

Visualization of bioinformatics workflows for ease of understanding and design activities

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Abstract: Bioinformatics analyses are growing in size and complexity. They are often described as workflows, with the workflow specifications also becoming more complex due to the diversity of data, tools, and computational resources involved. A number of workflow management systems (WMS) have been developed recently to help bioinformaticians in their workflow design activities. Many of these WMS visualize workflows as graphs, where the nodes are analysis steps and the edges are interactions and constraints between analysis steps. These graphs usually represent a data flow of the analysis. We know that in software visualization, similar graphs are used to show a data flow in software systems. However, the WMS do not use any widely accepted standards for workflow visualization, particularly not in the bioinformatics domain. As a result, workflows are visualized in different ways in different WMS and workflows describing the same analysis look different in different WMS. Furthermore, the visualization techniques used in WMS for bioinformatics are quite limited. Here, we argue that applying some of the visual analytics methods and techniques used in software field, such as UML (unified modelling language) diagrams combined with quality metrics, can help to enhance understanding and sharing of the workflow, and ease workflow analysis and design activities.

1 INTRODUCTION

Software structure has been depicted with design diagrams since the very start of computer programming (Diehl, 2007). Furthermore, control-flow graphs (Goldstine and von Neumann, 1947) were among the first kinds of software diagrams and are very similar to the data-flow graphs used in the bioinformatics domain. Every diagram typically emphasises a particular aspect of a software system, such as a software static model or the time ordering of messages between software components. Still, many diagram elements of a diverse nature can occur in the same diagram. An effective system understanding requires ways to correlate diagram elements and software metrics, which represent software quality attributes, in a single view.

Visualizations that combine software structure and software attributes are arguably among the most universal types of software visualizations, and among the first that were proposed in the history of software visualization (Diehl, 2007; Spence, 2007). A good understanding of the structure of a potentially large, complex, and relatively unfamiliar software system is

best served by visualizing the structure.

Adding attributes such as "quality" metrics to this picture helps correlate the various quantitative insights with structural and architectural insights (Lanza and Marinescu, 2006). In some cases, software designers also identify and use groups of elements in the system analysis without constructing a separate diagram. These group of elements can also have their own group-level metrics (Byelas and Telea, 2009).

An increase of size and complexity in bioinformatics analyses means there is now a need to use advanced visualization techniques to depict analysis structure and workflow "quality" metrics. If the structure of the analysis is represented by the graph, both graph nodes and relations can accommodate several "quality" metrics. These metrics can also be defined at different levels of detail, such as groups of graph elements or sub-members of them. Furthermore, workflow visualization should be unified in some way to improve workflow sharing between people and interchanging between different WMS. Some attempts to support workflows interoperability were done in the SHIWA project (SHIWA, 2012), however, to the best

of our knowledge, a question of the visual workflow representation was not addressed in that project.

After interviewing the final WMS users in our team, which are researchers and Ph.D. students, we identified main "quality" metrics for bioinformatics workflows, that they are interested in:

- a number of parallel executions of workflow elements, which is usually the case if the workflow is developed to run in a computational cluster or grid;
- sizes of input and output data;
- an analysis execution time;
- tools used in an analysis, their dependencies and the operation systems used;
- resources required to run an analysis (e.g. CPU, RAM, storage requirements).

Besides showing these workflow attributes together with the workflow structure, users want to see workflow *behaviour* and *evolution*. We identified several views on workflows, which are most required in Life sciences. These are:

1. a structural overview of workflow elements showing or hiding "quality" metrics; and zooming into to a particular element or a group thereof and its dependencies combined with "quality" metrics;
2. an overview of how different parameters influence the results of analysis; and it is often the case, when bioinformatics workflows should be re-run many times with different analysis parameters;
3. a workflow evolution view, showing what elements were introduced or removed, when and who made these changes;
4. a run-time execution monitor, which shows the workflow progress information; and a statistical overview of workflow runs, success/failure rates, use of tools and user statistics.

The first three views are the *design* views and the last one is the *execution* view of the workflow. All these views should be readily understandable and scalable.

Here, we first give some examples of visualizations used in the WMS and specific for bioinformatics and in generic WMS (Section 2). Then, we discuss visualization techniques to show software structure combined with software metrics (Section 3). Finally, we present our conclusions and outline potential directions for future work (Section 4).

2 WORKFLOW VISUALIZATION IN POPULAR WMS

Galaxy (Blankenberg and Taylor, 2007) is one of the popular WMS for bioinformatics. It is a web environment, where users can create workflows by combining a large variety of bioinformatics tools. Figure 1 shows an example of the proteomics workflow created and used by Berend Hoekman.

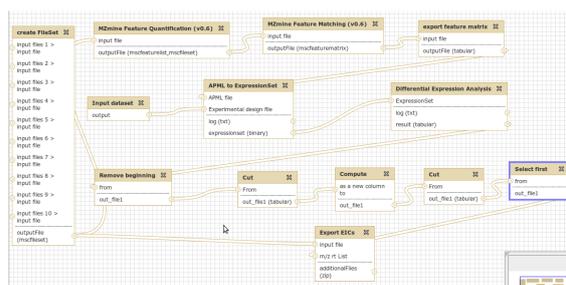


Figure 1: An example of a workflow visualization in Galaxy (Blankenberg and Taylor, 2007)

The workflow graph represents the data flow of the proteomics analysis used in the University Medical Centre Groningen (UMCG), Netherlands. The graph edges connect analysis steps from the workflow input (in the left-top corner) to output (in the left-bottom) showing the data flow. Input and output data files are listed in the body of the graph node icons. If you are not an expert in this workflow, it is difficult to evaluate a run time for the whole analysis, sizes of data, complexity of tools configuration *etc.* There is no visual difference between the workflow elements and it is difficult to distinguish those elements that are data nodes (*i.e.* workflow inputs/outputs) or processing analysis operations. Furthermore, parallelism in workflow design/execution can be shown in Galaxy by creating separate workflow nodes (*i.e.* one node per every parallel execution of the workflow element), that is a good solution if we consider up few parallel execution. However, this solution does not work with hundreds or thousands or parallel executions of the workflow element.

Another popular generic WMS is Taverna (Oinn and Greenwood, 2005). This is a suite of tools to design and execute workflows. It allows users to integrate third-party software tools, which are described as web services, into workflows. An example of a simple workflow that retrieves a weather forecast for a specified city is shown in Figure 2.

A workflows is presented as graphs constructed using the Taverna visual language. This graph (Fig. 2) also shows the data flow from top to bottom. Here, colours are used to show the nature of graph elements.

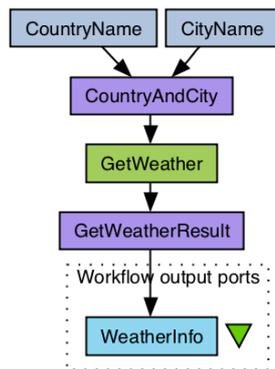


Figure 2: An example of a workflow visualization in Taverna (Oinn and Greenwood, 2005)

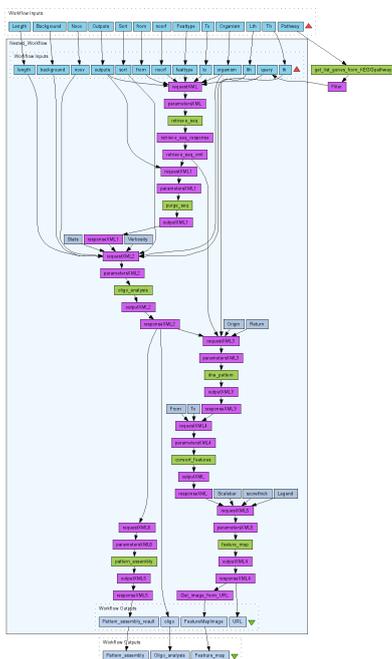


Figure 3: An example of a nested workflow in Taverna (Oinn and Greenwood, 2005)

We can clearly distinguish between data elements and Taverna services, although, the colour pattern is not really intuitive.

Workflows in Taverna can have conditional branches and loops, which are not widely used in bioinformatics, where actual analysis scripts can contain conditional statements as a part of the analysis script. In Taverna, workflows can also be nested into other workflows, which makes the workflows reusable and easier to maintain. An example of a larger workflow with nesting is shown in Figure 3. Here, the nested workflow is surrounded by a rectangle and an addi-

tional operation is shown outside of it. This operation can be *e.g.* a special input data preparation. We can treat this rectangle as showing one "quality" metric of the elements in it, but the analysis properties of the workflow elements can not be seen in such a workflow diagram.

3 TECHNIQUES THAT CAN ENHANCE VISUALIZATION OF WORKFLOW STRUCTURE

Since there are so many structure-and-attribute visualizations, we outline here the main common features that can be re-used in workflow visualizations for bioinformatics, and we present their strengths or limitations. From our own experience, most such visualizations share two design elements:

- *structure*: software structure is typically depicted by using a node-and-link graph metaphor, where nodes are software entities, *e.g.* functions, classes, components, or packages, and links are the relevant (sub)set of considered relations, *e.g.* function calls, data dependencies, associations, or inheritance relations.
- *attributes*: software attributes are usually depicted by mapping them to a visual attribute of the corresponding nodes or links in the structure visualization. Visual attributes that can be used to show software attributes are the position, size, shape, colour, texture, lighting, line size, and annotations of diagram elements.

The same node-and-link graph metaphor is used for workflow visualizations, particularly in bioinformatics. Below we discuss which visual attributes can be re-used in bioinformatics workflow visualization.

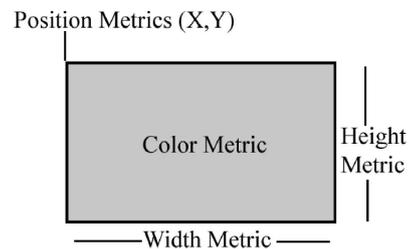


Figure 4: Using visual mapping to visualize "quality" metrics (Lanza and Ducasse, 2002)

In the lightweight software visualization framework, CodeCrawler (Lanza and Ducasse, 2002), "quality" metrics are visualized by mapping them to the colour, height, width, and position of the element

box icons (Figure 4). With these few visual attributes, it is possible to show, for example, analysis run time, sizes of input/output data, and CPU/memory requirements, combined with the workflow structure. Hence, the user can immediately get an idea about the requirements for running these workflow analysis steps.

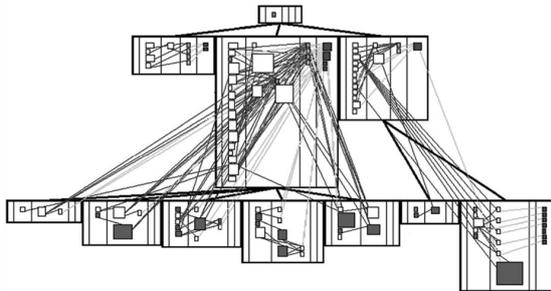


Figure 5: An example of a large software system in CodeCrawler (Lanza and Ducasse, 2002)

An example of a large software system visualized in CodeCrawler is shown in Figure 5. The system is divided into several modules, which are surrounded by rectangles. Here, a user can immediately see the division and spot outliers, which are shown as bigger rectangles with or without a colour. The same method can be applied to show large workflows that consist of many nested smaller workflows, and to emphasise the most computationally intensive steps. Visualization of both the analysis tool dependencies and the workflow structure can be combined into the same diagram using the method proposed in CodeCrawler method.

Another software visualization and exploration tool, MetricView (Termeer et al., 2005), combines traditional UML diagram visualization with metrics visualization. In contrast to the technique discussed above, MetricView uses existing and familiar to software engineers UML diagrams as a basis for software structure visualization 6. It follows the given diagrams layout and the positions and sizes of the diagram elements are not changed. This has an important advantage, because changing the diagram layout can destroy the users "mental map" and severely reduce how easily it can be understood; this is a well known fact in information visualization (see e.g. (Spence, 2006)). MetricView supports the visualization of metrics defined on UML diagram elements. Metrics can have boolean and numeric values; they are shown as icons, drawn atop of the UML elements for which the respective metrics are available.

Reusing this technique in workflow visualization allows a smooth transition from the familiar structural representation of a workflow, as used in Galaxy for example, to enhance the visualization of workflow with quality metrics. Metric icons simply take

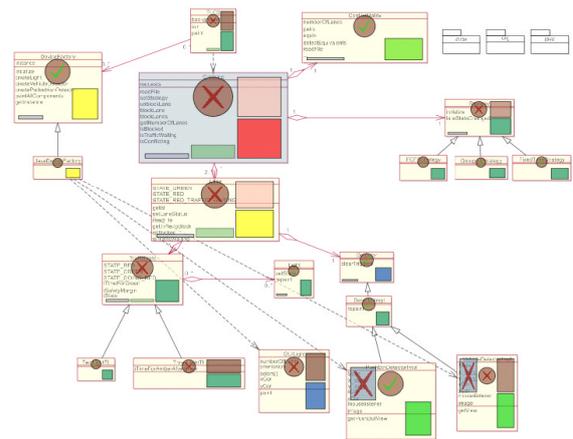


Figure 6: An example of 2D UML class diagram visualized with MetricView. (Termeer et al., 2005)

the space given by the Galaxy workflow diagram layout. In other words, metric information is added to diagrams in a non-intrusive way and users keep their "mental map" of the diagrams they are accustomed to work with.

The technique proposed in MetricView can usually be applied to show the attributes that are related to the whole workflow element. Besides visualization on the workflow element level, the metric lens visualization technique (Byelas and Telea, 2008) can be used to show metrics on members of the workflow elements. Let us look at a Galaxy visualization of a workflow element in Figure 7.

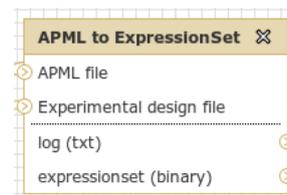


Figure 7: An example of workflow element visualized with Galaxy. (Blankenberg and Taylor, 2007)

An example workflow element has two inputs (*i.e.* APML file and Experiment design file) and two outputs (*i.e.* log and expressionset). However, users are not given any information about the sizes of these inputs/outputs or their nature from only the names. The task becomes even more complex, if users want to see not a single workflow element, but the whole workflow or a part of it, and if they want to see the metric-metric and metric-structure correlations of workflow elements. To achieve this, the metric lens techniques (Byelas and Telea, 2008) can be reused. It combines a classical UML viewer with a visualization of method-level metrics using an enhanced version of the well-

known table-lens technique (Rao and Card, 1994).

The basis of the metric lens technique is a traditional UML class diagram, which displays all its data members within each class frame (see Figure 8). Atop of this image, the metrics are displayed following a table model, where the rows are methods and the columns are metrics.

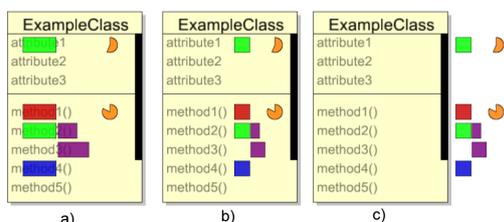


Figure 8: Metric layout options in of metric lens (Byelas and Telea, 2008)

The metric icon table can be placed within the class frames (Fig. 8 a,b), which yields a compact layout but does not allow users to read the method names, or on the right side of the class frames (Fig. 8 c), which does not occlude the method names displayed but yields a less compact layout. Different zooming mechanisms allow users to focus on a specific diagrams subsystem, and to smoothly navigate between seeing the entire contents of each class, as a set of coloured bar graphs, and seeing the individual signatures and names of methods and members. The same technique can be applied to navigate through the the workflow graph diagrams to spot the metric distribution of workflow element members and any metric value outliers, and help in the task of correlating such outliers among themselves and with the workflow structure.

4 CONCLUSION

We have presented a number of techniques that can be used to enhance visual analyses of workflows in WMS for bioinformatics, such as Galaxy or Taverna. We have reported some of the differences and limitations in these visualization techniques as used in these two WMS. We have also shown that there is no unified visual representation of workflows used in the bioinformatics domain. However, the same data flow graphs can be used to describe workflows visually.

Recently, we added workflow management to the existing data management built with the MOLGENIS system (Swertz and Jansen, 2007) and (Swertz and Jansen, 2010) to combine computational and data management into a single system (Byelas and Swertz,

2011) and (Byelas and Swertz, 2012). We use MOLGENIS to auto-generate web-user interfaces for biologists and program interfaces for bioinformaticians from a data model described in XML. Having the database background generated from the model web user interface, it is not surprising that we chose to use a simple table to show the workflow structure 9.

id	name	Workflow	protocol	PreviousSteps
1	FastqcElement	Lane file alignment	fastqc	
2	BwaElement	Lane file alignment	bwa	
3	BwaSampleElement	Lane file alignment	bwa-sample	BwaElement
4	SamToBamElement	Lane file alignment	sam-to-bam	BwaSampleElement
5	SamSortElement1	Lane file alignment	sam-sort	SamToBamElement1
6	BamIndexElement1	Lane file alignment	build-bam-index	SamSortElement1
7	MarkDuplicatesElement	Lane file alignment	mark-duplicates	BamIndexElement1
8	PicardQCElement	Lane file alignment	picard-qc	BamIndexElement1
9	BamIndexElement2	Lane file alignment	build-bam-index	MarkDuplicatesElement
10	RealignmentElement	Lane file alignment	realignment	BamIndexElement2

Figure 9: Showing workflow structure in the MOLGENIS framework (Byelas and Swertz, 2011)

In the future, we will investigate ways of using the visualization techniques described above for workflow visualisation. We are planning to visualise a workflow as a data flow graph as in Galaxy, but we want to advance its visualization by adding "quality" metrics. As the result, we expect to achieve a multiscale visualization similar to ones, that is used in geographical data visualization systems, such as *e.g.* Google Maps (Google Inc., 2012). In such a way, workflow "quality" metrics can be shown instead of photos and temperature in Figure 10.

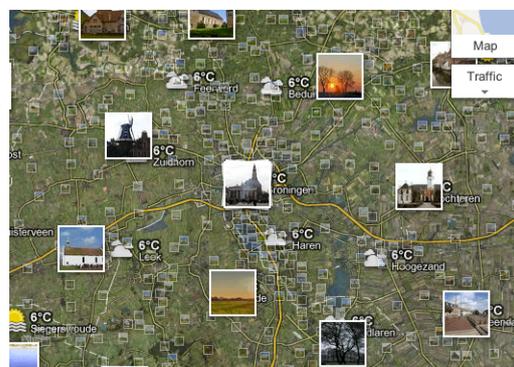


Figure 10: An example of multiscale visualization from Google Maps (Google Inc., 2012)

In this paper, we describe techniques which can enhance visual analysis of workflow structure. Besides, we want to enable users to get insight into workflow *behaviour* (run workflows, understand how parameters influence their output and refine the parameter space to achieve desired results) and *evolution* (detecting workflow changes over time). For *behaviour*, we will adapt multidimensional scaling (Borg and Groenen, 2005) and parallel coordinates

(Inselberg, 2009). For *evolution*, we will use timelines (Grafton and Rosenberg, 2010) visualizations to show how workflow structure and parameters change in time. Finally, we are planning to validate these visualization approaches by case studies on real-world workflows, that we use in our analyses.

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