The Taverna Developers Workshop Introduction

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http://www.taverna.org.uk
http://www.mygrid.org.uk
Day 1 – Thursday
10:00 - 11:00 Welcome and Introduction (Carole Goble)
11:00 - 12:00 The Apache Incubator (Stian Soiland-Reyes)
12:00 - 13:00 Lunch (provided)
13:00 - 14:00 Taverna 3 Demo/Update/Future (Stian Soiland-Reyes / Donal Fellows)
   • Command Line 3, Server 3, Workbench 3
14:00 - 15:00 Lightning talks by attendees (About 5 minutes each, please volunteer during the morning session)
   – Kevin Benson: Heliophysics and Astronomy with Helio/VAMDC
   – Susheel Varma: Medical simulation with VPH-Share and Taverna
   – Vadim Surpin (remotely): Taverna Online
   – Yassene Mohammed: PeptidePicker - A scientific workflow with web interface for selecting appropriate peptides for targeted proteomics experiments
   – Gabor Terstyanszky/Tamás Kiss: Workflow interoperability with Taverna in SHIWA
   – Pinar Alper: Using Taverna APIs, Workflow Provenance and Annotations
15:00 - 15:15 Coffee break
15:15 - 16:30 Round table (Chair: Aleksandra Nenadic)
18:30 Dinner (provided) – Kro Bar
Day 2 - Thursday

9:00 - 10:00 Taverna 3 code/API introduction (Stian Soiland-Reyes)
   – Taverna Platform, SCUFL2, Workflow Run bundles, Changes for plugin developers

10:00 - 12:00 Tutorials:
   – Working with the Taverna 3 code base
   – Creating a Taverna 3 plugin
   – Taverna Server REST API (Donal Fellows)

12:00 - 13:00 Lunch (provided)

13:00 - 14:00 Tutorials (continued) / Lightning talks (continued):
   – Stuart Owen: SEEK and Workflow Player - running Taverna workflows from a data portal
   – Ernesto Coto: Developing the VPH-Share Taverna plugin

14:00 - 15:00 Tutorials:
   – Converting an existing Taverna 2 plugin
   – Programmatically constructing and executing a workflow

15:00 - 15:15 Coffee break

15:15 - 16:00 Summary / Discussion (chair: Stian Soiland-Reyes)
   – What Taverna plugin/integration/feature do you wish existed?
   – Potential new collaborations
   – What should be the initial goals for the Taverna Apache Incubator?
Outline Ramble

• A few remarks on the past
• Encouraging examples of use
• Selected developments wrt Taverna
• Remarks on associated products
  – myExperiment, *Catalogue, SEEK, Research Objects
• Open development: the way forward
e-Science, Data-driven Science, Computational Science, Scientific Computing

- Support global scientific collaboration, enable large scale resource, tools and results sharing, assist scientific processing, avoid unnecessary repeated work.

- Accelerate scientific discovery, improving scientific productivity, stimulate technological innovation.

- Cope with scales and speed of scientific innovation and data.

- Reproducible methods & results
Back in the day...2001

Protocol

Create a gene list in Excel
Go to NCBI
Retrieve FASTA for each gene
Drag/DB Blast each sequence
Copy/paste IDs into a spreadsheet
Run Repeat Masker on each sequence
copy/paste masked sequence into Excel
Run MacVector cut each seq with EcoRI
Long Tail Little science
Self-organising groups
Disconnected, independent, distributed scientists
Disconnected, independent, distributed resources
Open in the wild.

Organised groups
Clubs of scientists
Organised, planned and in-house resources
Closed and well behaved services.

Organised science
Taverna Workflow Management
http://www.taverna.org.uk

• Dataflow
  – Computational Lambda Calculus with a monad extension*
  – Simple control flows, iterations over collections
  – Data type agnostic, domain independent
  – Data movement, monitoring, staging, reference
  – Custom (VO Tables), XML, JSON

• Mixed steps
  – Services, codes & command line tools
  – SOAP + REST Web Services
  – Scripts: R, “In Workflow Programming” Beanshell scripting ...
  – Codes: Java, libraries, HPC, Grid and Cloud platforms etc ...
  – Nested workflows
  – Interactions and Batch

*Turi et al  Taverna Workflows: Syntax and Semantics  e-Science 2007: 441-448;
Deployment view

Cataloguing and discovery view

Design view

Execution view
Lifecycle view

Research

Review, Revise/Discard
Personal

Explore Ideas

myexperiment

Scale

Harden

Compare

Deploy into tools

Reporting

IP[y]: Nb

SEEK

Scratchpad

Nature

BioVeL
In the workflow landscape

- LONI Pipeline
- KNIME
- PILOT
- Galaxy
- RAPID MINER
- Kepler
- Taverna
- R
- Python
- MATLAB
- CYLC
- Nipype
- pegasus
- P-GRADE

Specialist

Generalist

Application

Infrastructure
- Data cleaning
- Data movement
- Data retrieval and annotation
- Data analysis
- Data mining and knowledge management
- Data curation and data warehouse population
- Data visualisation
- Parameter sweeps over simulations
Workflow-based Computation

Trypanosomiasis resistance in African Cattle

Noyes, PNAS 2011 108(22) 9304-9309

BioDiversity Invasive Species Modelling

American Horseshow Crabs in the Baltic

Weeks -> Hours
Surprise predicted result tested in lab. DAXX Gene
Genetic differences between breeds

Dev. Years -> Weeks
Runs. Weeks -> Hours
Generalised ENM data mapping and overlaying pipelines.

Software as a Service / (Cloud) Appliance

Analytic bottleneck

Repetitive, unbiased, accurate record, taming data, transparency, avoiding shortcuts.

Interactive steps

Reproducible reporting
Lymphoma Prediction Workflow

MicroArray from tumor tissue

caArray

Microarray preProcessing

GenePattern

Lymphoma prediction

Ack. Juli Klemm, Xiaopeng Bian, Rashmi Srinivasa (NCI)
Jared Nedzel (MIT)
A systematic approach to a transcriptome analysis to asthma sputum inflammatory phenotypes,
transcription regulation network involving E2F6, IRF7 and STAT1,
modulation of oviductal transcriptome by X and Y-bearing spermatozoa

Maleki-Dizaji S, Holcombe M, Rolfe MD, Fisher P, Green J, Poole RK, Graham AI,
A Systematic Approach to Understanding Escherichia coli Responses to Oxygen:
From Microarray Raw Data to Pathways and Published Abstracts, Online J
Heliophysics
Integrated Observatory

Advanced instrument
discovery

HEC/HFC correlation

Event correlation between HEC tables
VPH-Share @neurist Aneurysm Morphology

Patients ➔ Patient Avatar

Disease Simulation Workflow

Systemic Factors

Gene Expression Profile

Patient Avatar updated

RISK

Patient Pseudoidentifier (PID)
- Demographics
  - Height
  - Weight
- Vital Signs
  - Heart Rate
  - Blood Pressure
  - Flow Rate
  - Transient Pressure
- Aneurysm Properties
  - Tissue Properties
  - Wall Thickness
  - Risk Factors
  - Medical Images
  - Medications

Updated Risk

Susheel Varma

http://www.vph-share.eu/
Preservation Planning & Watch

Long term preservation of digital data. Maintaining scans of newspapers, books, records of data; Metadata maintenance; large and automated. Preservation Policy: Collection level Control Policy: Low level actions & constraints

Merge a Preservation Action Plan...

... with an Access Workflow

Execution Workflow

Components

[Diagram showing workflow components and processes]

Use

Publish
Ecological Niche Modeling

**Step 1: Explorative modeling**
- Use unfiltered data
- Use fixed parameters: Mahalonobis distance
- Native projections
- Test the model, distribution of points, number of points

**Step 2: Deep modeling**
- Filtering environmentally unique points with BioClim algorithm
- ENM with Support Vector Machine and Maximum Entropy
- Parameter optimization (if necessary) on the model test results
- 2 masks (model generate, model project)

The workflows work over large geographical, taxonomic, and environmental scales, incl. terrestrial ecosystems

Baltic species invasions of various crabs/sea creatures

Interactions of different forest insects and trees
Interface Spectrum

Workflow design, compute  Concept Knowledge  Domain science

Technical PAL  Science PAL  Domain Scientist

Taverna Workbench  Component Builder  IP[y]:Nb  BioVeL  Scratchpads

Taverna Workbench  Component Builder  IP[y]:Nb  BioVeL  Scratchpads

High  Workflow Visibility  Low
Welcome to the BioVel Portal
For technical support or questions about the BioVel Project, please visit the contact page.

Choose an analysis...

Taxonomic Refinement
Ecological Niche Modelling
Metagenomics
Phylogenetics
Population Modelling
Ecosystem Modelling

BioVel has received funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement no. 283369.

Portal version: 1.1.0-11709
Data and Parameter Sweeps
Taverna Server

- Multiple clients, Multi-user
- SOAP and REST API
- Amazon Machine Image
  - Bundled R & Atom feed servers
  - Multiple instances in Cloud and as required, for multiple users/uses and different security scenarios
- Taverna Command Line
- Bundled Servers
- Taverna Virtual Machine
Taverna Player

- Embed workflows into any Web page
  - LifeWatch, Scratchpads, personal Web specialist web sites
  - Like embedding a YouTube video
- Ruby-on-rails plug-in for running workflows
  - Integrates into any Rails app
  - BioVeL Portal, myExperiment, SEEK

Scalability

- Job queuing system to scale runs with the number of workflows the servers can handle
- Each run in parallel with its own worker
- Prioritizes sweeps fairly (prefers interactive users)
- Reports saturation

Web Service interface (REST)

- Tight integration into other pipelines
- Run workflows from workflows
- Scratchpads

Manages:

- Input provenance, Runs, Results management, Service credential management:

Taverna Server

- Multiple clients, Multi-user
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- Taverna Command Line
- Bundled Servers
- Taverna Virtual Machine
iPython integration

http://goo.gl/hm0qCN

https://www.youtube.com/watch?v=QVQwSOX5S08

IP[y]: IPython Interactive Computing
Portable Taverna Application:  
“BioVeL in a box”

- Complete BioVeL infrastructure
  - Portal, Taverna Server + plugins
  - R + libraries, Open Refine
- Amazon Machine Image
  - Just start it up
- EGI Virtual Appliance
  - Just start it up, or
  - Download and run locally
- Automated build scripts for local install
- Application packaging
- Currently testing local install procedure with the Flanders Marine Institute (VLIZ)
Many workflows need user interaction. A workflow on a server does not need to be “press a button and wait.”

- VPH-Share opens a VNC connection to the spawned instance.

**Taverna Interaction Service**

- Users interact with a workflow (wherever it is running) in a web browser.
- Interaction Service Plug-in in workbench
Customised Taverna Workbench

- Focussed service set
- BioVeL Components
Taverna Workbench

• Customised domain-specific workbenches
  – Biodiversity Workbench: Defaults to BiodiversityCatalogue
  – myExperiment starter pack for biodiversity (query GBIF)
  – Some service types hidden (BioMoby, BioMart, …)

• Interaction Service plugin
  – Support simple interactions: Ask and Select
  – Support complex interactions: Preview Advance, Complex manipulation

• Special Services support
  – WebDAV support: Read and write data using WebDAV protocol
  – OAuth for authentication and authorization
  – JSON and JSON path support
  – WADL prototype released
  – WPS prototype in development with iMarine

• Components and component families
  – Component builder plugin
  – Adaptation of myExperiment to components
Challenging Complexity

Components: Well described, behaved, curated, annotated modularised workflow modules or snippets

- Semantic annotations, prescribed failover, formats, provenance
- Organised into common families
Ecological niche modeling workflow
Taverna Online: 3\textsuperscript{rd} party app

An online, in-browser application for assembling and running Taverna Workflows over a HPC platform  
http://onlinehpc.com/site/main

Dr Vadim Surpin and Vitaly Sharanutsa, Institute for Information Transmission Problems of Russian Academy of Sciences (IITP RAS)
Taverna Workflow Management
Open extensibility

- Plug-in framework
  - Command line tool
  - Data Services: VOTables for AstroTaverna
  - Optimisations: E.g. Holl. model parameter sweeps
  - Infrastructures: Grid, HPC, Web Services
  - Domains: CDK, BioMart, VOTable
  - Commodities: Excel Spreadsheets, Open Refine, R
- Plug into other frameworks & platforms
  - Portals: Scratchpads
  - Interactive platforms: iPython Notebook
  - Wfms: KNIME Node, Galaxy tool, Kepler Actor
- Third party applications
  - Taverna Online
  - XworX
  - OGC chainer
Workflow Management System Directions

**Embed**
- Workflows in common applications
- Integration into reporting & publishing
  - Underpin integrative platforms.
  - Service based science and science as a service

**Reporting**
- Workflow commodities, Research Objects
- Design practices for reuse. Credit
- Executable interactive notebooks. Provenance
  - A tool for reproducibility

**Process**
- Seamless, pluggable workflow as a service.
- Scale. Adaptability.
  - Easier development, user experience

**Access**
- Cloud and Scale
- Standards data formats, programmatic interfaces.
- Adapting to change. Security.
  - Governance of components
ServiceCatalographer
General platform
Specialized and skinned for specific instances
Categories
- Service level annotations
- Hierarchical taxonomy
- Fixed (will use an ontology in future)
- Search “similar services”
  - Parents, children, siblings

Tags
- All levels: Services, endpoints
- Keywords or short phrases
- Free choice
Catalogue Curation: Maturity

- Automated scan: Catalogue API
- Manual review

<table>
<thead>
<tr>
<th>Maturity level</th>
<th>Quality</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Service invalid</td>
<td>The service is not registered, or information is inadequate for basic use and support. The RServe service, for example, is not (and cannot be) registered because it does not provide a SOAP or REST interface.</td>
</tr>
<tr>
<td>1</td>
<td>Service is registered</td>
<td>The service provides top-level links to external documentation and contact information. Users can discover the service through BiodiversityCatalogue, but would need to use these external resources to use the service. Tool automation is limited to discovery.</td>
</tr>
<tr>
<td>2</td>
<td>Service is described</td>
<td>The service describes the available operations and parameters. Users have enough syntactical information in BiodiversityCatalogue to use the service, but need the external resources to understand the meaning of parameters and the effect of operations. Tool automation can suggest operations and parameters, and, given suitable parameters, can invoke operations automatically.</td>
</tr>
<tr>
<td>3</td>
<td>Service can be invoked</td>
<td>The service provides rich annotations. All service operations are defined, documented, and annotated within BiodiversityCatalogue. A user could make use of the service without referring to external resources. Tools can provide users with information about operations and parameters, including parameter constraints.</td>
</tr>
</tbody>
</table>

Maturity level of this service (from the BioVeL wiki) and actions to improve it: 


Actions to improve the service description

Provisional maturity level: 0
To obtain level 1, this service requires the following 1 actions:
- Add documentation link
Archiving
Publishing
Component Libraries
Preserving

PACKS

Recording
Storing
Exchanging
Versioning
Sharing
Cataloguing workflows

• Supporting workflow production lifecycle
  – Develop **and** publish workflows
  – Workflow versioning

• Supporting workflows for communities
  – Not just Taverna workflows
    • Kurator (UC Davis) - Kepler workflows
    • DataOne - Kepler and VisTrails workflows

• Persistent URI or Persistent id (Pid)
  – Manchester signed a DataCite contract so can issue DOIs
Data Operations in Workflows in the Wild

Analysis of 260 publicly available workflows in Taverna, WINGS, Galaxy and Vistrails

Monitor for decay
Workflow/Service Monitors
3rd Party Monitors
Workflow analytics

Detect and Repair
QUASAR toolkit

Fix on demand.
Notify as needed.

[Zhao et al. Why workflows break e-Science 2012]
Enabling **reproducible**, transparent research.

**Research Objects**

Outputs are first class **citizens** to be managed, credited and tracked: data, software

A Framework to Bundle and Relate multi-hosted (digital) resources of a scientific experiment or investigation using standard mechanisms & uniform access protocols. *Carriers of Research Context*

http://www.researchobject.org/
Nanopub: represents structured data along with its provenance in a single publishable and citable entry.

Galaxy workflows: re-enact the analysis

Research Object: aggregates the (digital) resources contributing to findings of (computational) research (results, data and software) as citable compound digital objects

http://isa-tools.github.io/soapdenovo2/
http://sandbox wf4ever-project.org/portal/ro?ro=http://sandbox wf4ever-project.org/rodl/ROs/SOAP2denovo2-Aurelius/
Research Object Bundle

Stian Soiland-Reyes

docker

 workflow4Ever

Sample

Lab technician

Sequence

Metagenome

Workflow run

Results

Workflow server

was GeneratedBy

was StartedBy

was AssociatedWith

was GeneratedBy

was InformedBy

"2012-06-21"

was StartedAt

was AssociatedWith

Workflow-centric RO simple requirements

Target Music Classification Study does not satisfy checklist for ready-to-release.

* Experiment hypothesis is not present
* Workflow design sketch is present
* All workflow definitions are accessible
* All web services used by workflows are accessible
* Input data is not present
* Experiment conclusions are present

See quality history with RO Monitoring Tool.

This application has been developed by PSI as part of the WF4Ever project.

Icons by Glyphicons and the Noun Project.
Tracking Provenance

- Granularity
- Scales
- Blackbox
- Hybrid

Workflow definition
+ server, plugins, version
ScufI2 workflow bundle

Run Provenance
Extension of PROV-O

Data (inputs, outputs)
Parameter configs
Research Object Bundle

Annotations
Open Annotation Model

RO Manifest (JSON-LD)

File Stores
Lab Books
Repositories
The Execution Provenance Gap
Data tracking

Big
Fine grain
1 White box

One System
Special tools
Collection
A Big Graph

What do I cite?
What did I do?
N Black boxes

What am I citing?
Many Systems
My Lab Book
Analytics
Smart in situ Presentation
Why am I citing?

Summarisation, Labelling, Distillations, Selective tracking Filtering

THEORY
APPLICATION
PRACTICE
fundamental
applied

Pinar Alper, Khalid Belhajjame, Carole A. Goble, Pinar Karagoz: Enhancing and abstracting scientific workflow provenance for data publishing. EDBT/ICDT Workshops 2013: 313-318


http://provenanceweek.dlr.de
Reg/Repos Prospects

• Workflow preservation, reproducibility and curation
  – Curating methods
  – Research Objects spawned activity (NIH BD2K programme, VIVOweb, journals)

• Underpinning platform
  – SEEK4Science
    • portal already, myExp migrating
  – FAIRDOM & BBSRC investment
    • 3 million Euro for 5 years
Taverna Prospects

• Open source software
  – https://github.com/taverna/
  – License allows integration in closed-source products

• Open development
  – Developer documentation and tutorials
  – Public mailing lists, issue trackers, wiki
  – Contributors from around the world
    – Accepted in the the Apache Foundation

• Applications to UK and EU funding councils
Realisation of Time Well Spent

Increase in Awesomeness

Valley of despair

Key:  
A - Non reusable product
B - Reusable product

Technological Debt

Time
Innovate and Prototype  
(create it)

Consolidate  
(adopt it)

Sustain & evolve  
(rely on it)  
becomes Legacy

Taverna Phases

Taverna 1  (2004)
Core: OMII-UK

Taverna 2  (2008)
Core: Scavenged.

Many application projects

Taverna 3  (2014)
Open development
Friendships: Contributors: Trust
Contributor Licence Agreement (Apache style)

Family
Work with

Friends
Collaborate with

Core Team

Know
Acquaintances

Don’t know
Strangers
• myGrid
  – http://www.mygrid.org.uk
• Taverna
  – http://www.taverna.org.uk
• myExperiment
  – http://www.myexperiment.org
• BioCatalogue
  – http://www.biocatalogue.org
• SEEK and SysMO-SEEK
  – http://www.seek4science.org
  – http://seek.sysmo-db.org
• RightField
  – http://www.rightfield.org.uk
• BioVeL
  – http://www.biovel.eu
• Wf4ever
  – http://www.wf4ever-project.org
• Research Object
  – http://www.researchobject.org
• Software Sustainability Institute
  – http://www.software.ac.uk
Calling DCI Grid/Cloud Services

• Expose services/tools as WSDL/REST services
  – HELIO: Fixed host name
  – VPH-Share: Services running on dynamically started instances
  – SZTAKI Desktop Grid – BOINC/Debian Package

• Specific service/extension to Taverna
  – UNICORE plugin: Ask grid what services are available, include services in a workflow, invoke services on the grid

• Library to control job submission to grid
  – PBS plugin: beanshells in a workflow include invocations of jobs
  – KnowARC plugin: Advanced Resource Connector to submit jobs to NorduGrid
Next Steps

• Themed & customised Tavernas

• Making things better
  – Improved interaction between server & clients
  – Start up and user separations, Native table support

• Taverna 3 server and command line
  – Scufl2, OSGI framework, faster, Runs as first class objects, Values bundled.

• Support resources
  – Updates to myExperiment, BioCatalogue, Portal, Clients, Apps
  – Curation tools

• Analytics
  – Service monitoring, workflow repair, using provenance

• Taverna Foundation
  – Developer community around Taverna 3
The Take Home Message

• Workflows are great plumbing
• But not just process plumbing
  – They are memes
  – They are commodities
  – Release outside their silo
• System ecosystems: towards application factories
• Social ecosystems: towards communities and marketplaces
• Metadata infrastructure and new WFMS programming models
All user interaction via web interface

User data stored in the Cloud

Data for all tools and Web Services stored in the Cloud

Unified access to different workflow engines with our common REST API

Tools and Web Services for each workflow are installed together for easy replication
The image depicts a schematic diagram illustrating the interaction between a clinical researcher and various software tools and services. The diagram is divided into two sections: CLIENT-SIDE and SERVER-SIDE.

On the CLIENT-SIDE, the diagram includes:
- External Application
- Taverna Workbench
- Taverna On-line
- Web-based Remote Desktop
- VPH-Share plugin
- Web services
- GIMIAS CLPs

On the SERVER-SIDE, the diagram includes:
- Workflow Manager API
- Taverna Server
- Taverna CmdLine
- VPH-Share plugin
- Cloud Façade
- VPH-Share Workflow
- LOBCDER
- Atomic Service without interaction
- Atomic Service with interaction

The diagram also includes arrows indicating the flow of interaction and data between these components. The Clinical Researcher is connected to the CLIENT-SIDE, and there is an arrow indicating that Taverna Workbench opens a VNC connection to a spawned instance on the SERVER-SIDE.
Upload data to your workspace

Upload Data

Start a run from a workflow

Start Run

Download data from your workspace

Download Data
Tavoop—Taverna & Hadoop

- Compiles Taverna Workflow to collection of Hadoop jobs
- Designed for handling very large amounts of data
  - Overhead to using Hadoop, but wins if enough data
  - Data ingest (expensive step) must have already been done
- Supports Taverna Platform Execution interface
- Parallelisable service types
- [http://wiki.opf-labs.org/display/SP/PPL](http://wiki.opf-labs.org/display/SP/PPL)
Applications

- Applications components of workflows
- Compose applications into workflows
- Incorporate workflows into applications

Infrastructure

- Provision physical resources to support application workflows
- Coordinate resources through workflows
- Optimise and adapt to change

[Foster 2005]
**Data-centric Computation**
Scientific workflows over Distributed Cyber-Infrastructure.

**Data sharing Social Methods**
libraries and catalogues for all types of scientific artefacts and all types of scientists.

**Knowledge Management**
Metadata, semantics digital exchange, preservation, publishing

**Software Engineering**
Software sustainability, software and data policy, training

**Applications**
- Astronomy
- Library
- Digital Preservation
- Biodiversity
- Biology
- Systems Biology
- Chemistry
- Public Health
- Astro-Physics
- Social Science
Science

Computer Science

Scientific Informatics Computational Science

Software Engineering

THEORY

APPLICATION

PRACTICE

fundamental

applied

PRINCIPLE

“USE CASE”

PRODUCT (Open Source)
Taverna Server family

• Taverna Server
  – Multiple clients, Multi-user
  – Local and large scale infrastructures
  – Site Replication

• Taverna Server Amazon Image
  – Local R server
  – Multiple instances as required, for multiple users/uses and different security scenarios

• Taverna Virtual Machine

• Taverna Command Line

• Bundled Servers, Services and Tools
Taverna Server for BioVeL

• Taverna Server Amazon Image
  – With Interaction, R and Google Refine Servers

• Replicated at BioVeL partner INFN

• Server Version 2.5
  – Interactions
  – Components plug-in