Portals and workflows: Taverna Workbench

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Summary

- Information and data integration in biology
- Web Services and workflow management
- Taverna Workbench
- A workflow enactment portal
Information in biology: well known facts

- Biomedical research produces an increasing quantity of new data and new data types
  - EMBL size: ver 82 7.3% more vs ver 81 (3 months), 112.9% vs ver 74 (24 months)
- Emerging domains, like mutation and variation analysy, polymorphisms, metabolism, as well as new technologies, e.g., microarrays, will contribute with even huger amounts of data

- Analysis softwares must interoperate with databases
  - Databases as input for softwares
  - Results as new data to record and analyze
Heterogeneity of databanks

- A few dbs are managed in an almost homogenous way (e.g., sequences at EBI, NCBI, DDBJ)
- Secondary databases are of high quality (good and extended annotation, quality control)
- Many databases are highly specialized, e.g. by gene, organism, disease, mutation, etc…
- Many databanks are created by small groups or by single researchers

Databanks are distributed:
- Different DBMS, data structures, query methods
- Different information, semantics
In this context, data integration and work automation are needed to:

- Carry out analysis and/or searches involving more databases and softwares automatically
- Perform analysis involving large data sets effectively
- Achieve a better and wider view of all available information
- Carry out a real data mining
Data integration longevity

- **Integration needs stability**
  - Standardization……
  - Good domain knowledge
  - Well defined data
  - Well defined goals

- **Integration fears:**
  - Heterogeneity of data and systems
  - Uncertain domain knowledge
  - Fast evolution of data
  - Highly specialized data
  - Lacking of predefined, clear goals
  - Originality, experimentalism ("let me see if this works")
Integration of biological information

In biology:

○ A pre-analysis and reorganization of the data is very difficult, because data and related knowledge change very quickly
○ Complexity of information makes it difficult to design data models which can be valid for different domains and over time
○ Goals and needs of researchers evolve very quickly according to new theories and discoveries

Integration must therefore be carried out by using flexible systems that are easy to adapt and to extend
Integration methods

From syntactical to semantical links:

- Explicit (reciprocal) links (xrefs)
- Implicit links (e.g., names)
- Common contents (vocabularies)
- Shared data models and schemas
- Common Semantics (ontologies)
Web Services in brief

- XML based network services
- Implement standard transport protocols (SOAP, HTTP)
- Standards also available for retrieval and identification (UDDI), description (WSDL) and composition (WSFL)
- Allow software applications to access data “intelligently”: identification of contents, interpretation of semantics information
- Metadata needed
- Web Services already implemented by many Institutes and service centers
Workflow management

“A computerized facilitation or automation of a business process, in whole or part". (Workflow Management Coalition)

Main goal is:
- the implementation of data analysis processes in standardized environments

Main advantages relate to:
- **effectiveness**: being an automatic procedure, it frees bio-scientists from repetitive interactions with the web and it supports good practice,
- **reproducibility**: analysis can be replicated over time,
- **reusability**: intermediate results can be reused,
- **traceability**: the workflow is carried out in a transparent analysis environment where data provenance can be checked and/or controlled.
Workflow management software for bioinformatics applications:

- Biopipe, an add-on to bioperl
- GPipe, an extension of the Pise interface
- Taverna (EBI), a component of the myGrid platform
- Wildfire (Bioinformatics Institute, Singapore)
- Pipeline Pilot (SciTegic)
- BioWBI, Bioinformatic Workflow Builder Interface, from IBM

They all require knowledge of the systems and skills and time for development of the workflows.
Workflow management: Taverna

Taverna Workbench

- builds complex analysis workflows
- is able to access both remote and local processors
- defines alternative processors
- runs workflows
- visualizes the results

It includes a an ontology for bioinformatics data

Requirements: java, Windows or Linux
Open source: http://taverna.sourceforge.net/
Current version: 1.3.1 (stable, next version 2.0)
Graphical user interface (GUI) including:

- Advanced Model Explorer (AME)
- Workflow diagram
- Available services
- Run workflow
- Enactor invocation

Options: default services, workflow editor, debug
Extra features: FETA search engine
Taverna: available processors (services)

WSDL services
- Web Service Description Language (WSDL) file: adds WSDL based service nodes

Soaplab servers
- Soaplab server: adds a list of soaplab provided services

BioMOBY registries
- Moby Central repository: determines hosts and their services

Workflows
- XScufl definition file: either adds the workflow as a sub-workflow or imports processors

Biomart databases
- Biomart data warehouse: allows for searching all available data sets

Local processors
- Simple list/string processors, r/w, extra special remote links, constant values, beanshell scripts

Other processors
- Styx, Talisman, Seqhound, API Consumer
**Workflow Input: libs**

**Input Metadata**

<table>
<thead>
<tr>
<th>Semantic type</th>
<th><a href="http://www.mygrid.org.uk/ontology#CABRI_cell_lines_catalogue">http://www.mygrid.org.uk/ontology#CABRI_cell_lines_catalogue</a></th>
</tr>
</thead>
<tbody>
<tr>
<td>Syntactic type</td>
<td>text/plain/plain</td>
</tr>
</tbody>
</table>

**Description**

This input includes the name(s) of the CABRI human and animal cell lines catalogues involved in the query. Multiple values can be specified, in a unique string field, each name in a distinct text line (thus, names must be divided by a `\n` character). As of Feb 15, 2005, possible values are: `-iclc` (i.e., the Interlab Cell Line Collection, www.iclc.it) - `ecacc_cell` (i.e., the European Collection of Cell Cultures, www.ecacc.org.uk) - `dsmz_mutz` (i.e., the collection of human and animal cell cultures of the DSMZ, www.dsmz.de) Catalogues can be added (or, rarely, removed) without notice. See www.cabri.org for further information.

**Instructions**

To input data into this workflow you must first create either a single item or a list. Having done this you can select the item from the tree to the left of this panel and either enter the data manually, upload from a file on your local machine or load from a location on the internet. When all workflow inputs have been populated as required you can click the 'run workflow' button to...
This input includes the name(s) of the CABRI human and animal cell lines catalogues involved in the query. Multiple values can be specified, in a unique string field, each name in a distinct text line (thus, names must be divided by a `\n` character). As of Feb 15, 2005, possible values are:

- `iclcl` (i.e., the Interlab Cell Line Collection, www.iclcl.it)
- `ecacc_cell` (i.e., the European Collection of Cell Cultures, www.ecacc.org.uk)
- `dsmz_mutz` (i.e., the collection of human and animal cell cultures of the DSMZ, www.dsmz.de)

Catalogues can be added (or, rarely, removed) without notice. See www.cabri.org for further information.

**Instructions**

To input data into this workflow you must first create either a single item or a list. Having done this you can select the item from the tree to the left of this panel and either enter the data manually, upload from a file on your local machine or load from a location on the internet. When all workflow inputs have been populated as required you can click the 'Run workflow' button to...
<table>
<thead>
<tr>
<th>Name</th>
<th>Last event</th>
<th>Event timestamp</th>
<th>Event detail</th>
<th>Breakpoint</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regex_for_catalogue_name</td>
<td>ProcessComplete</td>
<td>8-mar-2006 13.33.31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substitute_blanks_with_SP</td>
<td>ProcessComplete</td>
<td>8-mar-2006 13.33.31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Extract_ids_by_removing</td>
<td>ProcessComplete</td>
<td>8-mar-2006 13.33.31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Separate_cell_line_ids</td>
<td>ProcessComplete</td>
<td>8-mar-2006 13.33.31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>getCellLineIdsByName</td>
<td>ProcessComplete</td>
<td>8-mar-2006 13.33.31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>getCellLinesById</td>
<td>ProcessComplete</td>
<td>8-mar-2006 13.33.32</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Workflow Diagram**

```
Text_lines_separator
  | Separate_cell_line_ids

ICLC:ICLC ATL95005
```

**Result**

```
ICLC:ICLC ATL95005
```
Workflow information

This report applies to the workflow titled 'Search CABRI human and animal cell lines catalogues by cell line name and retrieve full cell line descriptions' authored by Paolo Romano, IST, Genova, Italy (paolo.romano@istge.it) and with LSID 'urn:lsid:www.mygrid.org.uk:operation:US8XCRXJAA0'. The textual description, if any is shown below:

This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines’ unique IDs associated with the input (done via a call to the getCellLineIdsByName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesByIds web service).

Resource usage report

This display shows the various external resources used by the current workflow. It does not show resources such as local operations or string constants which are run within the enactment engine. Services are categorized by resource host and type, and the name of the instance of each service shown to the right.

Resources on www.o2i.it, 2 instances.

<table>
<thead>
<tr>
<th>Service</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soaplab</td>
<td>Service rooted at /axis/services</td>
</tr>
<tr>
<td></td>
<td>App category and name: Processors</td>
</tr>
<tr>
<td></td>
<td>/axis/services/cabri:getCellLineIdsByName</td>
</tr>
<tr>
<td></td>
<td>/axis/services/cabri:getCellLinesByIds</td>
</tr>
</tbody>
</table>
Oncology over Internet (O₂I)

We designed a web system that:

- allows for the carrying out of a set of predefined workflows (of oncology interest)
- supports workflows annotation by using a simple ontology for bioinformatics processors (domain, task, i/o)
- implements search of workflows on the basis of their annotation
- supports retrieval of workflows based on users’ registration and profiling
- allows storing and retrieval of workflows’ executions and related results
Oncology over Internet (O₂I)

We designed a web system that:
- makes access to and retrieves data from Web Services and registries of Web Services
- stores workflows using the Simple conceptual unified flow language (Scufl) format
- is partially based on open source tools (Taverna WB, FreeFluo and mySQL)

Prototype available on-line: http://www.o2i.it:8080/portal/
O2I architecture
Predefined workflows

Workflows are:

- created by internal staff using Taverna
- stored in Scufl format
- maintained (workflow vs version)
- submitted by:
  - users
  - service providers
Annotation of workflows

Workflows are annotated on the basis of:

- a simple ontology for bioinformatics processors:
  - application domains
  - task
  - inputs/outputs
- ontology derived from Taverna:
  - new structure
  - some additions (biological resources, images, …)
  - under further development
O₂I ERA schema
O₂I workflows annotation
Users’ registration and profiling

Users are profiled on the basis of:

- role in their organization
  - computer scientist / physician / researcher / patient / journalist / …
- domains of interest
- past workflows’ executions
O₂I (Oncology over Internet) Project
Your personalized project research web site.

Please login

username: 
password: 

Login

New user? Please register

Please install the new library. (Instructions)
Applets digital certificate.
## All workflows:

<table>
<thead>
<tr>
<th>Workflow</th>
<th>Description</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conditional Branch Choice</td>
<td>This is a demo workflow distributed with Taverna Workbench (see taverna site). If the input is true then the string 'foo' is emitted, if false then 'bar'. Just a simple example to show how the conditional branch processor works.</td>
<td>1.0</td>
</tr>
<tr>
<td>Retrieve Cell Lines Descriptions By Name</td>
<td>This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines' unique IDs associated with the input (done via a call to the getCellLineIdsByName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesByIds web service). Both these web services are available at the soaplab system at <a href="http://www.o2i.it:8080/axis/services">http://www.o2i.it:8080/axis/services</a>. A number of string or string list local elaborations are required: returned IDs are in a string and this must be transformed in a list (done by the 'Separate_cell_line_ids' processor, that is implemented by using a Split_string_into_string_list_by_regular_expression local processor) - returned IDs include catalogues' names and this must be removed before their utilization for further processing (done by the 'Extract_ids_by_removing_catalogues_names' processor, that is implemented by using a Filter_list_of_strings_extracting_match_to_a_regex local processor) - returned IDs include a blank character and this must be substituted by a '_' characters string before submitting the data to the 'getCellLinesByIds' web service (done by a trivial bashshell script). Special requirements on input data are: one or more of the following catalogues names can be specified: 'idc', 'ecacc_cell', 'dsmz_mutb'. Other names may lead to errors - when specifying more than one catalogue names, they must be in a unique input string but on distinct text lines, - cell lines names can only be made by a single word, excluding special characters as '/', ' ' and '' - cell lines names are case insensitive. Example of valid cell lines names are: - vero - hela - e172 - calu6</td>
<td>1.0</td>
</tr>
<tr>
<td>Retrieve descriptions of</td>
<td>Retrieve full descriptions of bacteria strains from CABRI catalogues (see CABRI site) by their scientific name (genus and species only). Inputs of the workflow are the name of the involved CABRI catalogues (text/plain string with one catalogue name per line) and the scientific name of the desired bacteria strain (text/plain string including genus and species separated by a blank space).</td>
<td>1.0</td>
</tr>
</tbody>
</table>
**O₂I (Oncology over Internet) Project**

*Your personalized project research web site.*

**My application domains workflows:**

<table>
<thead>
<tr>
<th>Workflow</th>
<th>Description</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Retrieve Cell Lines Descriptions By Name</strong></td>
<td>This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines' unique IDs associated with the input (done via a call to the getCellLineIdsByCatalogueName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesByIds web service). Both these web services are available at the soaplab at <a href="http://www.o2i.it:8080/axis/services">http://www.o2i.it:8080/axis/services</a>. A number of string or string list local elaborations are required: - returned IDs are in a string and this must be transformed in a list (done by the 'Separate_cell_line_ids' processor, that is implemented by using a Split_string_into_string_list_by_regular_expression local processor) - returned IDs include catalogues' names and this must be removed before their utilization for further processing (done by the 'Extract_ids_by_removing_catalogues_names' processor, that is implemented by using a Filter_list_of_strings_extracting_match_to_a_regex local processor) - returned IDs include a blank character and this must be substituted by a '<em>SP</em>' characters string before submitting the data to the 'getCellLinesByIds' web service (done by a trivial bash script). Special requirements on input data are: - one or more of the following catalogue names can be specified: 'col1', 'ecaco_cell', 'dsmu_mutz'. Other names may lead to errors. - when specifying more than one catalogue names, they must be in a unique input string but on distinct text lines, - cell lines names can only be made by a single word, excluding special characters as '/', '°' and '™', - cell lines names are case insensitive. Example of valid cell lines names are: - vero - hela - a172 - calu6</td>
<td>1.0</td>
</tr>
<tr>
<td><strong>Retrieve descriptions of bacteria strains</strong></td>
<td>Retrieve full descriptions of bacteria strains from CABRI catalogues (see <a href="http://www.o2i.it:8080/axis/services">CABRI site</a>). Inputs of the workflow are the name of the involved CABRI catalogues (text/plain string with one catalogue name per line) and the scientific name of the desired bacteria strain (a text/plain string including genus and species separated by a blank space). Data is retrieved from CABRI Web Services in two steps. First, all bacteria strains IDs are retrieved by using the getBacteriaIdsByNameName method, and after descriptions are retrieved by using the getBacteriaByBld method. Some list/text elaboration is required to remove catalogue names from returned IDs</td>
<td>1.0</td>
</tr>
</tbody>
</table>
Simple demo workflow
O₂I (Oncology over Internet) Project
Your personalized project research web site.

WORKFLOWS DETAILS

Name: Retrieve Cell Lines Descriptions By Name

Description: This workflow takes the cell line name and the catalogue(s) name(s) as input and retrieve the full cell line description(s) by first retrieving the cell lines' unique IDs associated with the input (done via a call to the getCellLineIdsByName web service) and then using IDs for retrieving the full cell lines descriptions (done via a call to the getCellLinesByIds web service). Both these web services are available at the soaplab system at http://www.o2i.it:8080/axis/services

A number of string or string list local elaborations are required: returned IDs are in a string and this must be transformed in a list (done by the 'Separate_cell_line_ids' processor, that is implemented by using a Split_string_into_string_list_by_regular_expression local processor) - returned IDs include catalogues' names and this must be removed before their utilization for further processing (done by the 'Extract_ids_by_removing_catalogues_names' processor, that is implemented by using a Filter_list_of_strings_extracting_match_to_a_regex local processor) - returned IDs include a blank character and this must be substituted by a '_SP_' characters string before submitting the data to the 'getCellLinesByIds' web service (done by a trivial beanshell script).

Special requirements on input data are: one or more of the following catalogues names can be specified: 'iclc', 'acacc_cell', 'dmz_mutz'. Other names may lead to errors, - when specifying more than one catalogue names, they must be in a unique input string but on distinct text lines, - cell lines names can only be made by a single word, excluding special characters as '/', '-' and 'w', - cell lines names are case insensitive.

Example of valid cell lines names are: - vero - hela - a172 - calu6

Author: Paolo Romano, IST, Genova, Italy (paolo.romano@istge.it)

Roles list:
- researcher - molecular biologist
- researcher - cellular biologist
- researcher - structural biologist
- researcher - microbiologist
- researcher - immunologist
- researcher - virologist

Version details

Version: 1.0

Date: 18:05 - 27/09/2005
**Version details**

**Version:** 1.0

**Date:** 18:05 - 27/09/2005

**Author:** Paolo Romano, IST, Genova, Italy (paolo.romano@istge.it)

**Filename:** RetrieveCellLinesDescriptionsByName.xml

**Changes:** Original version

**Image:** show in a new window

**Input list:**
- biological resource database (required)
- cell line name (required)

**Output list:**
- CABRI human and animal cell lines record

**Domains list:**
- Microbiology
- Cellular Biology

**Processors:**
Please be advised that only a list of main components of the workflow. They are not ordered.

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Task</th>
<th>Domains</th>
<th>Inputs</th>
<th>Outputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Get cell lines id by name</td>
<td>Retrieve CABRI cell lines' IDs after a search in CABRI Web Services by cell lines' name</td>
<td>biological resource retrieval</td>
<td>Microbiology</td>
<td>biological resource database cell line name</td>
<td>biological resource identifier</td>
</tr>
<tr>
<td>Get cell lines descriptions by id</td>
<td>Retrieves cell lines' descriptions by CABRI id</td>
<td>biological resource retrieval</td>
<td>Microbiology</td>
<td>biological resource database biological resource identifier</td>
<td>CABRI human and animal cell lines record</td>
</tr>
</tbody>
</table>
Version details

**Version:** 1.0

**Date:** 18:05 - 27/09/2005

**Author:** Paolo Romano, IST, Genova, Italy

**Filename:** RetrieveCellLinesDescriptions

**Changes:** Original version

**Image:** show in a new window

**Input list:**
- biological resource database (required)
- cell line name (required)

**Output list:**
- CABRI human and animal cell lines

**Domains list:**
- Microbiology
- Cellular Biology

**Processors:**
Please be advised that is only a list of main processors.

<table>
<thead>
<tr>
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<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Get cell lines id by name</td>
<td>Retrieve CABRI cell lines id after a search in Services by cell line name</td>
</tr>
<tr>
<td>Get cell lines descriptions by id</td>
<td>Retrieves cell lines' descriptions by CABRI id</td>
</tr>
</tbody>
</table>

Workflow Inputs

- `libs`
- `name`

Workflow Outputs

- `Text_lines_separator`
- `value`

Additional nodes:
- `regex`
- `string`
- `regex_for_catalogue_name_extraction`
- `value`

Legend:
- `text/plain`
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Please insert input:

CABRI Cell lines catalogues: [required input]

Description: This input includes the name(s) of the CABRI human and animal cell lines catalogues involved in the query. Multiple values can be specified, in a unique string field, each name in a distinct text line (thus, names must be divided by a 'n' character).

As of Sep 15, 2005, possible values are:
- 'icl' (i.e., the Interlab Cell Line Collection, http://www.icl.it/)
- 'ecacc_cell' (i.e., the European Collection of Cell Cultures, http://www.ecacc.org.uk/)
- 'dsnz_mutz' (i.e., the collection of human and animal cell cultures of the DSMZ, http://www.dsmz.de).

Catalogues can be added (or, rarely, removed) without notice. See the CABRI site for further information.

Cell line name: [required input]

Description: The input must specify the name of the required cell line(s). Due to the indexing rules in the CABRI network service (see the http://www.cabri.org/), only one word can be used in the search and no spaces are allowed in the cell line name.

Moreover:
- cell lines names cannot include the following characters: '/' and '*';
- cell lines names are case insensitive.

Example of valid cell lines names are:
- vero
- hela
- a172
- calu6

Execute
Your persistently saved results:

All the results in the same table have been produced by the same workflow execution.

<table>
<thead>
<tr>
<th>Execution Details</th>
<th>Workflow Inputs</th>
<th>Results list</th>
</tr>
</thead>
<tbody>
<tr>
<td>Date of Execution: 13:08 - 04/10/2005</td>
<td>termID = 'GO:0003677'</td>
<td>□ Workflow output</td>
</tr>
<tr>
<td>Workflow name: Show Gene Ontology Term Context</td>
<td></td>
<td>□ ancestorColour</td>
</tr>
<tr>
<td>(Workflow diagram)</td>
<td></td>
<td>□ childColour</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ inputTermColour</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ getImmediateChildren</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ getParents</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ getAncestry</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ create</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ getChildren</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ getResults</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Execution Details</th>
<th>Workflow Inputs</th>
<th>Results list</th>
</tr>
</thead>
<tbody>
<tr>
<td>Date of Execution: 14:44 - 23/05/2005</td>
<td>libs = 'idc' name = 'vero'</td>
<td>□ Workflow output</td>
</tr>
<tr>
<td>Workflow name: Retrieve Cell Lines Descriptions By Name</td>
<td></td>
<td>□ Text lines separator</td>
</tr>
<tr>
<td>(Workflow diagram)</td>
<td></td>
<td>□ Substitute blanks with SP</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ Regex for catalogue name extraction</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ Group for catalogue name extraction</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ Separate cell line ids</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ Extract ids by removing catalogues names</td>
</tr>
<tr>
<td></td>
<td></td>
<td>□ getCellLineIdsByName</td>
</tr>
</tbody>
</table>
|  |  | □ getCellLinesById
Some acknowledgements…

IST, Genoa
Paolo Romano,
Ulrich Pfeffer,
Domenico Marra,
Valentina Mirisola,
M. Assunta Manniello

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Matteo Fattore

ITB, CNR, Milan
Luciano Milanesi

DISCo, University of Milan Bicocca
Guglielmo Bertolini,
Flavio De Paoli,
Giancarlo Mauri

DIST, University of Genoa
Ivan Porro,
Silvia Scaglione

DMI, University of Camerino (MC)
Emanuela Merelli,
Ezio Bartocci

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