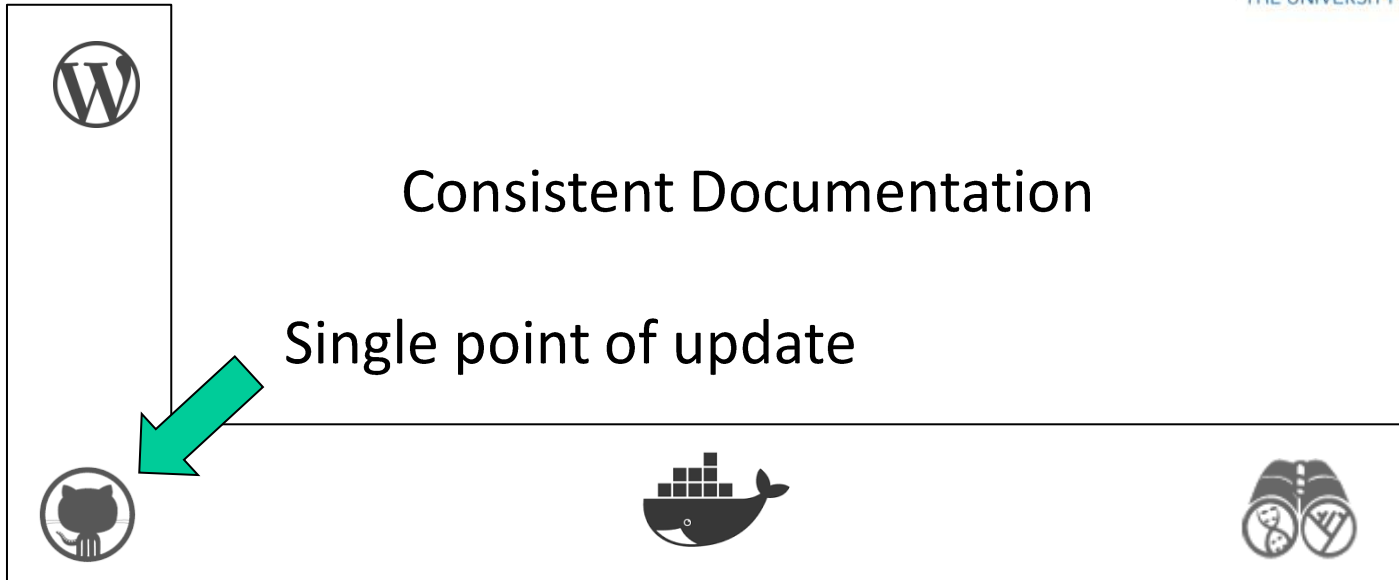
CyVerse UK Applications:

App CyVerse-isation Pipeline (cont.)

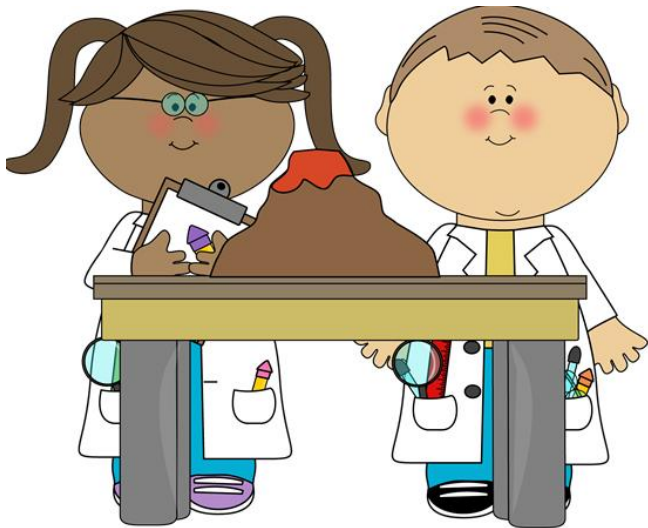


App CyVerse-isation Pipeline (cont.)

New pull request!			
1	cyverseuk	cyverseuk	Latest commit 3 days ago
2	cyverseuk	cyverseuk	3 days ago
3	cyverseuk	cyverseuk	3 days ago
4	cyverseuk	cyverseuk	3 days ago
5	cyverseuk	cyverseuk	3 days ago
6	cyverseuk	cyverseuk	3 days ago
7	cyverseuk	cyverseuk	3 days ago
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99	cyverseuk	cyverseuk	3 days ago
100	cyverseuk	cyverseuk	3 days ago



Application Testing



Internal:

- University of Warwick
- University of Birmingham
- University of York

External:

- John Innes Centre
- Max Planck Institute for Plant Breeding Research

Next

- More apps, more testing and collaboration
- Agave-rise apps with standardised process
- Upgrade DE services

Part 2: Applications