



BIOPLATFORMS  
AUSTRALIA

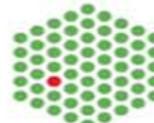


# BTP: a cloud-based bioinformatics training platform

Annette McGrath (CSIRO),  
Jerico Revote (R@CMon, Monash University)  
May 24, 2016



EMBL-EBI



TGAC The Genome Analysis Centre™

# Who we are

- CSIRO
  - Commonwealth Scientific and Industrial Research Organisation
  - Australia's National Science Agency
  - <http://www.csiro.au>
- Bioplatforms Australia
  - Manages the federal government's investment in
    - Genomics
    - Metabolomics
    - Proteomics
    - Bioinformatics
  - <http://www.bioplatforms.com>

# Training needs survey

A word cloud composed of various training topics, each associated with a specific color. The words are arranged in a roughly circular pattern, with some overlap. The colors used include dark red, maroon, dark green, olive green, yellow, orange, purple, and dark blue.

The words in the cloud include:

- Quality analysis
- Genome design
- Linux standards
- Perl Python
- Analysis
- Planning
- formats Databases
- SQL Workbench
- Statistics
- data experiments
- control NGS
- Genomics Bioinformatics Modern CLC Bio
- Regression Data Browsers

# A training collaboration

- CSIRO's challenge
  - Increasing bioinformatics literacy, capability and competencies in a
    - diverse,
    - relatively small and
    - geographically dispersed
- Group of bioinformaticians and many more biology end-users
- Bioplatforms Australia (BPA)
  - Provide training for a
    - diverse,
    - relatively small and
    - geographically dispersed
- Group of bioinformaticians and many more biology end-users

# Our goal

- Create a critical mass of trainers
- Engender a cohesive training community
- ‘Trainer’ – volunteers
- To deliver hands-on training workshops in the major cities in Australia



# Where do we start?

- A great deal of bioinformatics training experience
- Many successful workshops in a wide range of bioinformatics topics
- Dedicated resources
- Train-the-trainer
  - Attend workshops as trainees
  - Learn about how to train adults in a professional setting
  - Develop a course, using our own and EBI's material, to deliver in Australia



# Introduction to NGS 2012

- Introduction to Next Generation Sequencing  
March 12<sup>th</sup>-14<sup>th</sup> 2012 day workshop
- 8 trainers from CSIRO & BPA facilities
- Participants and observers
- 2 days of ‘Train-the-trainer’ workshop



# Metagenomics:

Managing, Analysing and Visualising Data Course

- 9-11<sup>th</sup> September 2013
- Expanding the trainer network
- Developed an outline for a 2 day “Introduction to Metagenomics” workshop



# Cancer Genomics

- 20-24<sup>th</sup> July 2015
- Further expanding our network and course offering
- 9 trainers attended course
- Developed a 3 day “Cancer Genomics” workshop



# De novo genome assembly

- 29-31<sup>st</sup> July 2015
- Expanding our course offering
- 10 (different) trainers attended the course
- Developed a 2.5 day “De novo genome assembly” course



# Target audience

- Bench biologists
- Aiming to increase research productivity
  - Scientists can independently look at their data
  - Engage in more productive conversations with bioinformaticians
- Used an application process
- Selection questions
  - To ensure that the audience expectations could be met
  - Attendees were of similar skill levels

# Introduction to NGS outline

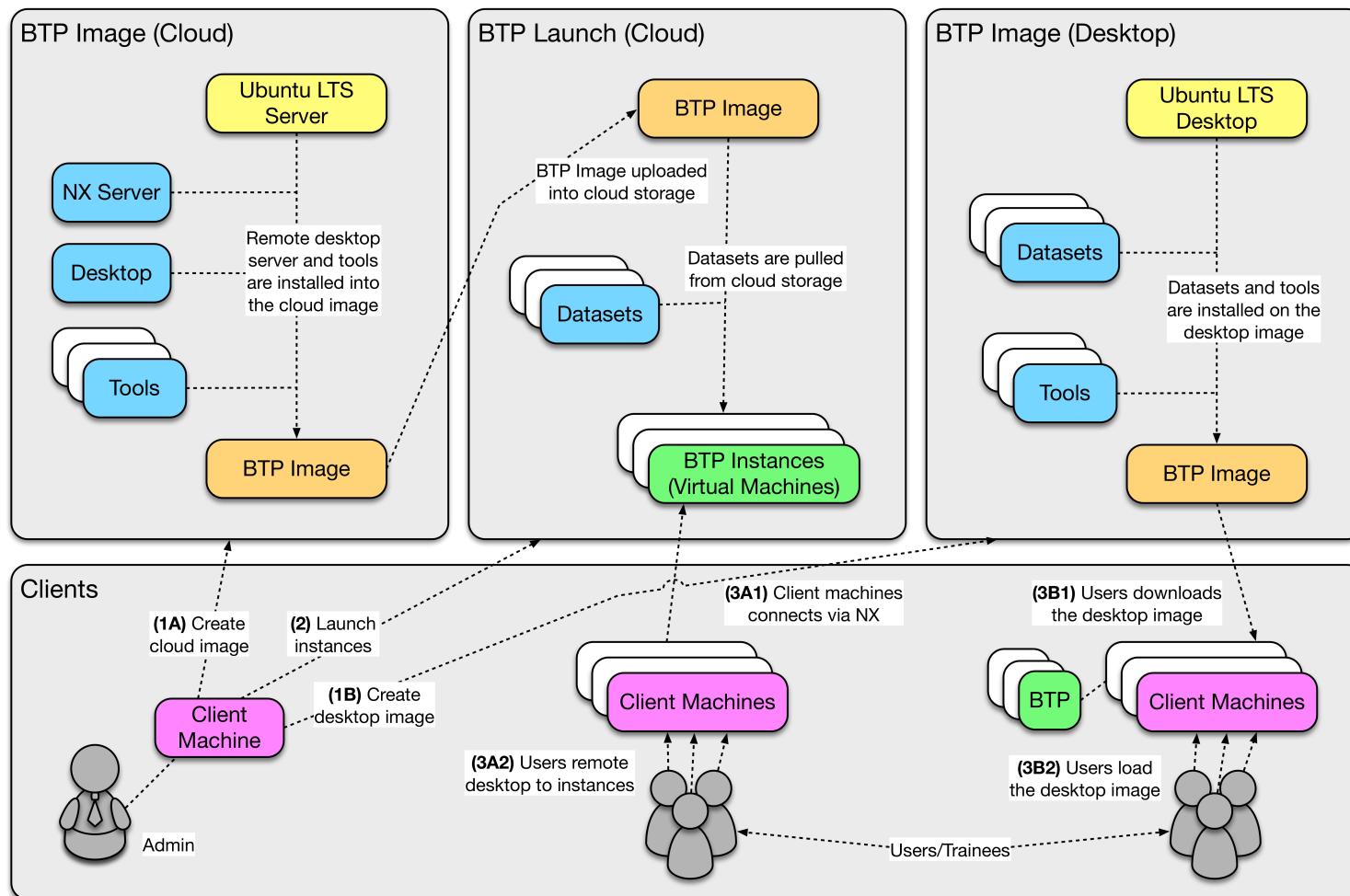
- Intro to Linux (lecture + hands-on)
- Intro to NGS (lecture)
- QC (lecture + hands-on)
- Alignment (lecture+ hands-on)
- ChIPSeq (lecture + hands-on)
- RNASeq (lecture + hands-on)
- *de novo* genome assembly (lecture + hands-on)



# Delivering the workshop

- We do not have dedicated training facilities
- We want to deliver the workshop in a roadshow format
- Minimise maintenance of the training environment
  - No monolithic installs
- Minimise cognitive burden on trainees
  - The training environment should go unseen
- Make everything publically accessible and as reusable as possible
- Engage local bioinformaticians

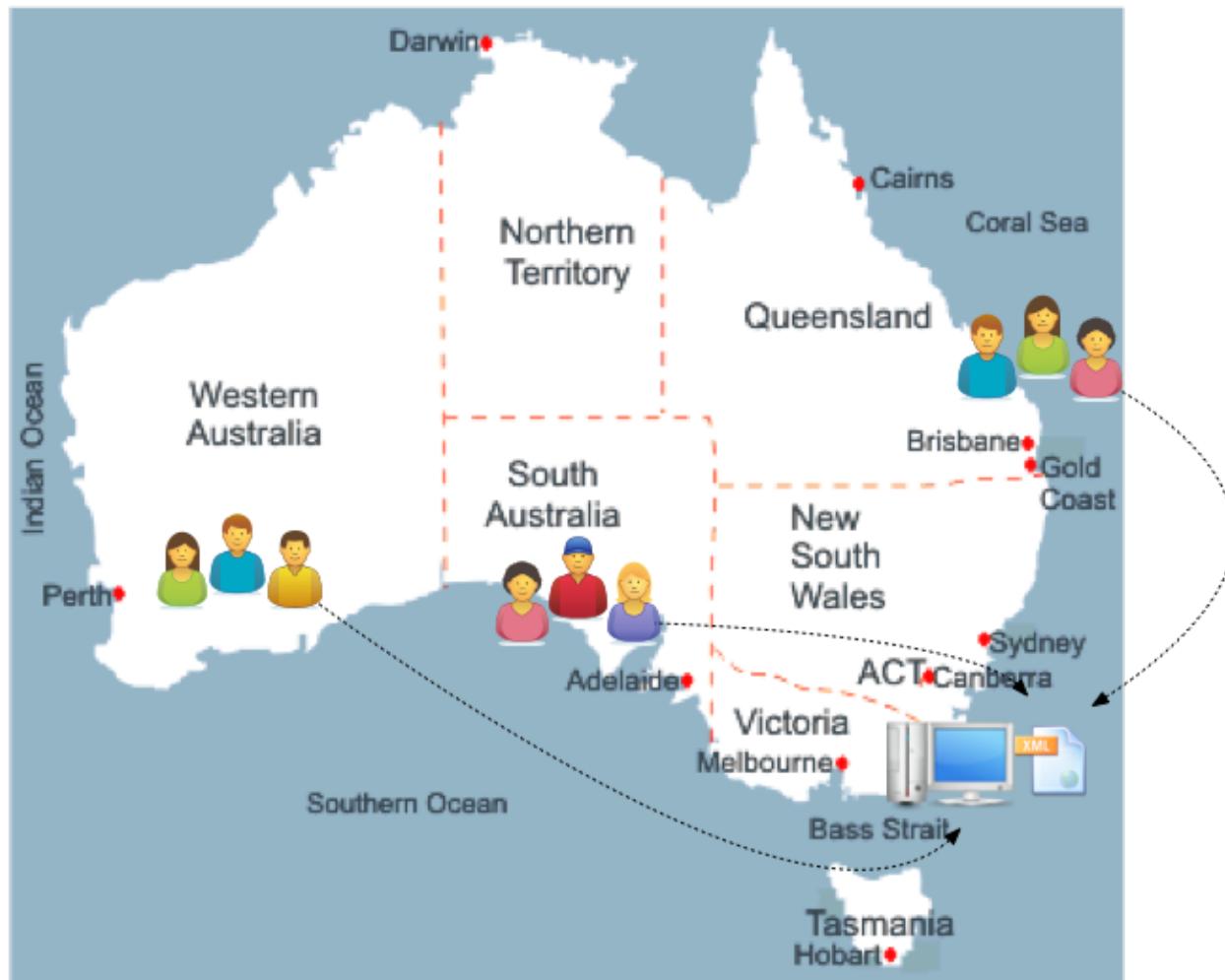
# The Big Picture



# Training Environment



# Training Environment



# Training Environment

- Ubuntu-based Environment
  - Standard Desktop
  - Command Line Interface
- 1:1 Resource Allocation
  - Trainees are allocated dedicated training server
- Intro to NGS, de novo assembly and metagenomics courses
  - 2 vCPUs, ~8GB RAM
- Cancer Genomics courses
  - 4 vCPUs, ~16GB RAM

# Training Environment



# Training Environment



# Training Workshop

- Modular eg running shorter, more focused workshops
- Compose of stand-alone training modules
  - Promotes "plug and play" setup
- BPA-CSIRO workshops can be used "as is"
  - Easily customisable and reusable
- Version-controlled (GitHub)
- Orchestration system for:
  - Creation of training image (BTP) image
  - Instantiation of training instances (cloud, VirtualBox, VMWare)

# Nuts and Bolts

- **GitHub** for managing training workshops and its modules
- **Travis CI** for auto building of training materials (LaTeX) and tools installers (deb)
- **Packer** for creating cloud images on NeCTAR and AWS, desktop images for VirtualBox and VMWare
- **FPM/FPM Cookery** for packaging analysis tools into stand-alone installers

# Nuts and Bolts

- **Puppet** for auto configuration of analysis tools and datasets into the images
- **OpenStack Heat** for provisioning training instances on NeCTAR
- **AWS CloudFormation** for provisioning on AWS

# Training Modules

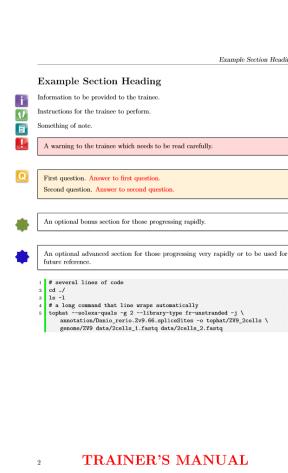
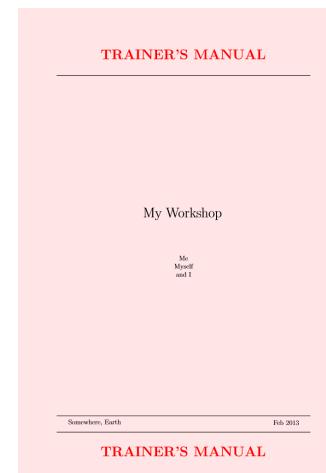
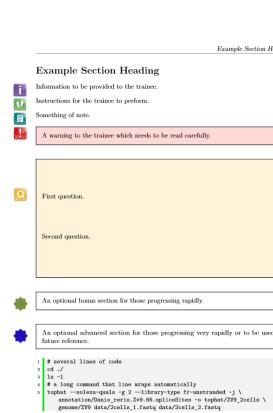
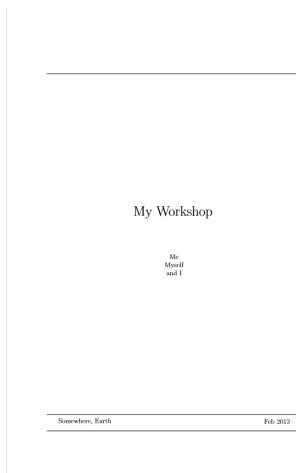
- Version-controlled (GitHub)
- Containers relevant metadata:
  - Tutorials
  - Training Datasets
  - Analysis Tools

Tree: c91426... ▾ [New pull request](#) [New file](#) [Find file](#) [HTTPS](#) ▾ <https://github.com/BPA->   [Download ZIP](#)

revote Just renaming datasets metadata.		Latest commit c914261 on Jan 27
	datasets	Just renaming datasets metadata.
	handout	Picard java jar files are now installed under /usr/share/java.
	presentations	Added presentation
	tools	apt -> dpkg.
	README.md	Moved compute requirements to workshop repo

# Tutorials

- LaTeX-based
- Version-controlled (GitHub)
- Automated Publishing
  - Continuous Integration (Travis CI)
- Trainee/Trainer Versions



# Tutorials

```
\begin{questions}
```

First question.

```
\begin{answer}
```

Answer to first question.



```
\end{answer}
```

Second question.

```
\begin{answer}
```

Answer to second question.

```
\end{answer}
```

```
\end{questions}
```

First question.

Second question.



First question. **Answer to first question.**

Second question. **Answer to second question.**

# Training Datasets

- Publicly Available/Downloadable
  - Open Access
  - Standard HTTP/GET
  - Amazon S3
  - NeCTAR Object Storage (Swift)
- Training Modules-Organised
  - One container/bucket for training module
- Automatically Pulled
  - Orchestration
    - BTP Image
    - BTP Instances

# Training Datasets

- Each training module has datasets metadata
- Describes the location of dataset to be installed on:
  - BTP Images (VirtualBox, VMWare)
  - BTP Instances (NeCTAR Research Cloud, AWS)
- Datasets metadata
  - YAML
  - Used by “Puppet” for automated installation (Orchestration)

# Training Datasets

30 lines (29 sloc) | 1 KB

Raw Blame History



```
1 btp::modules:
2   qc:
3     dirs:
4       - 'qc'
5     data:
6       good_example.fastq:
7         source: 'https://swift.rc.nectar.org.au:8888/v1/AUTH_809/NGSDataQC'
8         targets:
9           - 'qc/good_example.fastq'
10      adaptorQC.fastq.gz:
11        source: 'https://swift.rc.nectar.org.au:8888/v1/AUTH_809/NGSDataQC'
12        targets:
13          - 'qc/adaptorQC.fastq.gz'
14      bad_example.fastq:
15        source: 'https://swift.rc.nectar.org.au:8888/v1/AUTH_809/NGSDataQC'
16        targets:
17          - 'qc/bad_example.fastq'
18      bad_example.fastq.trimmed_fastqc.zip:
19        source: 'https://swift.rc.nectar.org.au:8888/v1/AUTH_809/NGSDataQC'
20        targets:
21          - 'qc/bad_example.fastq.trimmed_fastqc.zip'
22      qcdemo_R1.fastq.gz:
23        source: 'https://swift.rc.nectar.org.au:8888/v1/AUTH_809/NGSDataQC'
24        targets:
25          - 'qc/qcdemo_R1.fastq.gz'
26      qcdemo_R2.fastq.gz:
27        source: 'https://swift.rc.nectar.org.au:8888/v1/AUTH_809/NGSDataQC'
28        targets:
29          - 'qc/qcdemo_R2.fastq.gz'
```

# Analysis Tools

- FPM/FPM Cookery
  - “Effing Package Manager”
  - Inspired by “brew” and “brew2deb”
  - Packaging of analysis tools
  - Creates a “\*.deb” installer for the tool
  - Ruby-based Tool Recipes

# Tool Recipe

27 lines (23 sloc) | 710 Bytes

Raw Blame History



```
1 class Velvet < FPM::Cookery::Recipe
2   description 'Sequence assembler for very short reads.'
3   name 'velvet'
4   version '1.2.10'
5   revision 0
6   homepage 'https://www.ebi.ac.uk/~zerbino/velvet/'
7   source "https://www.ebi.ac.uk/~zerbino/velvet/velvet_#{version}.tgz"
8   md5 '6e28c4b9bedc5f7ab2b947e7266a02f6'
9
10  # Let's install build dependencies first:
11  build_depends ['curl', 'zlib1g-dev']
12
13  # Build:
14  def build
15    safesystem "make 'MAXKMERLENGTH=59' 'LONGSEQUENCES=1' 'OPENMP=1'"
16  end
17
18  # Install:
19  def install
20    velvetg_long = bin('velvetg_long')
21    velveth_long = bin('velveth_long')
22    bin.install ['velvetg', 'velveth']
23    ln_s 'velvetg', velvetg_long
24    ln_s 'velveth', velveth_long
25  end
26 end
```

# BTP Tools

- Version-controlled (GitHub)
  - Tool Recipes
- Easily Customisable
- Tool Installers Uploaded/Downloadable
  - NeCTAR Object Storage (Swift)
  - Amazon S3
- Automatically Pulled
  - Orchestration
    - BTP Image
    - BTP Instances

# BTP Tools

The screenshot shows a GitHub repository page for 'BPA-CSIRO-Workshops/btp-tools'. The repository has 322 commits, 3 branches, 0 releases, and 3 contributors. The latest commit was made 22 hours ago. The repository description states: "Analysis tools installers and fpm-cookery recipes for building .deb packages for the Bioinformatics Training Platform <http://bpa-csiro-workshops.github.io/btp-tools>".

Analysis tools installers and fpm-cookery recipes for building .deb packages for the Bioinformatics Training Platform <http://bpa-csiro-workshops.github.io/btp-tools>

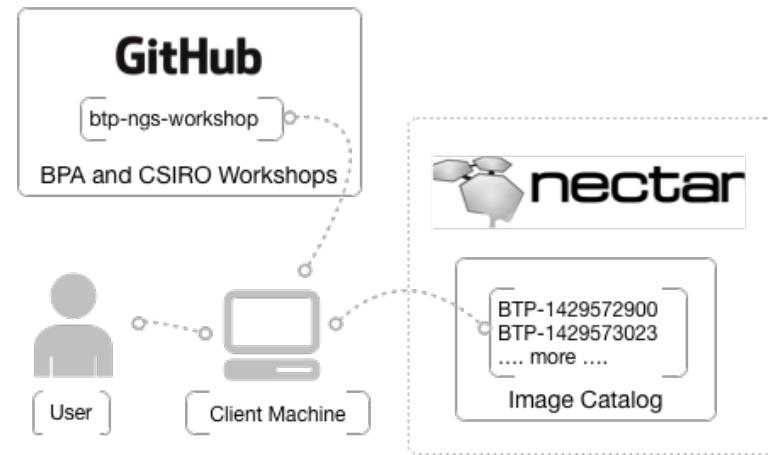
Commit	Message	Date
amos	Remove tags on, try deploying for every commit.	8 months ago
bedtools	Trigger bedtools.	8 months ago
blat	trigger blat.	8 months ago
bowtie	Merge branch 'master' of https://github.com/BPA-CSIRO-Workshops/btp-t...	7 months ago
bowtie2	Dummy commit for all these tools.	8 months ago
cufflinks	Dummy again.	8 months ago
fastqc	Testing commit.	8 months ago
fastx-toolkit	Dummy commit for all these tools.	8 months ago

# The BTP Image

- Ubuntu LTS OS
- Minimalistic Setup
  - Desktop Environment
  - Remote Desktop (NoMachine)
- Training Modules
  - Intro CLI, QC, Alignment, RNA-Seq, ChIP-Seq, de novo
    - Tutorials
    - Exemplar Datasets
    - Analysis Tools

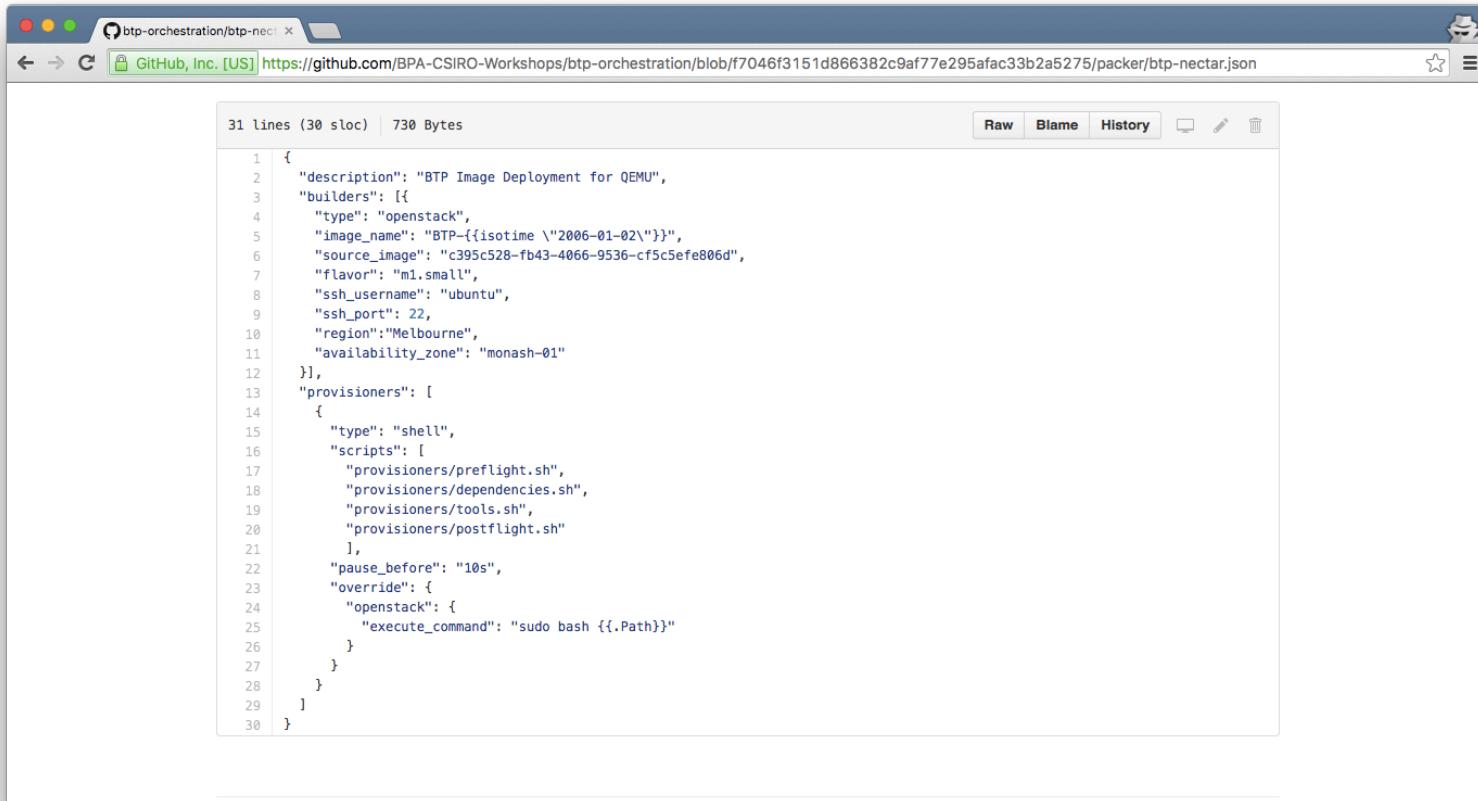
# The BTP Image

- Packer
  - Creates BTP images for
    - NeCTAR RC
    - AWS
    - VirtualBox
    - VMWare
  - Using a simple build recipe
    - Included in the workshop repository
  - Fully automated & configurable



# Packer Recipe

- YAML
- Defines how to build & configure the image

A screenshot of a web browser displaying a GitHub page. The URL is https://github.com/BPA-CSIRO-Workshops/btp-orchestration/blob/f7046f3151d866382c9af77e295afac33b2a5275/packer/btp-nectar.json. The page shows a JSON file with 31 lines and 30 source locations (sloc), totaling 730 bytes. The JSON content defines a Packer recipe for building a QEMU image. It includes configurations for builders (using OpenStack with specific image and flavor details) and provisioners (using shell scripts like preflight, dependencies, tools, and postflight).

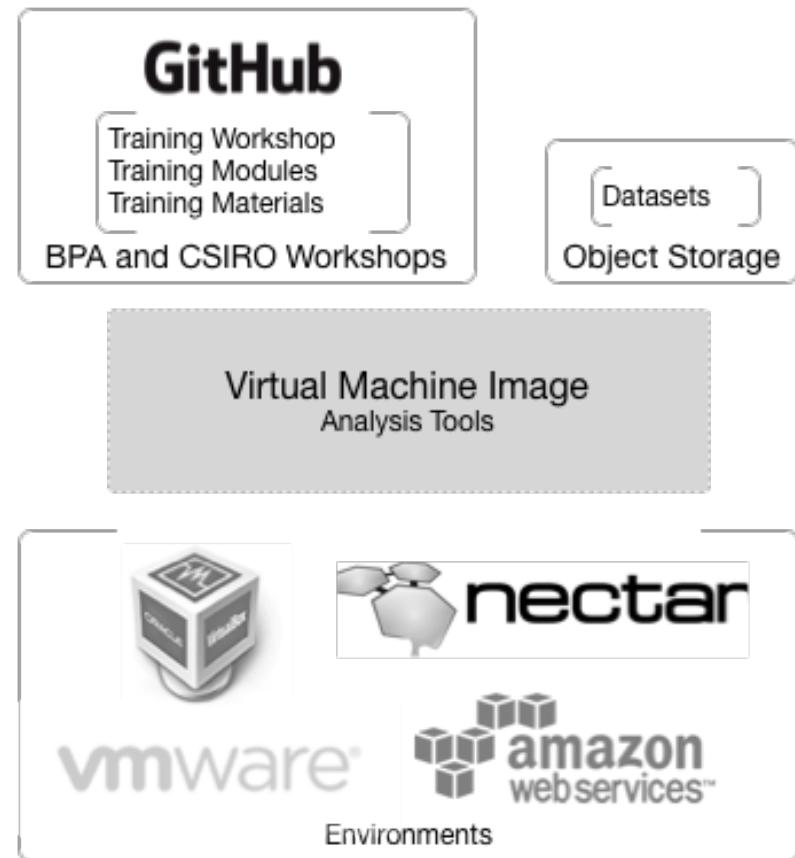
```
1  {
2    "description": "BTP Image Deployment for QEMU",
3    "builders": [
4      {
5        "type": "openstack",
6        "image_name": "BTP-{{isotime \\\"2006-01-02\\\"}}",
7        "source_image": "c395c528-fb43-4066-9536-cf5c5efe806d",
8        "flavor": "m1.small",
9        "ssh_username": "ubuntu",
10       "ssh_port": 22,
11       "region": "Melbourne",
12       "availability_zone": "monash-01"
13     },
14     "provisioners": [
15       {
16         "type": "shell",
17         "scripts": [
18           "provisioners/preflight.sh",
19           "provisioners/dependencies.sh",
20           "provisioners/tools.sh",
21           "provisioners/postflight.sh"
22         ],
23         "pause_before": "10s",
24         "override": {
25           "openstack": {
26             "execute_command": "sudo bash {{.Path}}"
27           }
28         }
29       }
30     }
31 }
```

# Reusable BTP Resources

- BTP Images
  - VirtualBox, VMWare
  - NeCTAR Research Cloud
  - AWS
  - Can be used “as is”
- Training Workshops
  - Training Modules
    - Training Datasets
    - Analysis Tools
    - Training Handouts

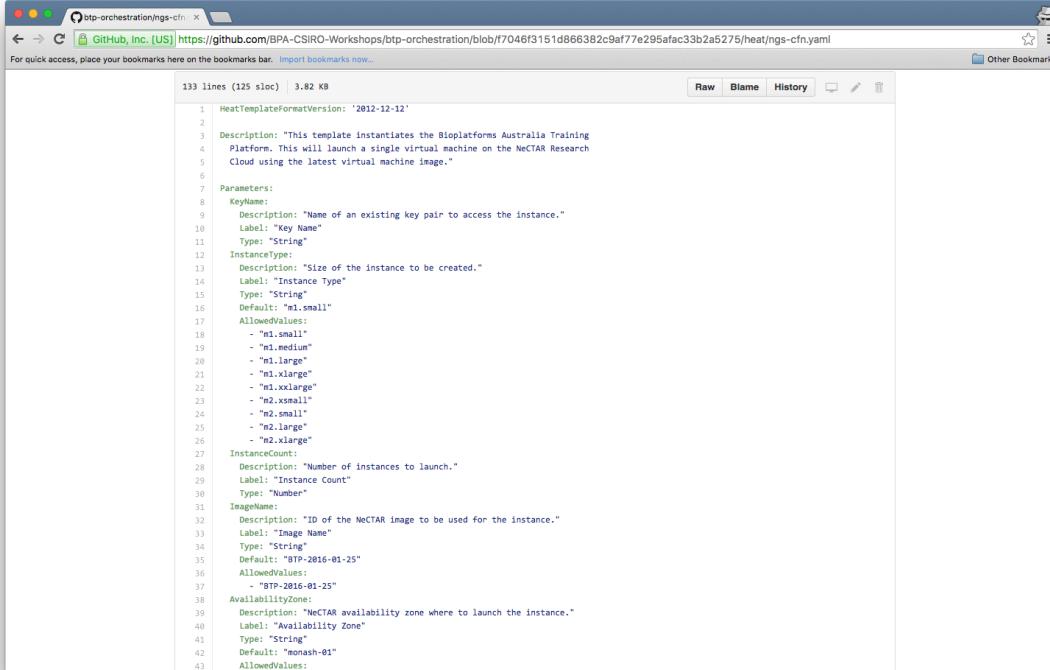
# Launching BTP Instances

- Orchestration
  - Fully Automated
    - Training Datasets
    - Analysis Tools
- Cloud Instantiable
  - NeCTAR RC
  - AWS
- Stand-alone VMs
  - VirtualBox
  - VMWare



# Orchestration Templates

- Templates developed for Heat and CloudFormation
- Instructs the cloud infrastructure how to build and configure the cloud server



A screenshot of a web browser displaying a GitHub page for a file named 'heat/ngs-cfn.yaml'. The page shows the YAML code for a CloudFormation template. The code defines a stack with parameters for key name, instance type, instance count, image name, and availability zone. It specifies the NECTAR Research Cloud as the platform and uses the latest virtual machine image.

```
1  HeatTemplateFormatVersion: '2012-12-12'
2
3  Description: "This template instantiates the Bioplatforms Australia Training
4    Platform. This will launch a single virtual machine on the NeCTAR Research
5    Cloud using the latest virtual machine image."
6
7  Parameters:
8    KeyName:
9      Description: "Name of an existing key pair to access the instance."
10   Label: "Key Name"
11   Type: "String"
12   InstanceType:
13     Description: "Size of the instance to be created."
14     Label: "Instance Type"
15     Type: "String"
16     Default: "m1.small"
17     AllowedValues:
18       - "m1.small"
19       - "m1.medium"
20       - "m1.large"
21       - "m1.xlarge"
22       - "m1.xxlarge"
23       - "m2.xsmall"
24       - "m2.small"
25       - "m2.large"
26       - "m2.xlarge"
27   InstanceCount:
28     Description: "Number of instances to launch."
29     Label: "Instance Count"
30     Type: "Number"
31   ImageName:
32     Description: "ID of the NeCTAR image to be used for the instance."
33     Label: "Image Name"
34     Type: "String"
35     Default: "919-2016-01-25"
36     AllowedValues:
37       - "919-2016-01-25"
38   AvailabilityZone:
39     Description: "NeCTAR availability zone where to launch the instance."
40     Label: "Availability Zone"
41     Type: "String"
42     Default: "monash-01"
43     AllowedValues:
```

# NeCTAR Research Cloud

- OpenStack Orchestration Service
  - Heat
    - OpenStack API CLI
    - NeCTAR Dashboard
    - Orchestration template, included in workshop repository
  - Automated Instantiation & Configuration
    - Puppet
      - Installation of training datasets
      - Trainee user access
      - Remote desktop service

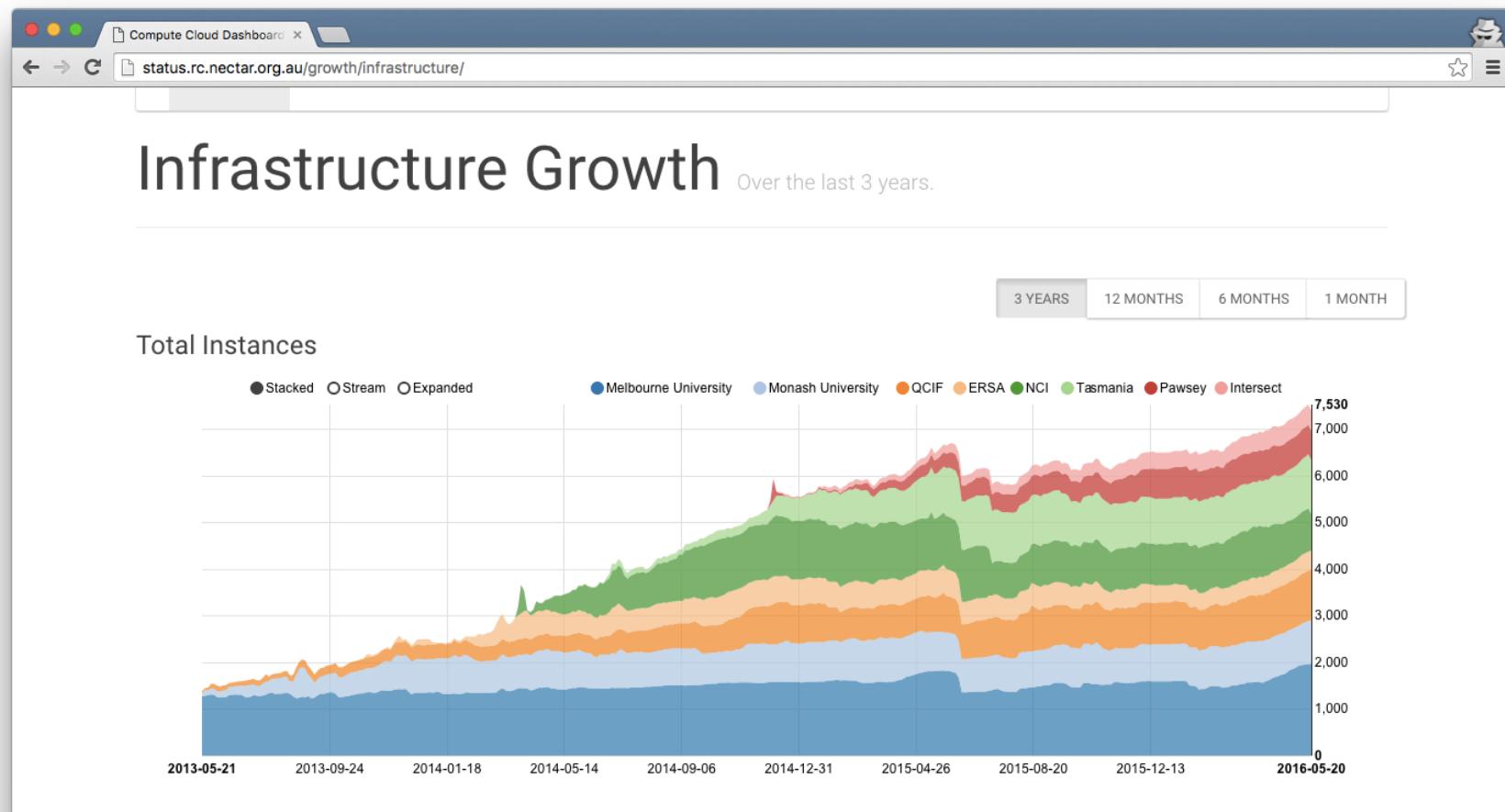
# NeCTAR Research Cloud

- Federated Research Cloud
  - Distributed across Australia
    - 8 Availability Zones
- Research Infrastructure as a Service (IAAS)
  - Dynamic Provisioning
  - Computing Infrastructure
  - Software & Services
- Dedicated Training Project/Allocation

# NeCTAR Research Cloud



# NeCTAR Research Cloud



# NeCTAR Research Cloud

The screenshot shows the NeCTAR Research Cloud OpenStack Dashboard interface. The main title is "Launch Stack". The left sidebar has sections for Project, Compute, Orchestration, and Stacks (which is currently selected). The right side contains fields for Stack Name, Creation Timeout (minutes), Rollback On Failure, Availability Zone, Image Name, Instance Count, Instance Type, Key Name, and Trainee Password. A "Description:" section with the placeholder "Create a new stack with the provided values." is also present. At the top right, there are buttons for "Report Ticket", "Jerico.Revote@monash.edu", "Search", "+ Launch Stack", and "Preview Stack". The bottom right shows a table with columns for Status and Actions.

nectarcloud

Project

Compute

Orchestration

Stacks

Resource Types

Object Store

Allocations

Stack Name \* ⓘ

Creation Timeout (minutes) \* ⓘ

60

Rollback On Failure ⓘ

Availability Zone ⓘ

monash-01

Image Name ⓘ

BTP-2016-01-25

Instance Count \* ⓘ

Instance Type ⓘ

m1.small

Key Name \* ⓘ

Trainee Password \* ⓘ

Description:

Create a new stack with the provided values.

Report Ticket Jerico.Revote@monash.edu

+ Launch Stack Preview Stack

Status	Actions

# Amazon Web Services

- AWS Orchestration Service
  - CloudFormation
    - AWS CLI
    - AWS Web Console
- AWS Educational Grant/Credits ☺
- BTP Image
  - ap-southeast-2 (Sydney)
  - eu-west-1 (Ireland)

# Amazon Web Services

The screenshot shows the AWS Management Console home page for the 'ap-southeast-2' region. The top navigation bar includes 'AWS' (dropdown), 'Services' (dropdown), 'Edit' (dropdown), and user information ('jrevote @ bpa-csiro-btp', 'Sydney', 'Support'). A 'Resource Groups' section is visible on the right.

**Amazon Web Services**

**Compute**

- EC2** Virtual Servers in the Cloud
- EC2 Container Service** Run and Manage Docker Containers
- Elastic Beanstalk** Run and Manage Web Apps
- Lambda** Run Code in Response to Events

**Storage & Content Delivery**

- S3** Scalable Storage in the Cloud
- CloudFront** Global Content Delivery Network
- Elastic File System** PREVIEW Fully Managed File System for EC2
- Glacier** Archive Storage in the Cloud
- Snowball** Large Scale Data Transport
- Storage Gateway** Hybrid Storage Integration

**Database**

- RDS** Managed Relational Database Service
- DynamoDB** Managed NoSQL Database
- ElastiCache** In-Memory Cache
- Redshift** Fast, Simple, Cost-Effective Data Warehousing
- DMS** Managed Database Migration Service

**Networking**

- VPC** Isolated Cloud Resources
- Direct Connect** Dedicated Network Connection to AWS

**Developer Tools**

- CodeCommit** Store Code in Private Git Repositories
- CodeDeploy** Automate Code Deployments
- CodePipeline** Release Software using Continuous Delivery

**Management Tools**

- CloudWatch** Monitor Resources and Applications
- CloudFormation** Create and Manage Resources with Templates
- CloudTrail** Track User Activity and API Usage
- Config** Track Resource Inventory and Changes
- OpsWorks** Automate Operations with Chef
- Service Catalog** Create and Use Standardized Products
- Trusted Advisor** Optimize Performance and Security

**Internet of Things**

- AWS IoT** Connect Devices to the Cloud

**Game Development**

- GameLift** Deploy and Scale Session-based Multiplayer Games

**Mobile Services**

- Mobile Hub** Build, Test, and Monitor Mobile Apps
- Cognito** User Identity and App Data Synchronization
- Device Farm** Test Android, iOS, and Web Apps on Real Devices in the Cloud
- Mobile Analytics** Collect, View and Export App Analytics
- SNS** Push Notification Service

**Application Services**

- API Gateway** Build, Deploy and Manage APIs
- AppStream** Low Latency Application Streaming
- CloudSearch** Managed Search Service
- Elastic Transcoder** Easy-to-Use Scalable Media Transcoding
- SES** Email Sending and Receiving Service
- SQS** Message Queue Service
- SWF** Workflow Service for Coordinating Application Components

**Analytics**

- EMR** Managed Hadoop Framework
- Data Pipeline** Orchestration for Data Driven Workflows

**Enterprise Applications**

- WorkSpaces** Desktops in the Cloud
- WorkDocs**

**Resource Groups** Learn more

A resource group is a collection of resources that share one or more tags. Create a group for each project, application, or environment in your account.

**Create a Group** **Tag Editor**

**Additional Resources**

**Getting Started** Read our documentation or view our training to learn more about AWS.

**AWS Console Mobile App** View your resources on the go with our AWS Console mobile app, available from Amazon Appstore, Google Play, or iTunes.

**AWS Marketplace** Find and buy software, launch with 1-Click and pay by the hour.

**AWS re:Invent Announcements** Explore the next generation of AWS cloud capabilities. See what's new

**Service Health**

All services operating normally.

Updated: May 23 2016 09:19:01 GMT+1000

[Service Health Dashboard](#)

# Amazon Web Services

The screenshot shows the AWS CloudFormation 'Create stack' interface. The browser title bar reads 'Create A New Stack'. The URL is <https://console.aws.amazon.com/cloudformation/home?region=ap-southeast-2#/stacks/new>. The top navigation bar includes 'AWS', 'Services', 'Edit', and user information 'jrevote @ bpa-csiro-btp', 'Sydney', and 'Support'. Below the navigation is a bookmark bar with 'Other Bookmarks'. The main content area is titled 'Create stack' and 'Specify Details'. It instructs the user to specify a stack name and parameter values. The 'Stack name' field contains 'BTP-NGS'. The 'Parameters' section contains fields for 'InstanceType' (set to 'm1.medium'), 'KeyName' (set to 'Search', with a dropdown menu open), 'SSHLocation' (set to '0.0.0.0/0'), and 'TraineePassword' (an empty field). At the bottom right are 'Cancel', 'Previous', and 'Next' buttons, with 'Next' being highlighted.

Create stack

Select Template

**Specify Details**

Options

Review

Specify Details

Specify a stack name and parameter values. You can use or change the default parameter values, which are defined in the AWS CloudFormation template. [Learn more](#).

Stack name

Parameters

InstanceType  EC2 instance type

KeyName  Name of an existing EC2 KeyPair to enable SSH access to the instance

SSHLocation  The IP address range that can be used to SSH to the EC2 instances

TraineePassword  The password to assign the trainee user for remote access

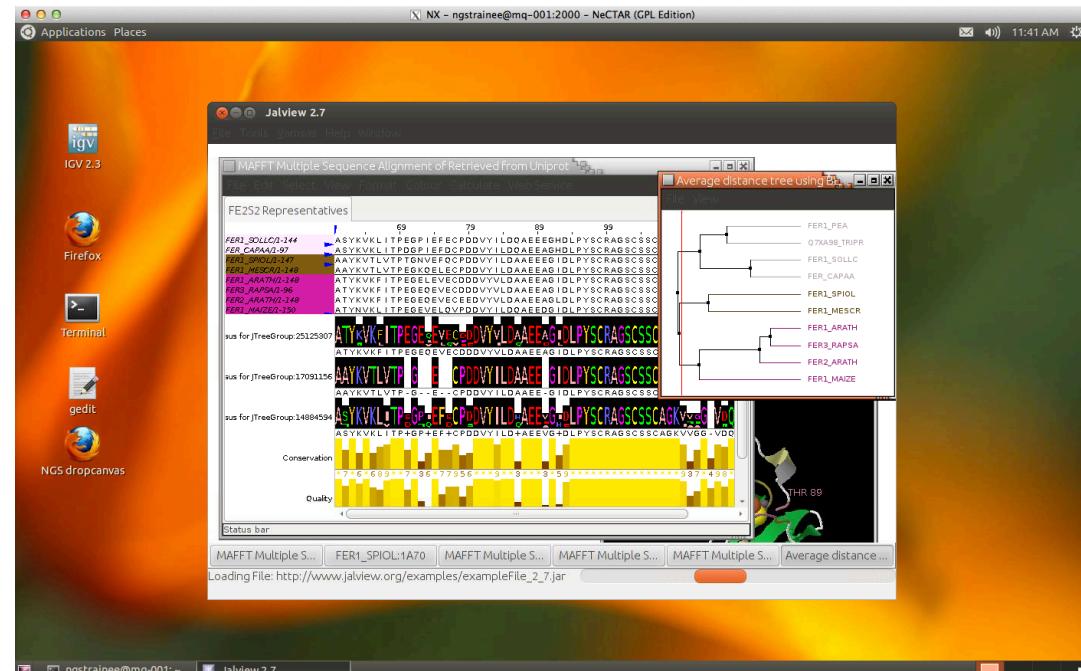
Cancel Previous Next

Feedback English

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# Accessing BTP Instances

- VirtualBox & VMWare
  - Simply download the image and launch ☺
- Cloud Training Instances
  - Remote Desktop Client
    - NoMachine
    - SSH



# Post Workshop

- Trainees continue with analysis
  - Cloud Resources
    - Trainees can request for research cloud allocation
  - Stand-alone images (VirtualBox/VMWare)
  - Orchestration
  - Customisation
  - Support

# Summary

- BTP
  - Training Workshops
    - Training Modules
    - Training Datasets
    - Analysis Tools
    - Training Handouts
  - Modular, “plug & play”
  - Reusable
  - Customisable
  - Orchestration
  - Open Access

# Future

- BTP -> AWS Marketplace
- BTP -> NeCTAR RC App Store
  - Murano
- BTP -> Docker, Google, Azure
- BTP -> Production Pipeline
  - Collaboration
  - Data Management

# Links

- BPA-CSIRO Project @ GitHub
  - <https://github.com/BPA-CSIRO-Workshops>
  - <http://bpa-csiro-workshops.github.io/>
- Introduction to NGS BTP
  - <http://bpa-csiro-workshops.github.io/btp-workshop/ngs/>
- Contacts
  - Annette.McGrath@csiro.au
  - Jerico.Revote@monash.edu

# Papers

- Watson-Haigh NS, Shang CA, Haimel M, et al. **Next-generation sequencing: a challenge to meet the increasing demand for training workshops in Australia.** *Briefings in Bioinformatics*. 2013;14(5):563-574. doi:10.1093/bib/bbt022.
- **Towards an open, collaborative, reusable framework for sharing hands-on bioinformatics training workshops**  
Nathan S. Watson-Haigh; Jerico Revote; Radosław Suchocki; Sonika Tyagi; Susan M. Corley; Catherine A. Shang; Annette McGrath  
*Briefings in Bioinformatics* 2016;  
doi: 10.1093/bib/bbw013
- **Development of a cloud-based Bioinformatics Training Platform**  
Jerico Revote; Nathan S. Watson-Haigh; Steve Quenette; Blair Bethwaite; Annette McGrath; Catherine A. Shang  
*Briefings in Bioinformatics* 2016;  
doi: 10.1093/bib/bbw032



Annette McGrath

Konsta Duesing

Sean Li

Sean McWilliam

Paul Greenfield

David Lovell

Philippe Moncuquet

Paul Berkman



Jerico Revote

Simon Michnowicz

Blair Bethwaite

Steve Quenette

Mark Crowe (QFAB)

Peter Sterk

(Oxford e-Research Centre)



**BIOPLATFORMS**  
AUSTRALIA

Catherine Shang

Ellen van Dam

Katherine Champ

Nathan Watson-Haigh (ACPFG)

Nandan Deshpande (UNSW)

Paula Moolhuijzen (Murdoch  
Uni)

Sonika Tyagi (AGRF)

Matthew Field (ANU)

Dan Andrews (ANU)

Susan Corley (UNSW)

Zhiliang Chen (UNSW)

Ann-Marie Patch (QIMR)

Gayle Phillips (VLSCI)

Torsten Seemann (VLSCI)

Erdahl Teber (CMRI)

Velimir Gayevskiy (Garvan)



**Cath Brooksbank** (EBI)

**Sarah Morgan** (EBI)

**Matthias Haimeil** (University of Cambridge)

**Myrto Kostadima** (University of  
Cambridge)

**Gabriella Rustici** (University of Cambridge)

**Remco Loos** (EBI)

**Alex Mitchell** (EBI)

**Hubert Denise** (EBI)

**Mathieu Bourgey** (C3G)



**Vicky Schneider**  
**Bernardo Clavijo**