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Data Management for Quantitative Biology

Project Paper

Project 1: Data Modelling and Visualization

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1 Background

Data management in life sciences connects different fields and people with different scientific backgrounds. One challenge, especially when data needs to be collected and presented, is to keep track of the metadata that is important for analysis and reproducibility of an experiment, while exposing only informative and easy to understand data and metadata to users that are not concerned with computation or data management. Hence, for a given data set, the project task was to define what parts of data should be shown to end users (life scientists) and to implement a web-based Graphical User Interface, using Java, to visualize given data. Users should also be able to add some annotation on their own and download a summarizing report of the results. In addition, the user interface should be intuitive and well documented to guide even first-time users easily through the task of data annotation.

2 Material and Methods

2.1 Data

The main data structure is provided in form of TSV-files. The file *projects.tsv* contains multiple projects together with several attributes, describing the project. Projects themselves can contain multiple different experiments (*experiments.tsv*), which in turn contain two different types of samples (*QCOFF.tsv* and *QMOUSE.tsv*). *QCOFF* is storing samples of a coffee diversity project, whereas *QCOFF* consists of samples for a mouse knockout project. The set of samples can be structured hierarchically, with patients/organisms at the top (Entity samples) from which tissue/cell samples are derived. Experiments or samples can contain datasets, stored in *datasets.tsv*. Datasets link to one or more files. These files are for instance further descriptions in plain text, images, quality control HTML documents or FASTQ files. All structures of the system contain unique identifiers to connect the set of TSV-files together in a logical way.

2.2 Java and Vaadin

The graphical user interface (GUI) was developed using the open source web application framework Vaadin 7. Vaadin enables the possibility to build single page web apps in server-side Java. All of the browser–server communication and data transfer objects are automated by the framework. The app's state resides on the server, but the end-users use an HTML5 web app in their browsers. In addition, Vaadin's default component set can be extended with custom Google Webtoolkit Widgets (GWT) and designed over cascading style sheets (CSS) [1]. In addition to the common vaadin distribution, an extra addon, that provides with basic PDF and Excel export functionality, was used for the report generation [2].

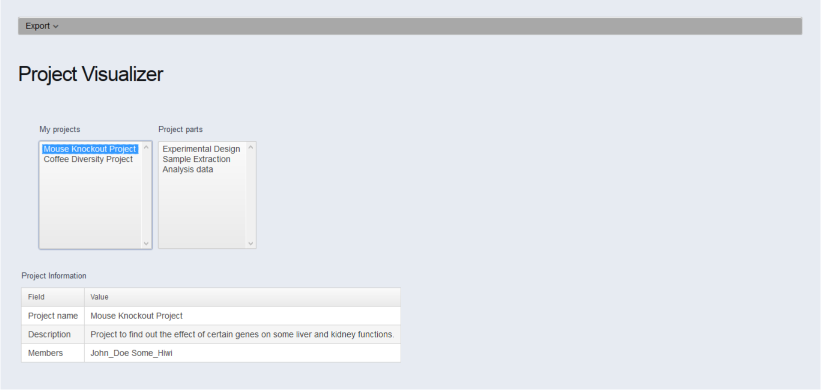
3 Results

3.1 Data Parser

... (Benni ?)

3.2 Project Visualizer

The resulting user interface tries to simplify the provided collection of data. Therefore, an clear navigation has been designed, to enable also new users handling all components of the web application in a fairly easy way. When the tool is started, all existing data is loaded in the background and available projects are displayed in a select-able list. If one choose a particular project, additional project information is shown in a extra table. In addition, a further select-able list appears, displaying all experiments under the project (Fig. 1).



Project Visualizer

My projects
- Mouse Knockout Project
- Coffee Diversity Project

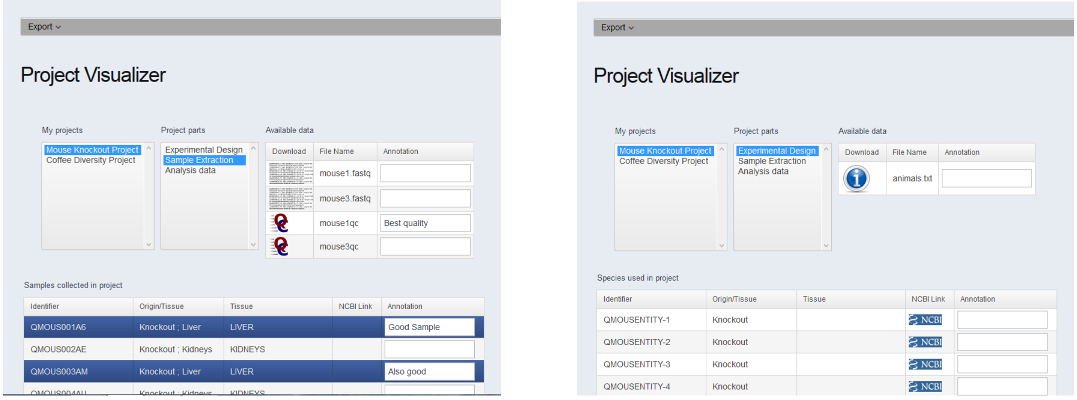
Project parts
- Experimental Design
- Sample Extraction
- Analysis data

Project Information

Field	Value
Project name	Mouse Knockout Project
Description	Project to find out the effect of certain genes on some liver and kidney functions.
Members	John_Doe Some_Hiwi

Figure 1: The GUI at the project level. Here, users can make a decision between various available projects and inspect additional information.

If the user clicks on a specific experiment, two additional tables are visualized (Fig. 2). One table showing available data files that are stored under a specific experiment and another one providing all existing experimental samples. The sample table has a multi selection feature, enabling the possibility to inspect the data sets that available for multiple samples. For instance, this can be seen in Fig. 2b. Here, two samples (QMOUS001A6 and QMOUS004AM) are selected, leading to a view at fastQ-files and quality control sites for each of the selected samples. All those datasets are click- and downloadable directly from the GUI.



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Available data

Download	File Name	Annotation
	mouse1.fastq	
	mouse3.fastq	
	mouse1qc	Best quality
	mouse3qc	

Samples collected in project

Identifier	Origin/Tissue	Tissue	NCBI Link	Annotation
QMOUS001A6	Knockout ; Liver	LIVER		Good Sample
QMOUS002AE	Knockout ; Kidneys	KIDNEYS		
QMOUS003AM	Knockout ; Liver	LIVER		Also good
QMOUS004AU	Knockout ; Kidneys	KIDNEYS		

(a) Example for a experimental design.

Project Visualizer

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Available data

Download	File Name	Annotation
ℹ	animals.txt	

Species used in project

Identifier	Origin/Tissue	Tissue	NCBI Link	Annotation
QMOUSENTITY-1	Knockout		NCBI	
QMOUSENTITY-2	Knockout		NCBI	
QMOUSENTITY-3	Knockout		NCBI	
QMOUSENTITY-4	Knockout		NCBI	

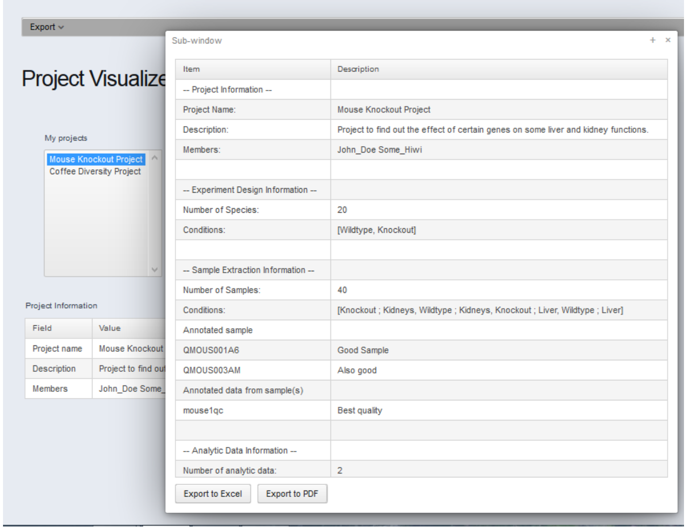
(b) Example for a sample extraction.

Figure 2: The GUI at the sample level. Here, users can inspect the collection of samples together with stored data sets.

A additional feature is the possibility to add some annotations for samples and datasets behind each row. Here end-users might leave some additional information, that is later included into to report for exportation. Additionally, the sample table comes up with an external connection to the NCBI Taxonomy Browser [3], if an taxonomy ID is deposited for a sample (Fig. 2b).

3.3 Data Exporter

With the aim to provide users with a printed summary of the visualized information, a data exporter has been developed. On clicking at the export menu bar, a new subwindow pops up, showing summarized information about a specific project in a new table. For instance, the project details, as well as the number of species together with their conditions for the specific experiments, are presented. As an extra feature, all samples/datasets, that have been annotated by the user, are also included together with their annotation into the summary table. An example for this can be seen in (Fig. 3) based on the navigation and annotation of Fig. 2b). At the end, the user has two option in form of press-able buttons. One button exports the summary table in Excel format, the other one generates a PDF download.



Field	Value
Project name	Mouse Knockout
Description	Project to find ou
Members	John_Doe Some_

Item	Description
-- Project Information --	
Project Name:	Mouse Knockout Project
Description:	Project to find out the effect of certain genes on some liver and kidney functions.
Members:	John_Doe Some_Hiwi
-- Experiment Design Information --	
Number of Species:	20
Conditions:	[Wildtype, Knockout]
-- Sample Extraction Information --	
Number of Samples:	40
Conditions:	[Knockout ; Kidneys, Wildtype ; Kidneys, Knockout ; Liver, Wildtype ; Liver]
Annotated sample	
QMOUS001A6	Good Sample
QMOUS003AM	Also good
Annotated data from sample(s)	
mouse1qc	Best quality
-- Analytic Data Information --	
Number of analytic data:	2

Figure 3: The export function. Here, inspect and download a project summary in Excel or PDF format.

4 Discussion

The complete project was structured in different phases. The first phase was the theoretical planing. A question which was adressed, was which data has to be visualised and which should not be visualised. In general only data serving as information gain, is important to the user. All other data is only important for the program.

Discussion of the columns, which are important for visualisation What did we additional need (IDs or stuff?) How do we want to visualize, what is expected at the experiment level. how should users navigate. Experiment subpoints

References

[1] Vaadin Ltd. vaadin - user interface components for web apps, 2015.

[2] Haijian Wang. vaadin - exporter version 0.0.5.5, 2014.

[3] Eric W. Sayers, Tanya Barrett, Dennis A. Benson, Stephen H. Bryant, Kathi Canese, Vyacheslav Chetvernin, Deanna M. Church, Michael DiCuccio, Ron Edgar, Scott Federhen, Michael Feolo, Lewis Y. Geer, Wolfgang Helmberg, Yuri Kapustin, David Landsman, David J. Lipman, Thomas L. Madden, Donna R. Maglott, Vadim Miller, Ilene Mizrachi, James Ostell, Kim D. Pruitt, Gregory D. Schuler, Edwin Sequeira, Stephen T. Sherry, Martin Shumway, Karl Sirotkin, Alexandre Souvorov, Grigory Starchenko, Tatiana A. Tatusova, Lukas Wagner, Eugene Yaschenko, and Jian Ye. Database resources of the national center for biotechnology information. *Nucleic Acids Research*, 37(suppl 1):D5–D15, 2009.