

# Jenkins as a Scientific Data and Image Processing Platform

Ioannis K. Moutsatsos, Ph.D., M.SE. Novartis Institutes for Biomedical Research www.novartis.com

June 18, 2014

#jenkinsconf

## Life Sciences are Computational Sciences

- Modern life sciences (biomedical research, systems biology) are heavily dependent on
  - Data Management
  - Computational Analysis
  - Computational Modeling
- Modern laboratory technologies and instrumentation generate data that are
  - Big
  - Heterogeneous
  - Complex

#### Computational Challenges & Opportunities

#### **Scientists**

- Face daily challenges by continuing increases in computational complexity
- Focused on the biology and not the compute problem
- Have varying and rapidly changing requirements

#### Life Sciences Research

- Benefits from computational systems that are
  - Easy to use
  - Fast to implement
  - Flexible
  - Support
    - Collaboration
    - Transparency
    - Automation
    - Reproducible Research
    - Open standards

#### **Talk Outline**

- A life sciences computational challenge
  - High Content Image Analysis
    - What is it?
- Jenkins-Cl as a scientific data/image processing platform
  - Functionality with standard plugins
  - How Jenkins-Cl provided a HP image analysis platform for lab scientists
- Jenkins as a data analytics platform
  - Domain specific analysis and visualization plugins
  - The Jenkins pros and cons
    - What are we missing?
- Where do we want to take Jenkins?

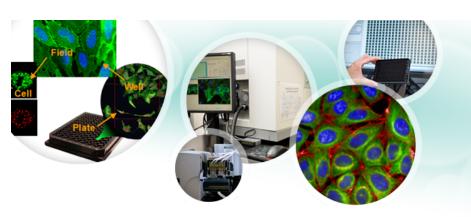


#### **High Content Screening: HCS**

High throughput automated fluorescent microscopy for drug discovery

- Wet Lab Workflow
  - Cells grown on high density arrays
  - Cells treated with large number of chemical or biological factors
  - Cells stained with fluorescent antibodies
- Data Acquisition
  - Stained cells are imaged in high throughput mode using a computerized microscope

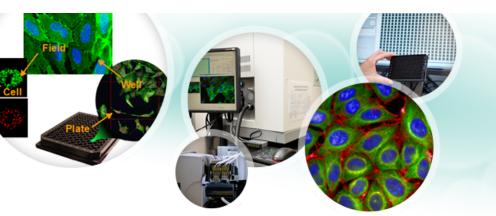
- Computational Workflow
  - Cell images processed to extract phenotypic measurements
  - Measurements analyzed to understand factor effects



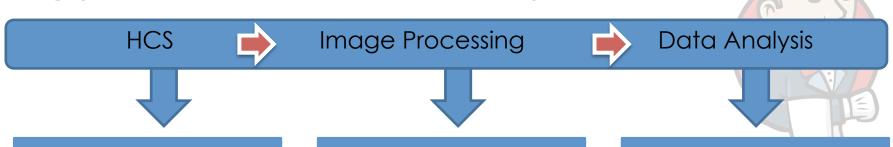
## **High Content Screening**

- Novartis
  - High Throughput Biology (my group)
    - Data from 2010-2013
- Captured
  - 83 Terabytes of high content image data
    - 17.5 million wells
    - 27 million images
    - ~540 days of imaging time
    - ~1.5 years of computing time





#### **HCS: Workflow and Data Stream**



#### Raw Data

- Images
  - channels
  - fields
- Metadata
  - Acquisition
  - Experiment

#### Measurements

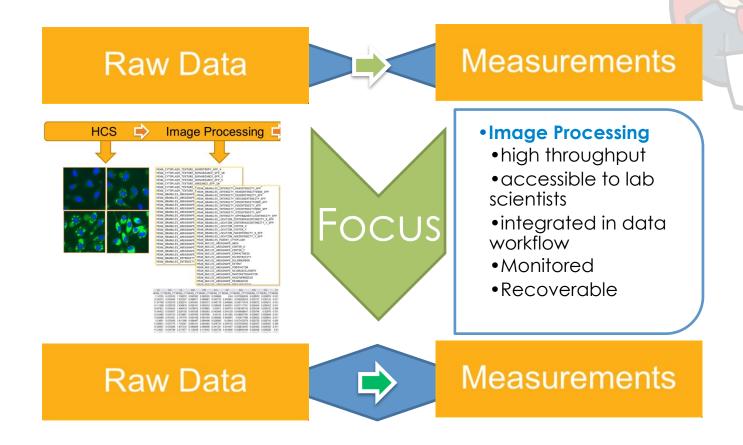
- Raw (>500 parameters)
  - Aggregated or cell by cell
  - filtered
- Metadata
  - Image Processing

#### Results

- Assay QC
- Hit Identification
- Multiparametric
   Statistics
- Correlations
- Machine Learning etc.

**HCS-High Performance Image Analysis** 

Intial Focus: Remove Image Processing Bottleneck



**HCS: Image Measurements and Analytics** 

Easily Accessible, High Performance Image Analytics

- Vision
  - Image and data analysis using high performance (HP) image processing tools
    - Accessible, scalable, affordable, flexible and well-supported
- Strategy
  - Evaluate and adopt open-source, community supported tools
    - CellProfiler, ImageJ, Jenkins-Cl
  - Utilize NIBR-IT systems and resources
    - Linux Compute Engine (cluster) / Network Attached Storage
    - Development expertise (UI, data management and web-services)
  - Increase usability of NIBR-IT systems and resources
  - Engage and provide timely and practical functionality to both expert and casual imaging platform users

#### Tactics

- Develop functional prototypes (Jenkins-CellProfiler, Test Mosaic, R-Analytics)
- Collaborate to develop new image/data analysis systems
- Explore imaging tools and data space. Define HP image processing requirements.
- Provide training, support and engage in community building



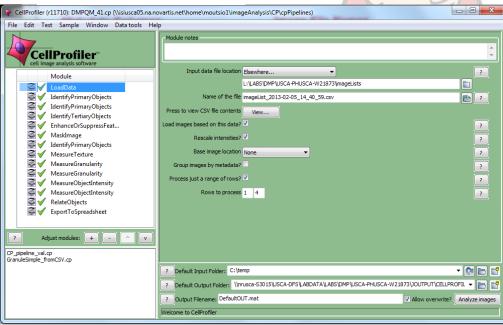




#### **CellProfiler**

- Open Source Image Processing
- Platform independent
- Desktop client for defining an arbitrarily complex image processing pipeline
- Pipeline can be used by the command line CellProfiler executable
  - Suitable for high throughput analysis
  - Suitable for deployment on a Linux grid engine
  - Can process large image sets (300K + images)

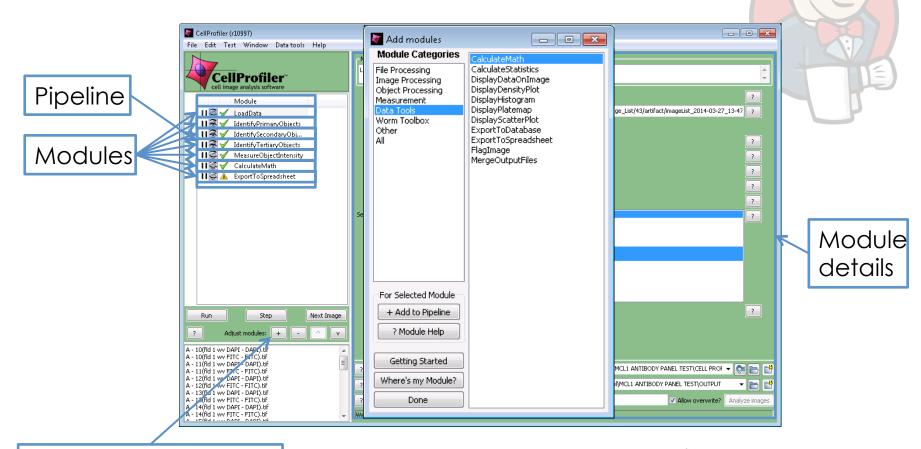




- Developed and supported by the Broad Institute and a sizable scientific user community
- Supports additional imaging tools (ImageJ)

CellProfiler – general anatomy

Nuclear Translocation Assay



Add/Subtract Modules



### **HCS Image/Data Processing**

Programming and Prototyping Functional Requirements

- Scripting
  - Pros
    - Quick prototyping
    - Flexibility
    - Platform independence
  - Cons
    - Unsuitable for end users
      - Requires installation of scripting tools
      - Command Line Interface

- Scripting for end users
  - Requires a user interface
    - Most UI prototypes are either
      - » hard
      - » Pretty but not functional
      - » Or...



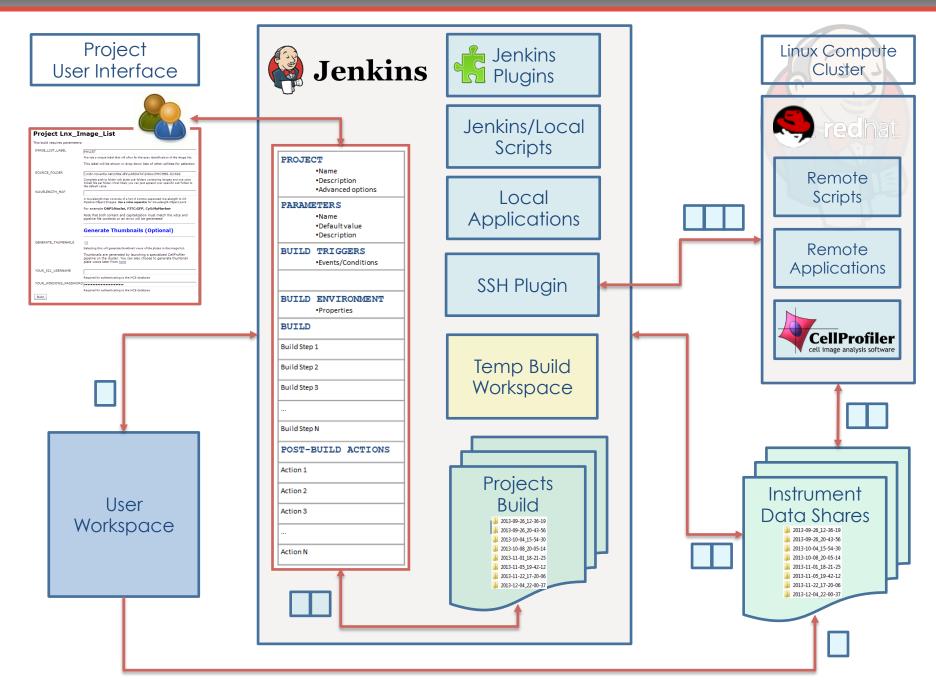
An extendable open source continuous integration server

- ...not very pretty
  - But quite functional

## Why choose Jenkins-CI?

- Why Jenkins-CI?
  - Jenkins allows us to rapidly wrap any command line script or program in a web interface
    - Excellent support for <u>Groovy</u> a Java based, dynamic, modern scripting language
    - Straight forward integration with other languages, tools, OS, frameworks
  - Jenkins has broad community support that provides access to over 800 plugins
    - Plugins allow easy customization of Jenkins for a variety of tasks

- Jenkins provides basic workflow and web server functionality
  - Which works well in combination with CellProfiler
- Jenkins is used extensively by the NIBR-IT group to build all kinds of internal software
  - Many software developers know a lot about Jenkins
- Jenkins is now emerging as a useful Bioinformatics tool
  - The <u>BioUno</u> project



#### Jenkins-CellProfiler

HP Image Processing Workflow: Outline

Contribute Image Processing Pipeline



Assemble Images, Metadata



CellProfiler
HP Image
Processing





#### Upload your CellProfiler pipeline

Upload a CellProfiler image processing pipeline from y The pipeline will be available for use on the Jenkins-HC



#### Generate a CellProfiler image list

The source folder must contain one or more subfolders

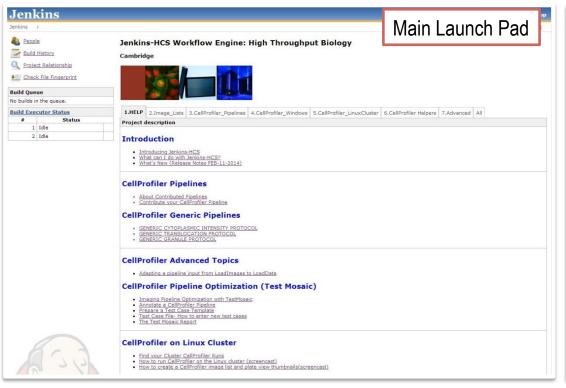


#### **Process images using CellProfiler**

The CellProfiler pipeline and the image list are selected Processing can be **restricted** to a subset of the plates <u>Help Screencast</u>



## Jenkins-HCS Workflow Engine High Level UI Components



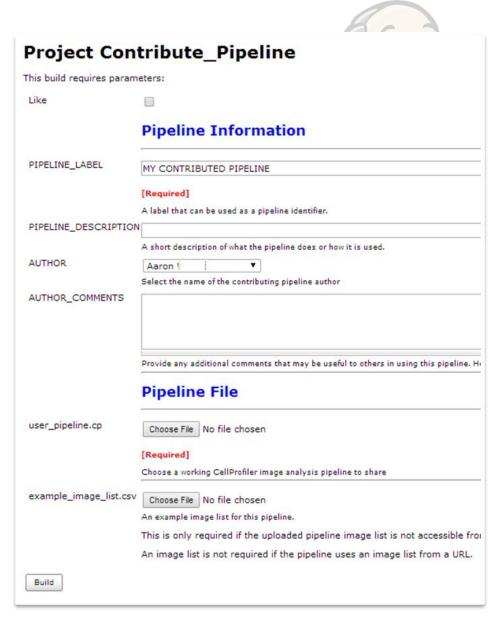
Project CellProfiler_JClustSelect This build requires parameters:  CELLPROFILER_VERSION [2.x.11364 v]		Project Launch Pad			
	Select the version of callProfiler to use.  CellProfiler  Welcome to CellProfiler on th	e Linux-Cluster!			
	1) Annotate your run:				
RUN_LABEL	CP_CLUSTER_RUN  A unique label that can be used to identify this run. Use no spaces and try to keep it <32 characters.				
RUN_DESCRIPTION	Provide a brief description about this Cell Profiler run  2) Select a processing pipelin	me:			
PIPELINE	Contribute_Pipeline 2014_02_12_DRAQS Select a Call Profiler Contributed Pipeline.  3) Select an image list (or su	bset):			
GENERATED_IMAGE_LI	ST Lnx_Image_List 20140211_Cheng_DRAQ5_10x_Li A previously generated Lnx_Image_List	INUX ▼			
QUERY_KEY	A QUERY_KEY must adhere to the format <b>Key1=Value1.K</b> Groups are composed from any combination of the  • Key names are case sensitive • The following comparison operators are supported	following Keys: Barcode, RowNumber, Column, FieldIndex  =, >, <, >=, <= s are separated with 'Y (colon). In that case an OR is implied.			
MERGE_CSV		output from CellProfiler. After merging all intermediate output files are deleted automatica -check this option so you have more control over what should be merged at th			
Build					

Build Pipeline: CellProfiler Cluster Run  Dynamic overview of CellProfiler image processing on the Linux Cluster  Data Pipeline Visualizatio				Pipeline Visualization				
	CellProfiler_JCl	•	Monitor_JCPClu	•	Merge_CPS	Simpl	<b>*</b>	CU_CleanThum
Pipeline 2014_02_12_DRAQ5_10x	2014_02_12_DRAQ5_10x CellProfiler_JClustSelect  _Feb 12, 2014 422033 PH	•	#17 Monitor_JCPClusterV2 Feb 12, 2014 4:20:56 PM 10 min	•	#11 Merge_CPS	F7 DW	<b>*</b>	JCP_2014-02-12_16-20-33 CU_CleanThumbnail_Folder  ■ Feb 12, 2014 4/32/20 PH  0 1.1 sec

### **Typical Workflow**

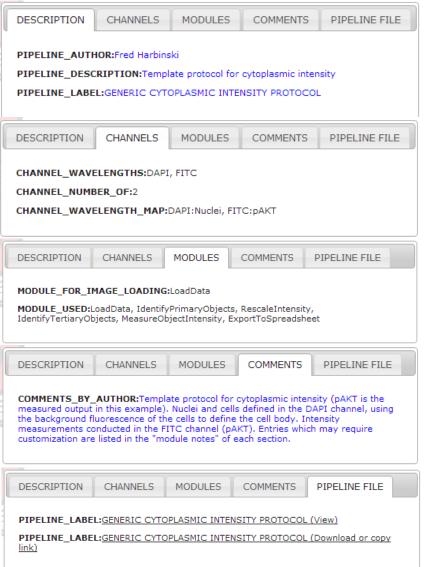
Step 1: Contribute a pipeline

- Project: Contribute\_Pipeline
  - Upload and annotate a standard CellProfiler image analysis pipeline.
     Uploaded pipelines are usable in other projects
  - Assumptions
    - The pipeline has been designed and successfully tested on the CellProfiler desktop client
  - Outcome
    - The CellProfiler pipeline file will be uploaded and stored on Jenkins
    - Additional annotation will be extracted and attached to the pipeline



### Build report from a contributed pipeline

Uses: Summary Display Plugin

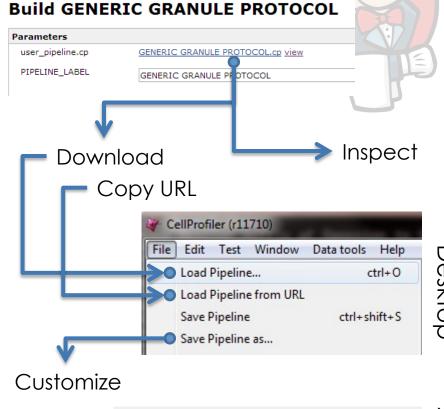


- Contributed pipelines are annotated by a combination of user provided and autoextracted metadata
  - Presented as a tab panel
  - Pipeline can be downloaded and further modified

FILE tab to download or quickly browse the pipeline

Additional Usage

- CellProfiler pipelines on the Jenkins server can be used as follows:
  - For inspection
  - For re-use
    - On CellProfiler desktop client
    - On Jenkins-CellProfiler
  - For further experimentation
    - Load in desktop client and further customize



2) Select a processing pipeline: PTPFI TNF CellProfiler Pipeline GENERIC GRANULE PROTOCO CellProfiler Pipeline GENERIC CELL INTENSITY PROTOCO CellProfiler\_Pipeline YAP Test CellProfiler\_Pipeline pAKT Cell Panel CellProfiler Pipeline HUH-1 pS6 CellProfiler Pipeline HUH-1 P62 Endogenous CellProfiler\_Pipeline KDM4\_ImageStats **OUERY KEY** oups are composed from any combination of the following Keys: Barcode, RowNum

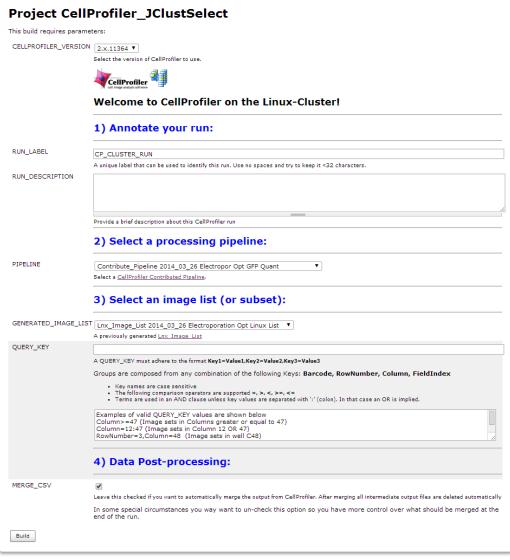
Jenkins-C

### **Typical Workflow**

Step 3: Execute CellProfiler on the Linux Cluster



- Project:
  - CellProfiler\_JClustSelect
  - Executes a series of image processing steps using the Jenkins-CI CellProfiler
  - Uses the <u>SSH Plugin</u>
  - Typical Assumptions
    - CellProfiler pipeline and a CP formatted image list are stored on the Jenkins server
      - Jenkins build artifacts
  - Outcome
    - Summary <u>report</u>
    - A file containing combined measurements from all the images processed.
      - Results file is in CSV format



#### Monitoring CellProfiler runs on the cluster

Uses: Build Pipeline Plugin

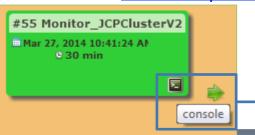
Users switch
to the
graphical
review of the
workflow!

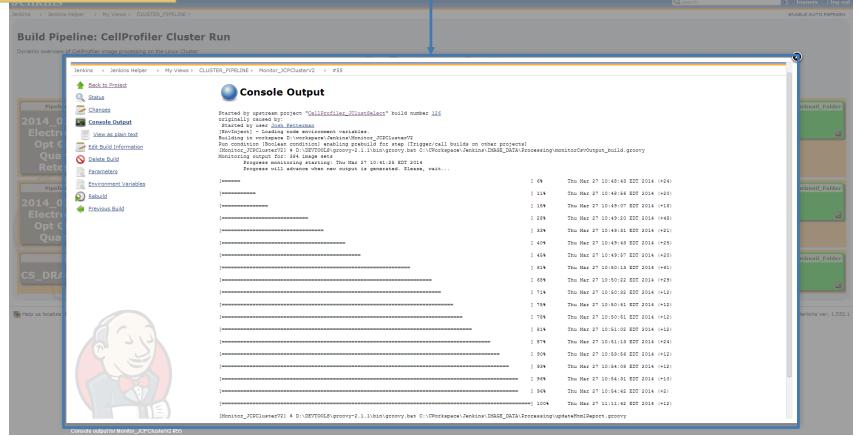




Monitoring CellProfiler runs on the cluster

Uses: <u>Build Pipeline Plugin</u> and the Console





Run Report & Measurement Retrieval

Uses: <u>Associated Files</u> and <u>HTML Publisher</u> plugins



If all goes well final results are found in the merged measurements folder





CellProfiler col lange adapts actions				
CS_DRAQ5_384_10x_AB00085165_1				
CellProfiler-on Clusto	er Report: 2014-03-24_14-15-53 (build 124)			
Build Parameters	Review			
CellProfiler Pipeline	Review			
Total Source Images	384			
Mapped Image List Parameters	Review			
Measurements Folder	/labdata/incell/cluster_runs/CPJENKINS\JCP_2014-03-24_14-15-53			
Merged Data Folder	\\nibr.novartis.net\usca-dfs\LABDATA\LABS\\incell\cluster_runs\JOUTPUT\CELLPROFILER\2014-03-24_14-15-53\ALI			
Progress Monitor	Progress Monitor			

Jenkins -CI: CellProfiler Image Processing

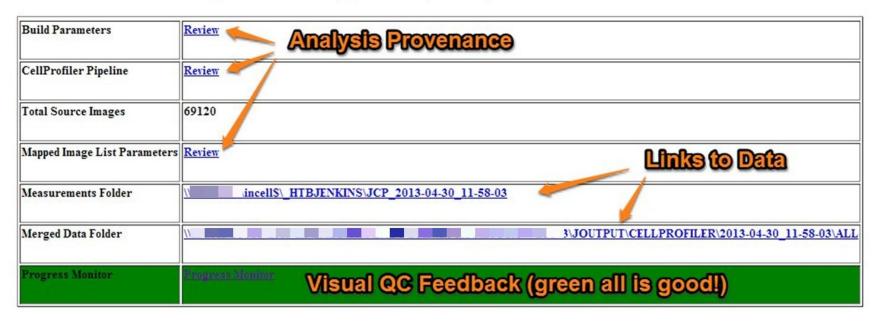
Uses: <u>HTML Publisher</u> plugin

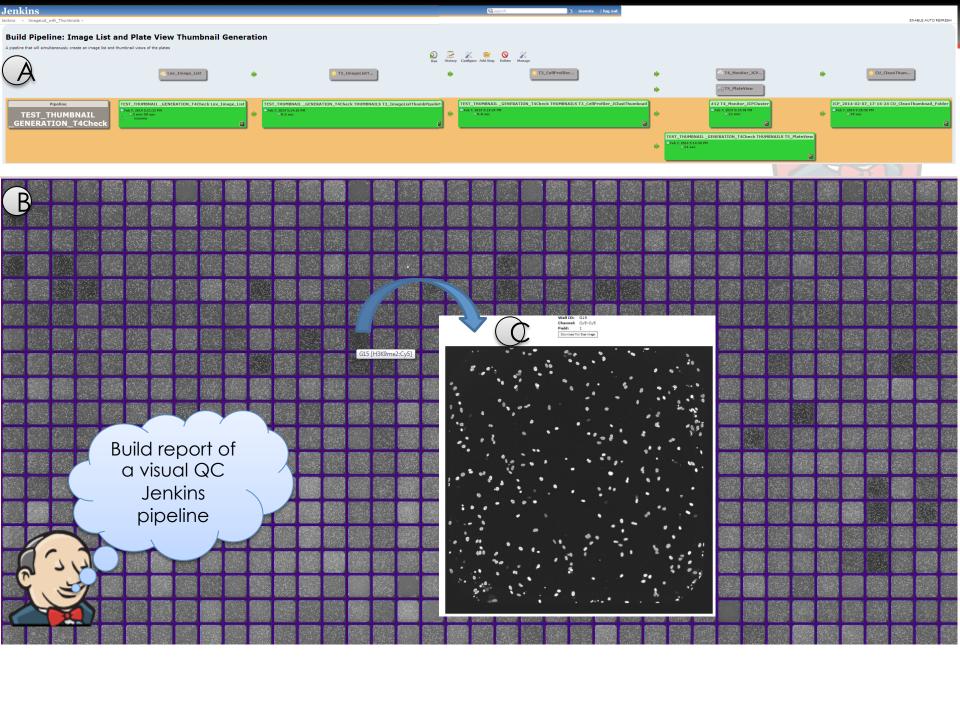
CellProfiler ordinage adulysis software

20130430

2 IC50

CellProfiler-on Cluster Report: 2013-04-30\_11-58-03 (build 26)





#### **Advanced/Experimental Functionality**

Exploring the parameter space (a.k.a. Test Mosaic)

Count\_Junko\_Default -> 54

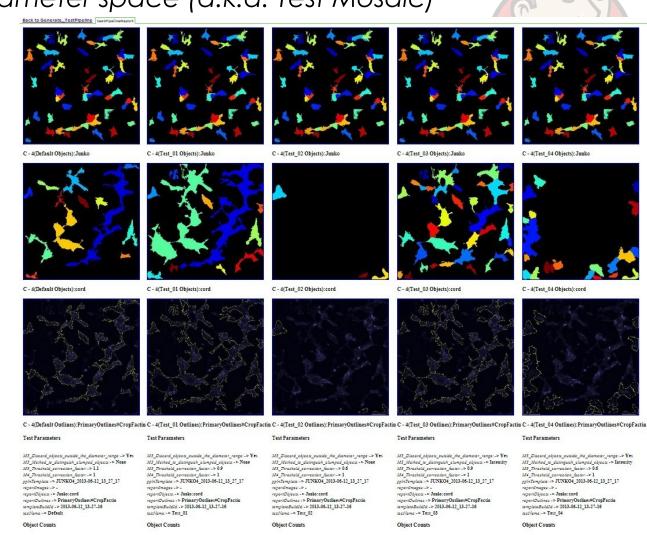
Count cord Default -> 13

Count\_cord\_Test\_01:-> 11

Count Junko Test 01:-> 54

25/3

- Optimization of imaging module parameters
  - A typical pipeline development requirement
- Test Mosaic
  - Allows systematic and documented exploration of the parameter space
  - Evaluation is based on visual and quantitative interpretation of the results



Count\_cord\_Test\_02:-> 3

Count Junko Test 02:-> 54

Count\_cord\_Test\_03:-> 38

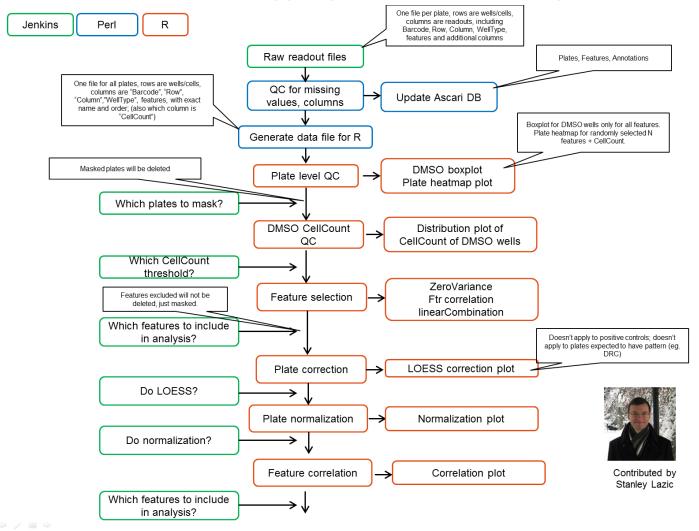
Count Junko\_Test\_03:-> 54

Count\_cord\_Test\_04:-> 20

Count Junko Test 04:-> 54

**HCS-Multi-Parametric Data Analysis** 

Current Focus: Prototype powerful and easy to use analytics



## Statistics, Visualization, Reporting

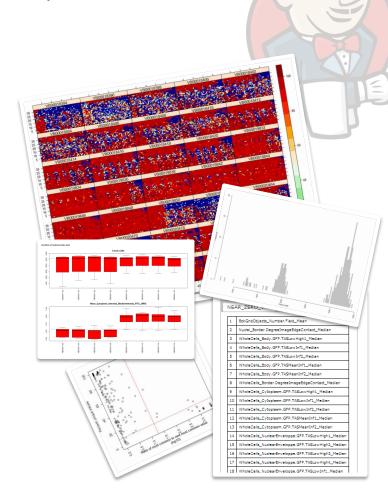
My current Jenkins toolkit

- Jenkins R-Plugin
  - Supplies build step for executing R scripts
    - This plug-in was created by the <u>BioUno</u> project (sponsored by <u>TupiLabs</u>), and released to Jenkins as well.
- Image Gallery Plugin
  - This plug-in reads a job workspace and collects images to produce an image gallery
  - Useful for visualizing various statistical plots and graphs
    - This plug-in was created by the <u>BioUno</u> project (sponsored by <u>TupiLabs</u>), and released to Jenkins as well.
- Reporting Plugins
  - HTML Publisher, Summary Display

Jenkins for Interactive Analytics

Using R in a Jenkins pipeline interactively

- Opportunities
  - Quickly prototype functional analysis for multi-parametric data
    - Improve analysis requirements
    - Experiment with required data management and analysis workflows
  - Provide lab scientists with an easy to use, yet sophisticated, standardized and validated platform for MP data analysis tools



## Jenkins for Interactive Analytics

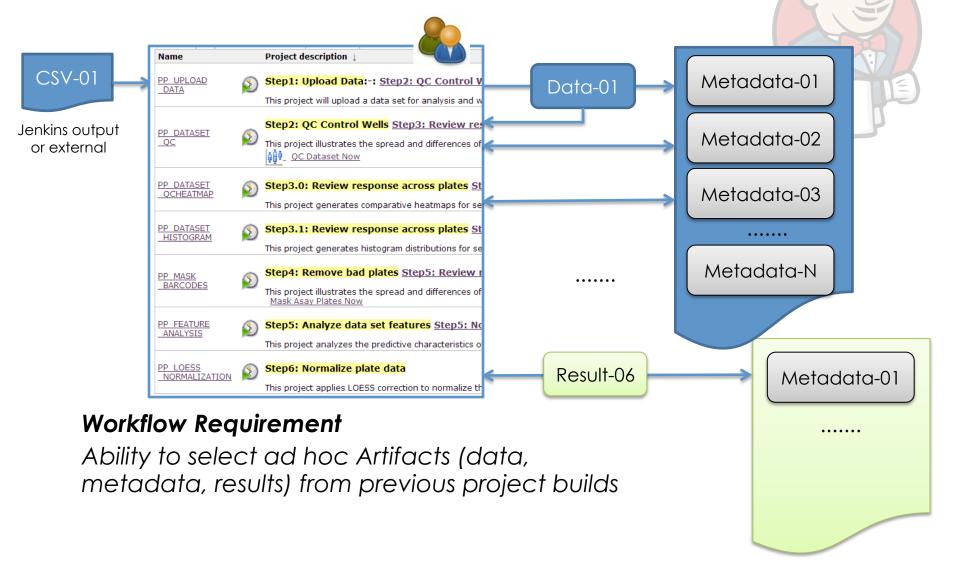
Using R in a Jenkins pipeline interactively

- Challenges
  - Limitations of the Jenkins user interface
    - Limited interaction between UI controls
  - Large and varied HC measurement metadata
    - A challenge for creating HC data schemata as well
- Strategies
  - Open source collaboration with BioUno project
    - Uno-choice UI control greatly facilitates dynamic updating of the UI
  - Initial design supports flexible (but still controlled) data schema
    - Low tech, cumulative, shared key-value Java properties



#### **Analytical Builds**

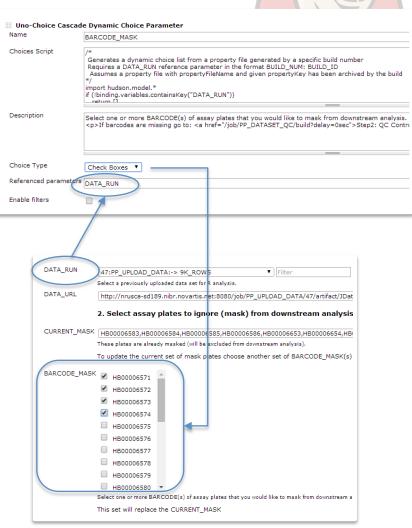
A build may create a new transform of the data or simply add metadata



### The Uno-Choice plugin

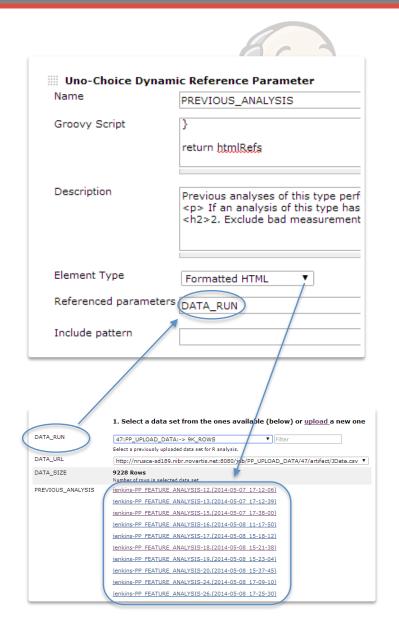
- Provides a list of dynamically generated options
  - Driven by a Groovy script
  - Single/Multi-select (Check Boxes, Radio Buttons)
  - References one or more other UI parameters
  - Dynamically refreshes when referenced UI parameters change

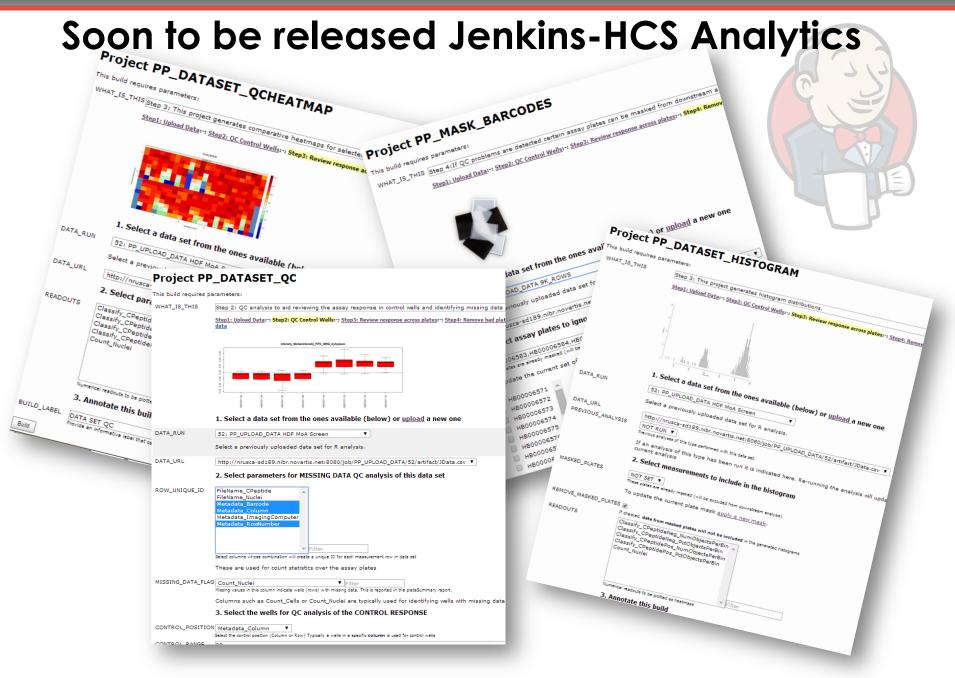




## The Uno-Choice plugin

- Provides reference parameters
  - Dynamically rendered in the UI but not used in the build
  - Rendered as lists, 'free-form'
     HTML, or an image gallery





#### Introducing Jenkins to Life Sciences!

Let's start by explaining away 'artifacts'!



ar-ti-fact ◁) [ahr-tuh-fakt] ? Show IPA

- 1) any object made by human beings, especially with a view to subsequent use
- a handmade object, as a tool, or the remains of one, as a shard or pottery, characteristic of an earlier time or cultural stage, especially such an object found at an archaeological excavation.
- any mass-produced, usually inexpensive object reflecting contemporary society or popular <u>culture</u>: artifacts of the pop rock generation.
- a substance or structure not naturally present in the matter being observed but formed by artificial means, as during preparation of a microscope slide.
  - a spurious observation or result arising from preparatory or investigative procedures.

http://dictionary.reference.com/browse/artifact

Developer

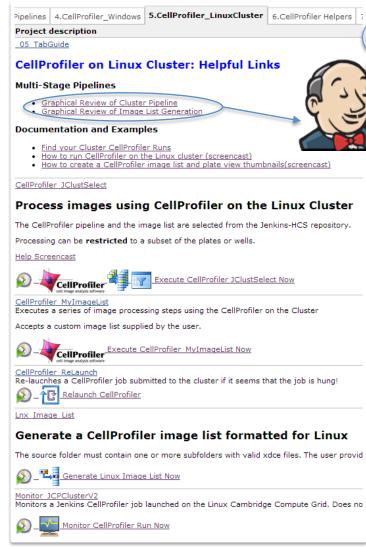
Impedance Mismatch!

Scientist

Introducing Jenkins to Life Sciences

Let's improve the User Interface/Experience

- Let's start by improving the default Jenkins UI
  - Layout
  - Navigation
  - Refreshing
  - Interactivity
- This is an active
   Jenkins
   community
   discussion

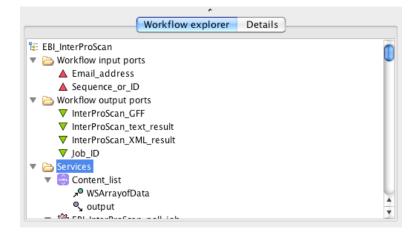


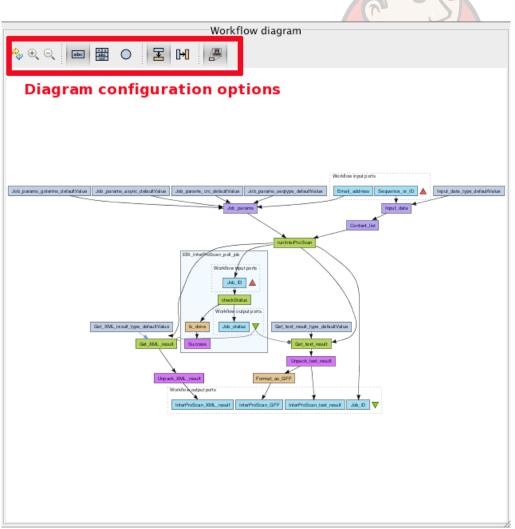
Hyperlinks to Build Pipeline Views of 'Jenkins Helper' user

#### What We are Missing

Configuration Explorer

- Structured
- Graphical
- Dynamic





## What We are Missing Bi-Directional Build Interaction



- Limited support by Run Type parameter
  - Missing flexible and dynamic filtering
- Build D modifies build/ publisher artifacts of Build C
  - Sometimes not do-able
  - Sometimes requires a reload



Build C produces an intermediate report that will get updated once Build D is finished successfully.

output of long

Build C

running job and updates report of

▼ cell image analysis software					
014_05_21_PGC1A_Set1Reimg					
CellProfiler-on	Cluster Report: 2014-05-23_13-31-11 (build 27)				
Build Parameters	Review				
CellProfiler Pipeline	Review				
Total Source Images	4608				
Image Source	D:DEVTOOLS\Jenkins\workspace\CellProfiler_MyImageList				
Measurements Folder	/Jabdata/incell/cluster_runs/CPJENKINS/JCP_2014-05-23_13-31-11				
Merged Data Folder	Unibr.novartis.nefusca-dfs\LABDATA\LABS\incell\cluster_runs\JOUTPUT\CELLPROFILER\2014-05-23_13-31-11\ALL				
Progress Monitor	Progress Monitor				
	Build D mor	nitors			

'Progress Monitor' Link and cell color are updated

Progress Monitor

#### What We are Missing

A good, deep search and metadata framework

- Supported
  - View Searches
  - Build Browsing
    - By timeline
    - By view
    - By user

- Missing
  - Build Searching
    - Parameter Search
    - Metadata Search
      - Metadata plugin (currently limited to adding metadata at project level)
    - Artifact Search
  - Tagging
  - Dynamic Metadata

#### What We are Missing

Life-Sciences Domain Plugins (Bio/Chem Informatic)

S	
S.	MrBayes Plug-in
	FigTree Plug-in
sis	
IS.	Structure Plug-in
ar	Structure Harvester Plug-in
ıs	CLUMPP Plug-in
	Distruct Plug-in
	Structure Harvester Plug-in  CLUMPP Plug-in  Distruct

- The BioUno project is filling the gap
- Interested in plugins that
  - Integrate bio-informatic, statistical and visualization tools
  - Connect to life-science data repositories
  - Generate artifacts and reports in LifeSci formats

	UI		
<u>Uno-</u> <u>Choice</u> <u>Plug-in</u>	A proposal for a new Jenkins UI plugin for selecting one or multiple parameters. Attempting to fill the gaps left by current plugin options.		
<u>lmage</u> Gallery Plug-in	This plug-in reads a job workspace and collects images to produce an image gallery using colorbox lightbox Javascript library.		
Misc			
R Plug-in	A simple plug-in to invoke R interpreter and execute an R script.		

## In Summary

- We have demonstrated that Jenkins-CI can be used for life-science applications
  - Using standard functionality
  - Using domain specific plugins
  - In demanding environments of big data and high performance
- We have observed that scientist are able and willing to use the platform despite it's 'domain impedance mismatch'
- There is some fundamental interest in the larger Jenkins-CI community to expand the boundaries of the framework beyond continuous integration

#### Where do we want to take Jenkins-CI?

- Discussion
  - No changes?
  - Gradual improvements?
    - User interface
    - API
    - New life-science plugins
  - Fundamental changes?
  - Integration framework for orchestrating more granular pipelines?
    - CellProfiler
    - Galaxy
    - Knime
    - Others?

## **Acknowledgments**

- Novartis
  - Fred Harbinski
  - Christian Parker
  - Stanley Lazic
  - Imtiaz Hossain
  - Josh Snyder
  - Erik Sassaman

- BioUno
  - Bruno Kinoshita
- The Jenkins Community

### Thank You To Our Sponsors





