





http://taverna.org.uk/

Stian Soiland-Reyes & Robert Haines myGrid, School of Computer Science University of Manchester, UK

# TAVERNA WORKFLOW MANAGEMENT SYSTEM



ITER IM workshop Château de Cadarache, 2011-06-08

# What is myGrid?

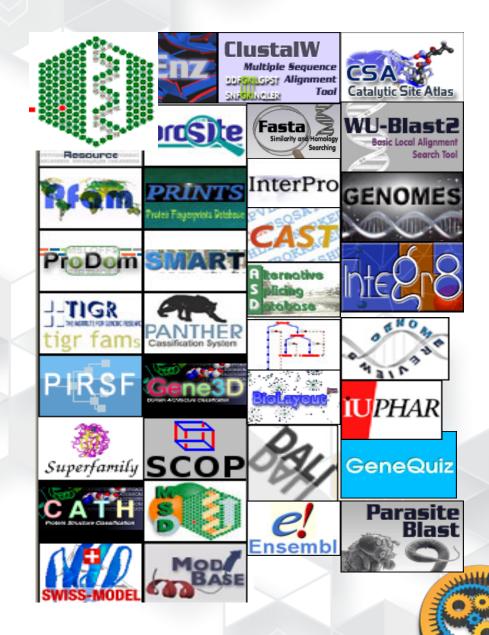
- An e-Science Collaboration Since 2001
- Not a grid!
- Numerous partners involved:
  - University of Manchester
  - University of Southampton
  - University of Oxford
  - EMBL-EBI
- Provides sustainable and production quality software
  - Supported by OMII-UK, EPSRC and BBSRC
- Mixture of developers, bioinformaticians and researchers

Software | Services | Content | Skills | Community



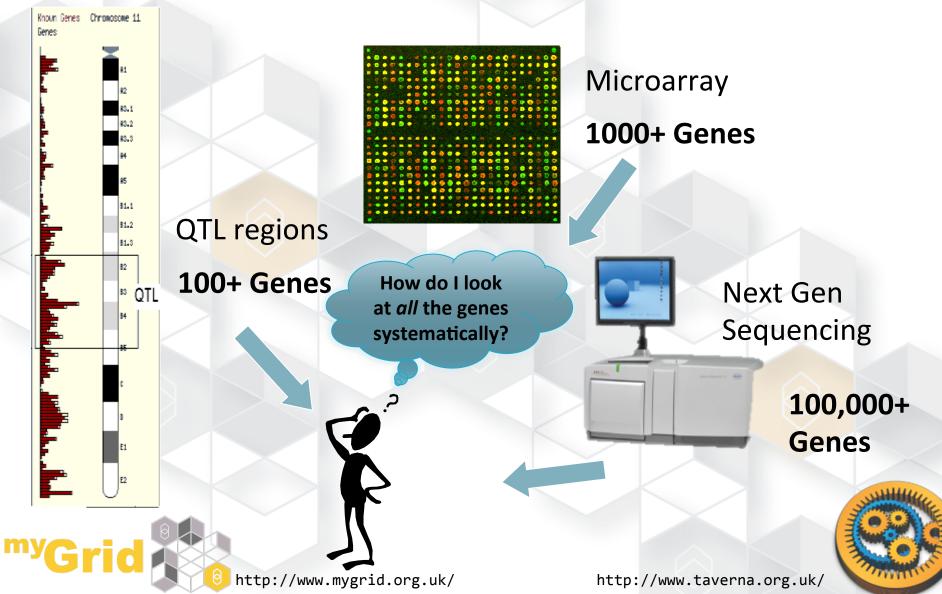
# Motivation: **Bioinformatics**

- Challenge:
  - Large amounts of data
  - Many open questions
  - Numerous freely available public datasets and analysis tools





# Huge amounts of data



# Manual approach

- Search using public web sites and databases
  - Pubmed
  - Uniprot
  - EBI BioMart
- Copy and paste to web tools for analysis
  - NCBI Blast
  - EBI InterPro
- Further processing locally
  - R
  - Perl
  - Python





# Manual: disadvantages

- Scale of analysis task overwhelms researchers
   lots of data
- User bias and premature filtering of datasets cherry picking
- Hypothesis-Driven approach to data analysis
- Constant changes in data problems with reanalysis of data
- Implicit methodologies (hyper-linking through web pages)
- Error proliferation from any of the listed issues
   notably human error



#### Web services and workflows

#### Web services

- Technology and standards for exposing code and data resources that can be programmatically consumed by a remote third party
- Description on how to interact with the service, parameters, documentation

#### Workflows

- General technique for describing and executing a process
- Describe what you want to do running which services





#### **The Taverna Open Source Suite of Tools**

Web Portals

#### Workflow Repository



#### Service Catalogue

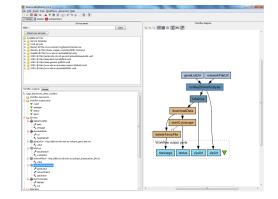


### Activity and Service Plug-in Manager





#### **GUI** Workbench



Workflow Engine



Provenance Store Workflow Server



Secure Service Access





Client User Interfaces

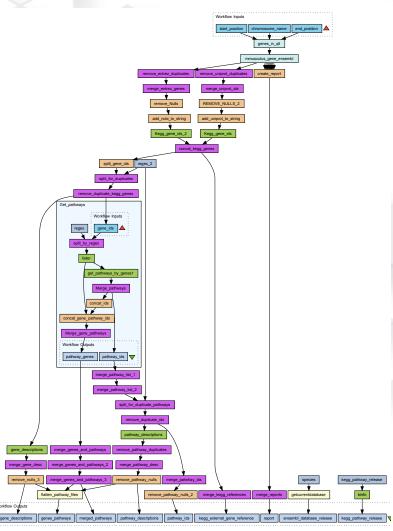






Programming and APIs

### Taverna workflows



- A set of (local and remote) services to analyze or manage data
- Nested workflows are also services
- Data-links connects services
  - i.e. output from service A is input to service B and C
  - Describes the desired dataflow instead of process coordination
- Automatic iterations
- Can customize list handling and control links



### What types of services and data?

- WSDL/SOAP web services
  - Secured invocation with HTTPS/SSL/WS-Security
- RESTful web services
  - Secured invocation with HTTPS/Basic Auth
- Spreadsheet import
- Command line tools (local, SSH)
- Inline scripts (Beanshell, R)
- Excel/CSV spreadsheets
- Java APIs
- Customizations:
  - BioMart, BioMoby / SADI
  - Soaplab
  - Grid services (EGEE gLite, caGrid, PBS, UNICORE)
  - ... your tool (Plugin tutorial in wiki)





### Service limitations

- Web service creation involves wrapping existing tools or writing WS code
- Web services can go down

  - Service monitoring
- Transferring data up/down to WS slow
  - Support references in WS interface
- Executing command line tools directly requires execution access
  - Trickier to share workflows, require either SSH/grid credentials or installing tools locally

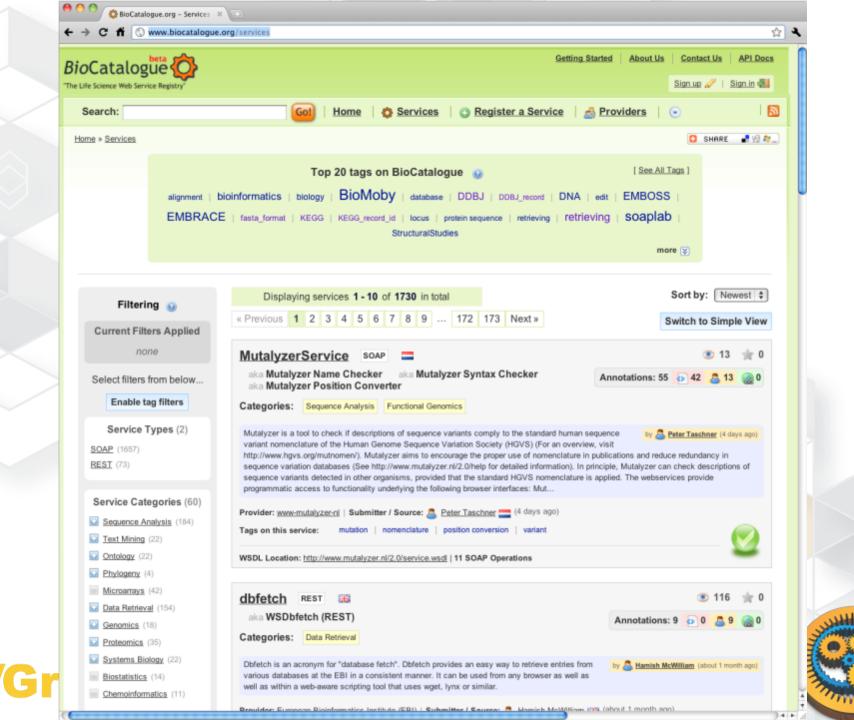


#### Which services?

- Taverna is general, can connect to standard web services and command line tools for any domain
- in bioinformatics..
  - From professional third-party organisations providing robust & open data/analysis services
  - ..to under-the-desk web services for one particular purpose, ran by PhD students
  - http://biocatalogue.org/ 2000+ services from 140+ providers – crowd sourced and quality monitored

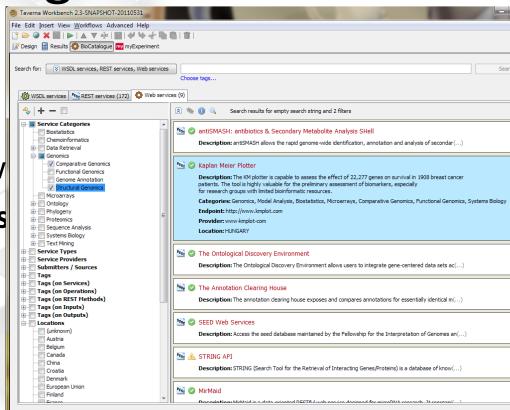






# BioCatalogue integration

- Search services from workbench
- Add services to workflow
- View service descriptions and uptime status from within workflow



# BioCatalogue



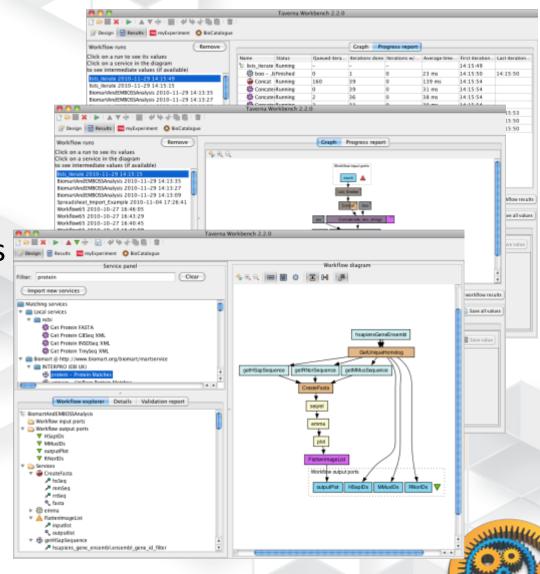
"The Life Science Web Services Registry"



http://www.taverna.org.uk/

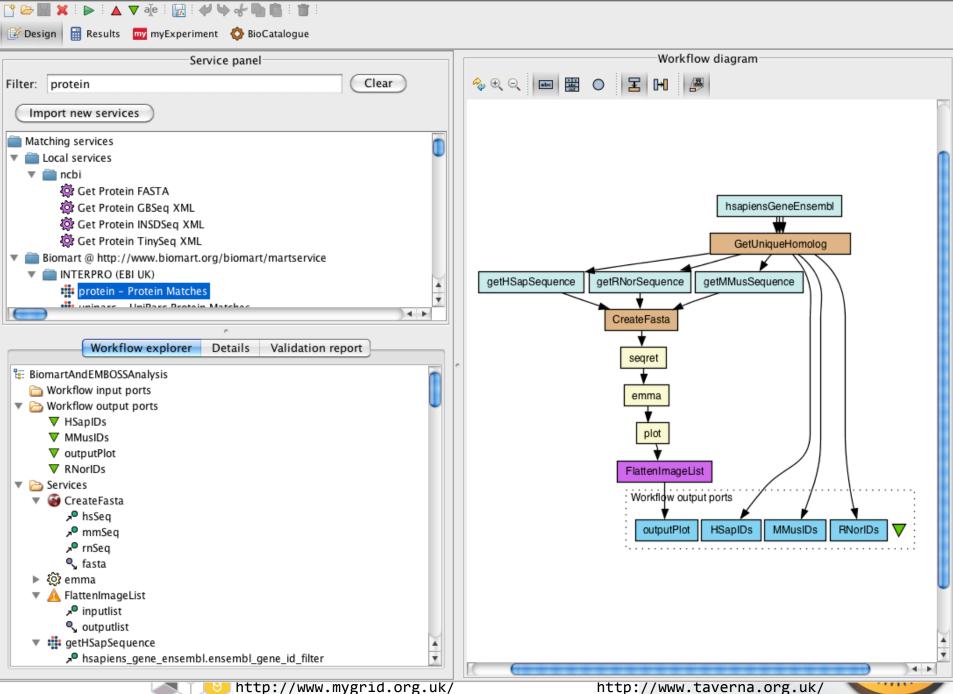
# Taverna workbench

- Graphical desktop tool
- No server installation required
- Drag-and-drop services into diagram
- Connect services, run, reconnect, rerun
- Integrates diverse set of tools





http://www.taverna.org.uk/



### Sharing workflows

- myExperiment.org allows users to share, find, download and rate workflows
- "Facebook for the scientist"
- 4000+ members, 1400+ workflows
- Open source code, can set up own instance

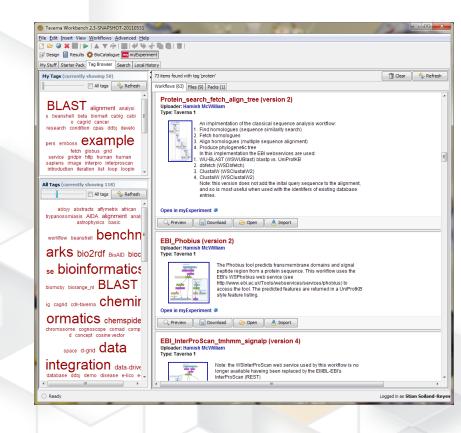




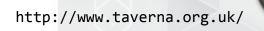


# myExperiment integration

- Search and browse workflows
  - By tags
  - Free text search
  - Own/group workflows
  - Packs, e.g. "Examples"
- Upload/share workflows







#### Taverna workflow features

- Nested workflows
  - Reuse existing components
- Implicit iterations
  - With customizable list handling
- Pipelining
  - Process partial iteration results early
- Parallelisation
  - Run as soon as data is available
- Retries, failover, looping
  - For stability and conditional testing
- Plugin-extensible execution control
  - Ideas: caching, error detection, dynamic service lookup





# Extensible UI and engine

- Plugins can provide new "perspectives"
  - e.g.: BioCatalogue, myExperiment
- Provide service-specific customization
  - e.g.: BioMart interface replicates web site
- Adding new functionality
  - New service types, eg: ...
  - Execution control like looping/branching
  - Design helpers, "Find matching service"





### Workflow limitations

- Initially designed for dataflows
  - Not suitable for business processes like "HR procedure for hiring new staff"
    - Long-running workflows require Taverna Server
  - .. But suitable for coordinating command line and grid executions, the data might just be job references
  - Execution control extensible, eg:
    - Looping, Branching
    - Dynamic service lookup
    - Data manipulation, Error detection





# Data and provenance handling

- Data references passed between services in workflow
  - http, file, sftp, gridftp, etc (extensible)
- Data downloaded/uploaded or references translated when needed
- Provenance captured for workflow runs
  - Trace execution steps, view intermediate values while running
  - Export as Open Provenance Model (OPM) / RDF
  - Proof and origin of produced outputs
  - Extensible annotations
- Wf4Ever: reproducible research objects
  - Workflow/data as a scientific publication → preservation
  - Need to capture more service data and metadata





#### Data limitations

- Running Workbench limited by:
  - Local disk space for storing data
  - Network speeds for up/download
  - Firewall access
  - Execute wf using Taverna Server or command line remotely with ssh/job submission
- No standardized WS reference mechanism
  - Agree on mechanism within WS 'family' with shared disk (eg. deconstruct local path from HTTP URI)



### Parameter sweeps

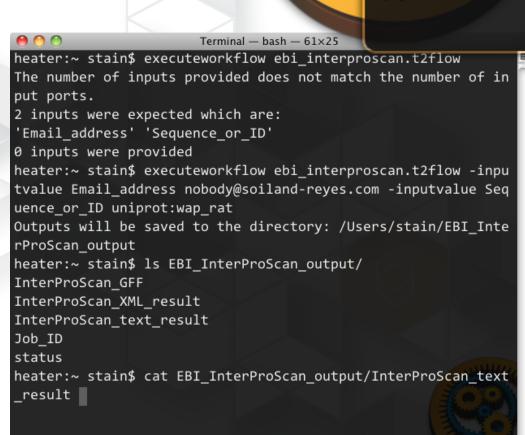
- Implicit iterations with pipelining provides an intuitive way to set up parameter sweeps
- Advanced looping and extensible execution control allows iterative & recursive reductions/approximations





#### Taverna command line

- Executes from a Windows/Linux/OSX shells
- Takes a predefined workflow with files as inputs and outputs
- Quick way to "productionize" a workflow





http://www.mygrid.org.uk/

http://www.taverna.org.uk/

#### Taverna Server

- REST/SOAP interface to execute workflows
- Client libraries for Ruby and Java
- Two demonstration web interfaces
  - Ruby
  - Java Portlets
- Upcoming:
  - Security delegation
  - AWS image



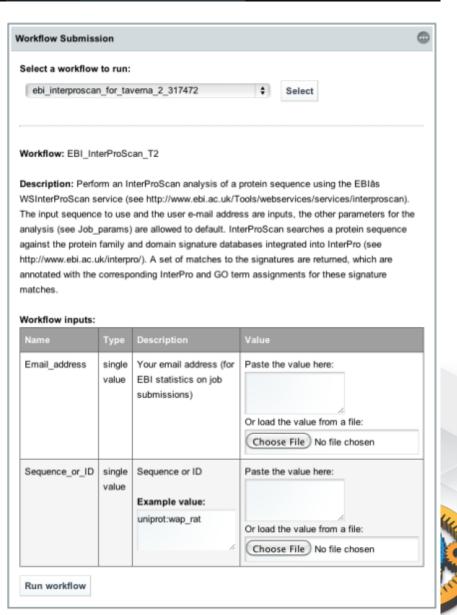


http://www.taverna.org.uk/

# Taverna portlet

- Example portlet interface
- Executes workflows using Taverna Server



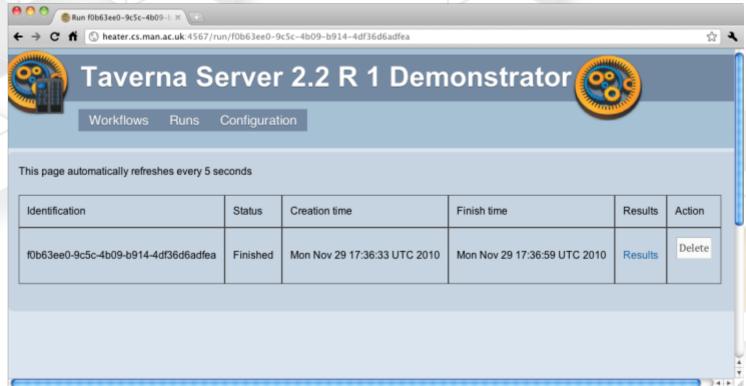




Workflow Results			
	results of a workflow submission h job statuses, click on the "Refr	•	s id, once its status becomes "Finished".
Workflow	submission jobs:		Refresh
Job Id	ob Id		ne Start date Status Delete job
02eac9e	)2eac9ec-e590-4628-8830-6367ea5c5794		al_workflow_877727 Mon, 29 Nov 2010 17:30:45 GMT Operating
d0280ad	0-1119-4d08-aa76-45fc829308a7	ehi interprosca	an for taverna 2 317472 Mon. 29 Nov 2010 17:27:56 GMT Finished 面
2162e9 7aa833	Job Id: d0280ad0-1119-4d08-aa7 Workflow: ebi_interproscan_for Results:		
ce4f5fl	Output port	Data	Data preview
22b056	Job_ID - single value text/plain	Value	sp P01174 WAP_RATFPrintScan 4DISULPHCORE 76 85 1.0E-6 InterProScan ; IPR015874 4-disulphide core
33365a	InterProScan_text_result -	Value	sp P01174 WAP_RATFPrintScan 4DISULPHCORE 101 108 1.0E-6
	single value text/plain		InterProScan; IPR015874 4-disulphide core sp P01174 WAP_RATFPrintScan 4DISULPHCORE 118 126 1.0E-6 InterProScan; IPR015874 4-disulphide core
	InterProScan_XML_result - single value text/xml	☐ Value	sp P01174 WAP_RATProfileScan WAP 27 73 0.0 InterProScan ; IPR00 Whey acidic protein, 4-disulphide core sp P01174 WAP_RATProfileScan WAP 76 127 0.0 InterProScan ; IPR00 Whey acidic protein, 4-disulphide core
ny	status - single value text/plain	Value	sp P01174 WAP_RATHMMPfam WAP 79 126 5.2999999999999999999999999999999999999
	Table promise		sp P01174 WAP_RATsuperfamily WAP 77 129 1.699999222840496E-8

# Ruby web interface

- Example customized web interface
- Uses Ruby gemt2-server





#### Grids and clusters

- Taverna have been integrated with several leading grid and middleware infrastructures, such as:
  - PBS
  - caGrid/Globus
  - EGEE/gLite
  - NorduGrid's ARC
  - JSDL/GridSAM
- Plans for SAGA integration





### Taverna on the cloud

#### Use-case:

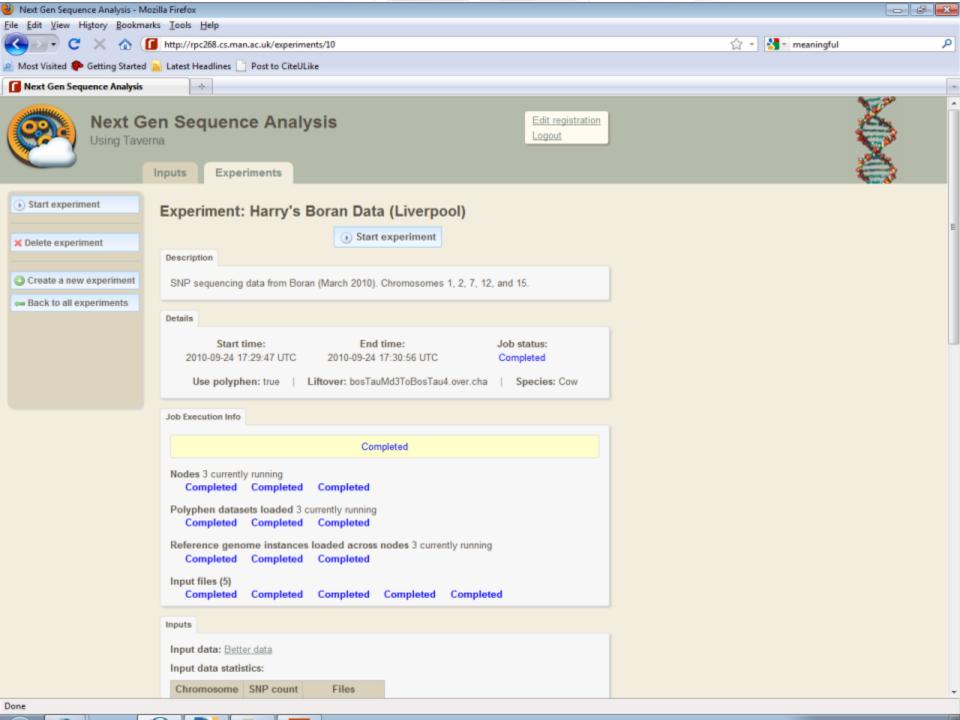
 SNP analysis and annotation of genome sequenced from breeds of cows in Africa – why are some of them resistent to X?



- Amazon EC2 with Taverna Server and local services
- Ruby on Rails web interface
- Runs through 31 chromosomes in 2 hours using 10 instances - \$10







# Taverna 3 roadmap

- OSGi plugin system
- Workflow language: Scufl2
  - Compound format; embedding metadata, dependencies, independent API for creating/ inspecting workflows
- Components
  - Finding/sharing command line tool descriptions
  - Richer way of finding compatible services





### Open source, open development

- Taverna suite of tools are all open source, free to use and customize
- Large user community, active mailing lists
- Lead developers: myGrid in Manchester UK
- Contributors from across the world
- PAL programme
- myGrid provides training, tutorials and documentation





### Who uses Taverna?

- Bioinformatics: EMBL-EBI, ONDEX
- Astronomy: HELIO, AstroGrid, SAMPO
- Engineering: NASA Jet Propulsion Lab (JPL)
- Chemistry: CDK, CIC
- Biodiversity: BioVel
- Preservation: Wf4Ever, SCAPE
- BioMedicine/Cancer research: caGrid
- Data/text mining: eLico, AID



### Taverna in numbers

#### Taverna:

- 361 organisations
- 48 countries
- 70,000+ downloads
  - ~4000 source

#### • myExperiment:

- 4000+ registered users
- 56 countries
- 1400+ workflows

#### BioCatalogue:

- 2000+ services
- 150+ service providers
- 500+ members
- 27 countries





# Acknowledgements









NIBHI







netherlands bioinformatics centre









**EMBL-EBI** 





open middleware infrastructure institute uk

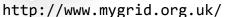














#### More information

http://www.mygrid.org.uk/

http://www.taverna.org.uk/

http://www.myexperiment.org/

http://www.biocatalogue.org/



