myGrid Tools for Scientists

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Overview

- Taverna
- BioCatalogue
- myExperiment

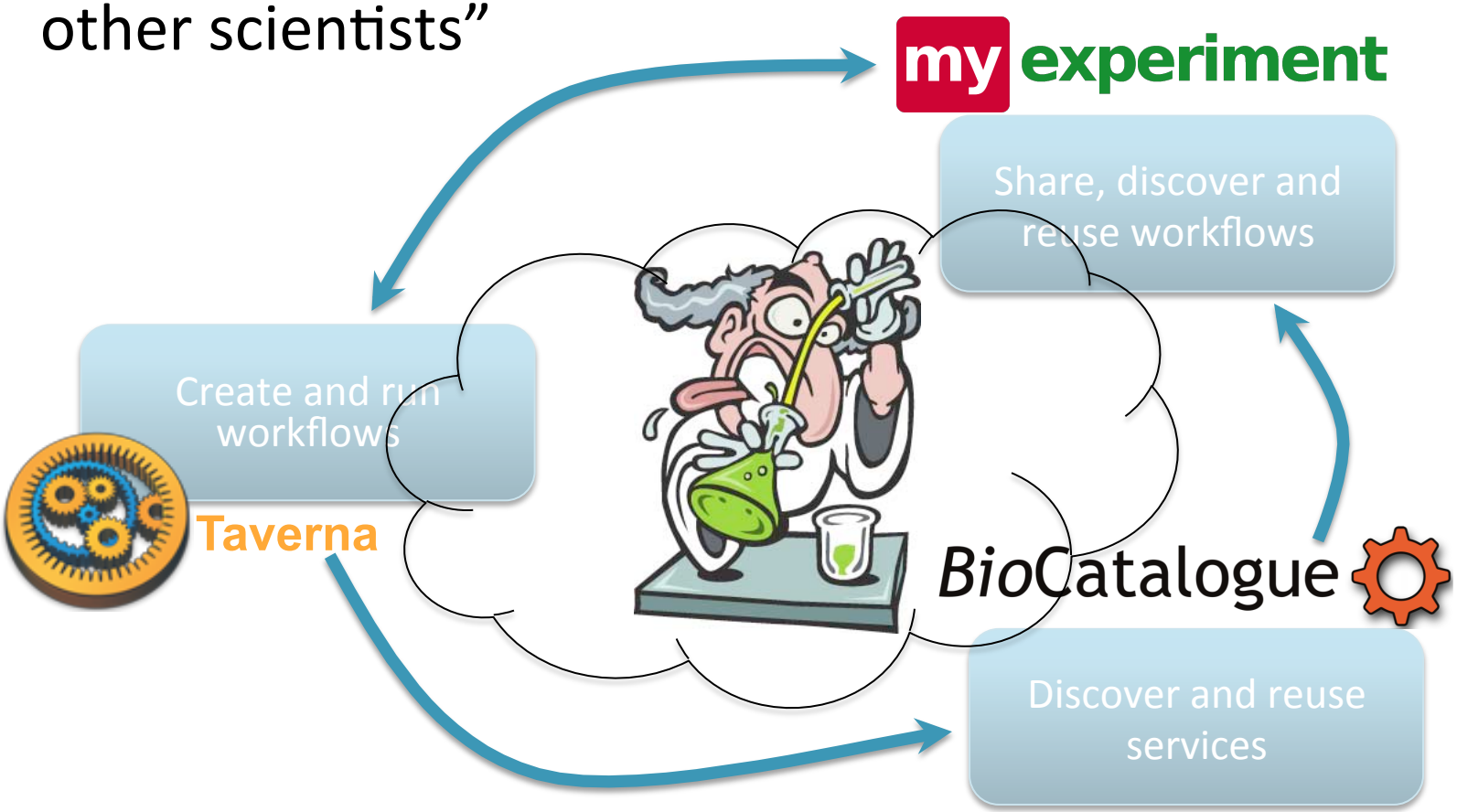
What is myGrid?

- "… a product of the e-Science initiative in the early 2000s to seize on the advantages of [grid] computing and translate them into the biological sciences."
- Mixed team of developers, domain scientists and researchers
- Building technical infrastructure and tools supporting the ***in silico* experiments**
- Various domains: bioinformatics, biodiversity, systems biology, social science, astronomy, chemistry, …
- Open source tools

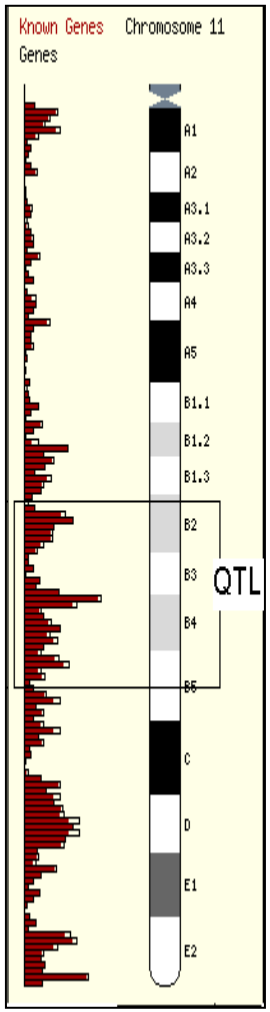
Software | Services | Content | Skills | Community

(Some of) myGrid Tools

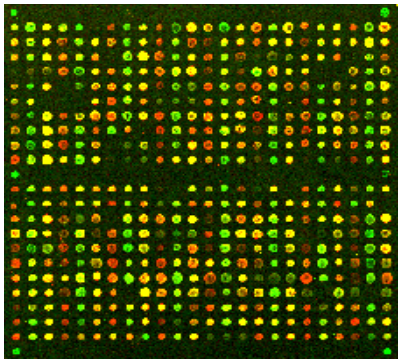
- " Help scientists get on with science and get on with other scientists"



A Problem: Huge Amounts of Data



QTL regions
100+ Genes



Microarray

1000+ Genes

Next Generation Sequencing

10,000+ Genes

How do I look at ALL the genes systematically?

How do I identify candidate genes?

(Some) Issues with Current Approaches

- Scale of analysis task overwhelms researchers – **large amounts of data**
  - Cannot use full data sets
  - Cannot rerun experiments due to data size
- Constant change in data - need for reruns of experiments (re-analysis) to check for new and updated information
- Scientists often have to manually click though various Web sites and pass their data
- Incompatible data formats
- Error proliferation from any of the listed issues – notably human error

Solution ⇨ Automate

One Solution - Workflows

- General technique for explicit **describing** and **executing** a process/scientific experiment
- Describes **what** you want to do on a high level
- Automation of scientific process enables:
  - Avoiding manual steps
  - Easier rerun
  - Parameter tweaking
  - Easier comparison of results
  - Science reproducibility

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SCAPE

BioVeL

myGrid

Creation and execution of workflows

Taverna

Taverna

- http://www.taverna.org.uk
- Workflow management system for creating and executing workflows
- A bit of history:
  - First released in 2004
  - Currently 2nd generation of software
    - Version 2.5 released in May 2014
  - 3rd generation in alpha
- Freely available, open source (LGPL license)
  - Windows, Mac OS and Linux
- Extensible
  - Via various plugins

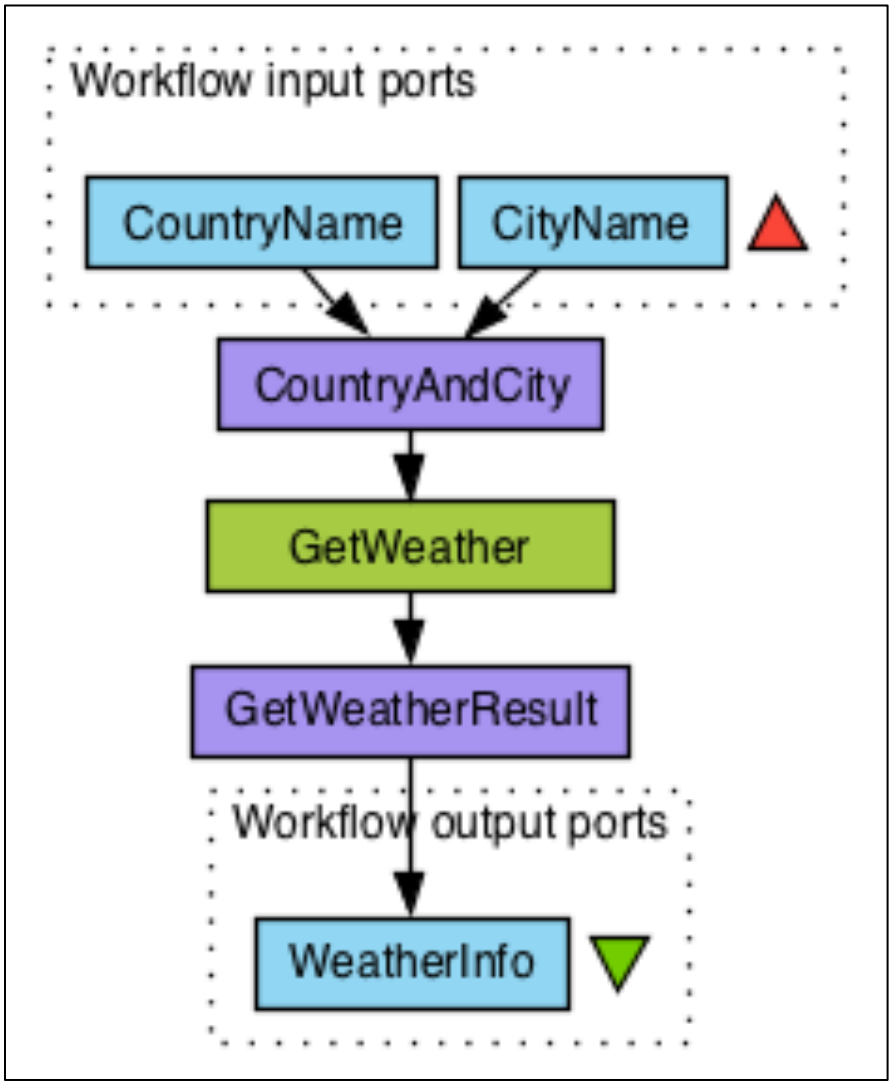
Taverna Workflows

- Sophisticated automated analysis pipelines for **data-driven** research or processes:
  - Define **how** you want your data to flow
  - Describe **what** you want to do with data, including the **services** to use
- Facilitate **data flow** links between the services:
  - Output data of service A is the input of service B
- Service **types**: data resources, analysis tools, knowledge resources
- Service **location**:
  - **Remote** services: Web services or scripts on remote machines
  - **Local** services: scripts and libraries on users' machines

Taverna Workflows – cont'd

- Advanced flow control:
  - **List handling/iteration strategy** for data inputs
  - **Loops** (until a condition is met)
    - Asynchronous services
  - **Control links** to determine execution order
- Help overcome problems with service **interoperability** and **integration**
  - Shim services

Example Taverna Workflow

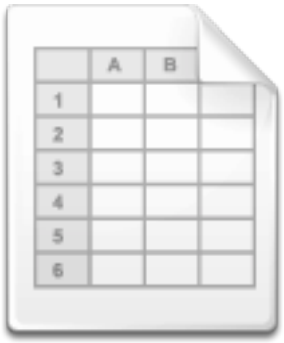


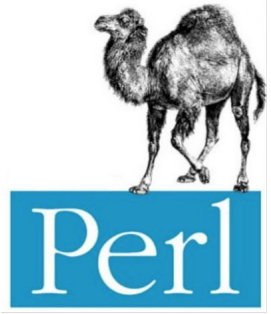
- Get the weather forecast of the day given the city and the country
- Green box is a Web service
- Purple boxes are local XML services to assemble/ extract XML (**shims**)
- Blue boxes are workflow input and output ports
- Arrows define the direction of data flow

Supported Services

- SOAP/WSDL Web services
- REST Web services
- R statistical services
- Local or remote (via ssh) scripts:
  - Python, Perl, Java, …
- Spreadsheet data import
- XPath and text manipulation services
- WebDav data management services
- BioMart
- and more!

- Third party extensions





Who Provides the Services?

- Open domain services and resources
- Third party
- myGrid does not own them
- myGrid did not build them
- myGrid does not enforce any common data model
- You can include your own services and resources too!

Data and Provenance Collection

- Collection of workflow run **provenance** – **who**, **when**, **where**
- Workflows can generate vast amount of data – Taverna can help manage and track:
  - **Data**, **metadata**, and workflow **provenance**
- **Data lineage** - data life cycle - origin and how it moves over time
- Allows checking back over past results, comparing workflow runs and sharing workflow runs with colleagues
  - Facilitates collaboration and reproducibility in science
- Inspecting **intermediate results** when designing and debugging workflows
  - Test with small dataset before running over a million of datasets

Success Story: Sleeping Sickness Case Study

- Successful use of Taverna to assist with gene analysis relating to sleeping sickness (trypanosomiasis) in African cattle
  - Joint study: Universities of Manchester, Liverpool, and International Livestock Research Institute (Nairobi)
  - Some cattle breeds more disease-resistant than others
  - Genetical diff. between resistant and susceptible cattle?
  - Can we breed cattle resistant to infection?
- Two key genes have been identified
- Breeding trials have started with one of the genes to see if new lines of resistant cattle can be raised

Sleeping Sickness Case Study – cont'd

- BBC news:
  - http://www.bbc.co.uk/news/10403254
- EPSRC Pioneer Magazine 2014:
  - http://www.epsrc.ac.uk/newsevents/pubs/pioneer-edition-12-issued-june-2014/
- Watch a video on YouTube:
  - http://www.youtube.com/watch?v=hmIErdZwFS0

Taverna Summary

- Data Analysis Pipelines
- Machinery for coordinating the execution of services and linking together resources
- Repetitive and mundane boring stuff made easier
- Demo at the end

Discover and reuse services

BioCatalogue

- http://www.biocatalogue.org
- A public centralised and curated registry of Life Science Web services that can be used in workflows
- Allow anyone to register, discover and curate Web services
- Community oriented with expert guidance
- Open content
- Open source (BSD license)

Motivation

- Guesstimate: thousands publicly available on-line services in Life Sciences
- **Where**
  - can I find them? advertise them?
- **What**
  - do they do? can I use them for?
  - is the cost? the licenses?
- **How**
  - do they work? up to date are they?
- **Who**
  - provides them? uses them?
  - recommends them?

Google is good, but …

- Unified way of describing services
  - How to invoke a service
  - Input and output data examples
  - Documentation
  - Who else is using this service
  - How reliable a service is
  - Monitoring history
  - Service variants, deployments

What Can BioCatalogue Users do?

	Non-registered user	Registered user	Curator
Search	✔	✔	✔
Register a service	✖	✔	✔
Receive notifications	✖	✔	✔
Add annotations	✖	✔	✔
Manage all services	✖	✖	✔

Benefits for Service Providers

- Free!
- Easy to REGISTER services
- Great exposure
  - The right demographic
  - Instantly searchable/discoverable
- Notifications
  - When your service goes down
  - When someone 'likes' your service
  - When someone annotates your service
- Community-aided ANNOTATION

Benefits for Community Members

- EXPLORE Web services
  - Full text search
  - Browse+xFiltering
- Comprehensive service descriptions
  - Annotated and verified by the community

Benefits for Community Members – cont'd

- Web service MONITORING
  - Services change and get outdated
  - Long term reliability
  - Testing on a daily basis

Monitoring status: **FAILED**

The last check failed

Note : Test is failing since Saturday December 08 , 2012

Last checked: about 14 hours ago

Monitoring status: **PASSED**

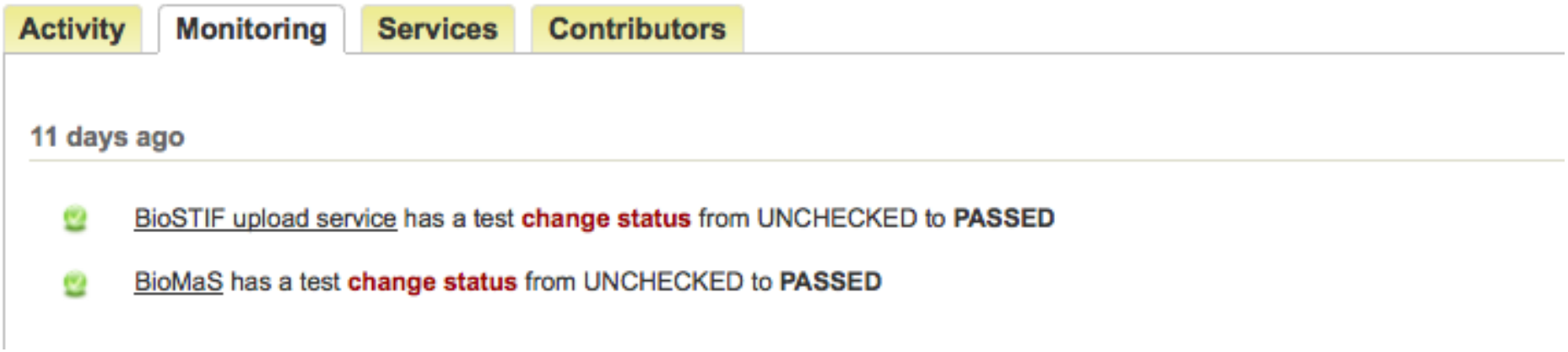
The last check for this test was successful

Last checked: about 14 hours ago

Various Information Feeds

- Latest services
- Latest activity/annotations
- Latest monitoring changes
- Top contributors

Subscribe to updates with an RSS reader



BioCatalogue Summary

Discover *"Web services are hard to find"*

Register *"My Web services are not visible"*

Annotate *"Web services are poorly described"*

Monitor *"Web services can be volatile"*


BioCatalogue

Demo


Share, discover and reuse workflows

myExperiment

- http://www.myexperiment.org
- Social networking site for scientists
  - "Facebook for Scientists"
  - Virtual Research Environment
- A pool of scientific workflows
- Enables scientists to **share**, **reuse** and **repurpose** workflows
- Helps to **reduce time-to-experiment**, **share expertise** and **avoid reinvention**
- Helps to build communities and form relationships

myExperiment Resources

- Workflows
  - Taverna
  - KNIME
  - Galaxy
  - Kepler
  - …
- Groups
  - myExperiment provides a central location for workflows from one community/group

myExperiment Resources – cont'd

- General files
  - Presentations
  - Data files
  - Auxiliary files
  - …
- Packs
  - Sets of resources in myExperiment
  - Like a **Research Object** or a full scientific experiment
    - Workflows, input data, results, logs, provenance, metadata, publications, presentations, etc.

Workflow Sharing, Ownership and Attribution or Resources

- Fine control over privacy
- myExperiment allows you to say
  - Who can look at your workflow
  - Who can download your workflow
  - Who can modify your workflow
  - Who can run your workflow
- Workflow ownership and attribution
  - Users do not need to start from scratch – reuse or modify existing workflows
  - Attribute/credit original author

myExperiment Summary

Discover	*"Find workflows suitable for your science, see what other are doing."*
Share	*"Share your and other people's expertise"*
Reuse	*"Reduce reinvention, form relationships with people working on same or similar things"*
Repurpose	*"Reduce time-to-experiment, attribute original author"*


myExperiment

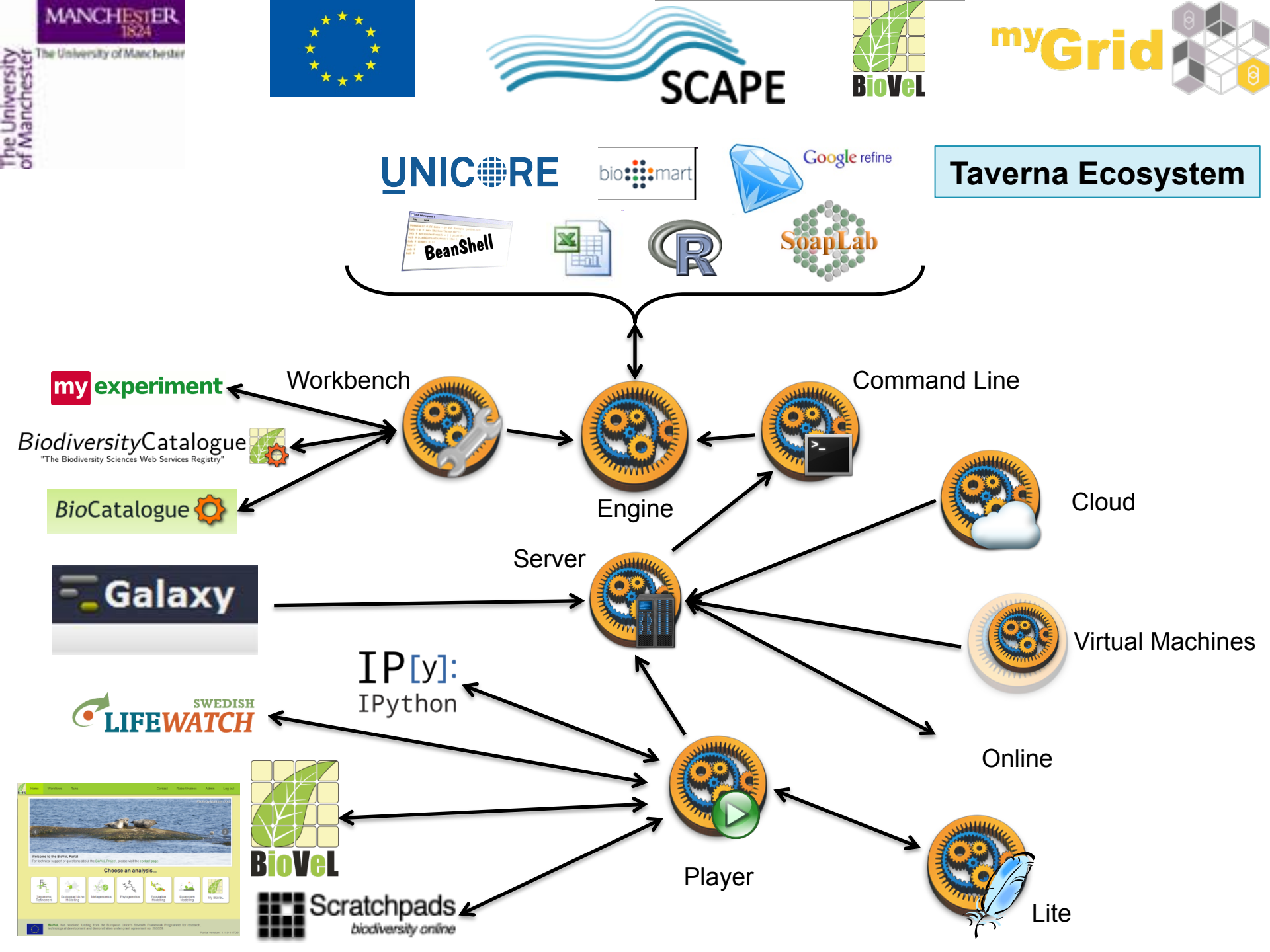
Demo

The Rest of the Day …

- Taverna introduction demo
- Taverna introduction – tutorial
- Taverna advanced features – tutorial
- Take a deep breath – there is more to myGrid!

Take a Breath - There is More

- Taverna Command Line Tool, Server, Player, On-line
- Taverna integrations with:
  - IPython
  - Galaxy
- SysMO SEEK
  - Data, models and SOPs (Standard Operating Procedures) repository
- BioVeL
  - Portal for sharing and executing Taverna workflows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Google refine
Taverna Ecosystem
BeanShell
SoapLab
my experiment
Workbench
Command Line
BiodiversityCatalogue
"The Biodiversity Sciences Web Services Registry"
BioCatalogue
Engine
Cloud
Server
Galaxy
Virtual Machines
IP[y]:
IPython
SWEDISH
LIFEWATCH
Online
BioVeL
Player
Scratchpads
biodiversity online
Lite

More information

- myGrid
  - http://www.mygrid.org.uk
- Taverna
  - http://www.taverna.org.uk
- BioCatalogue
  - http://www.biocatalogue.org
- myExperiment
  - http://www.myexperiment.org

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