Towards a Web-based Visualization for the CELLmicrocosmos 4 PathwayIntegration

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1   Introduction

The CELLmicrocosmos 4.2 PathwayIntegration (CmPI) is a tool to localize and visualize protein and gene data in the context of a virtual cell environment [1]. Here, an alternative, easy-to-use web browser-based tool is presented (CmPIwv, "wv" for web viewer), providing only the basic functionality of CmPI.

First, the basic workflow of CmPI should be discussed. A cell model is constructed based on different available cell component models, or an existing cell model is loaded. Then, protein-related or gene-related data or networks are imported. Finally, information is required to combine the virtual cell with the appropriate data. For this purpose, subcellular localization entries from different biomedical databases is acquired. This data has to be analyzed, because for some proteins or genes many different potential localizations are available, for other ones there is no data available at all. The analysis of this data is supported by different visualization approaches, particularly the subcellular localization charts [2]. The result can be interactively visualized as a virtual cell model representing a specific localization scenario.

CmPI is implemented in Java and Java 3D 1.5.2 and has to be installed to a PC. Basically, there are three user groups for CmPI: "authors" who can create and edit a specific virtual localization scenario, "reviewers" who are interested in a specific application case but do not want to analyze the basic data, and the "viewers" who are interested in exploring the final model. CmPI can be used by authors after a short adaptation phase. It takes advantage of Java WebStart technology, but requires some time to finish the installation process. Moreover, the functionality and features of CmPI are far beyond the (re-)viewer's scope. The obvious idea would be to create a simplified version of CmPI by developing a Java applet which runs in the browser. But the nowadays very restricted access to applets in the browser – caused by security issues – plus the requirement to install Java 3D in the background onto the client computer makes it a very complicated task for the developer and the user. Therefore, an alternative approach is required optimized for the (re-)viewer groups.

2   CmPI Web Viewer Concept

The optimal tool would be an application, where only a click on a web link is required to load a complete virtual localization scenario into a browser window, compatible to different systems, such as PCs, tablets, mobile phones, etc. In this way it will be possible to send a link to the collaborators, or to publish a link online or in the context of a manuscript, which can then be explored by the (re-)viewers. For this purpose, a web tool is being developed based on a three tier architecture:

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[1] Three.js is a WebGL framework which provides a scene graph–based API and direct visualization in most browsers, such as Chrome®, Firefox, Internet Explorer® [3].

[2] D3 is a JavaScript–based visualization library which enables fast visualization of 2D graphics inside a browser [4].

[3] PHP is used for interchanging content with the server-based application and the local computer. It enables to visualize local files as well as to load cell environments into the application which are uploaded to an external webspace.

The layout of the web tool is based on the basic layout of CmPI. Two different subcellular localization charts are available: the localization overview chart which summarizes all localizations found for the complete pathway, and the protein localizations chart, which shows all available localization for each protein at a time [2]. Figure 1 shows a KEGG example based on a previously published application case [1], [5].
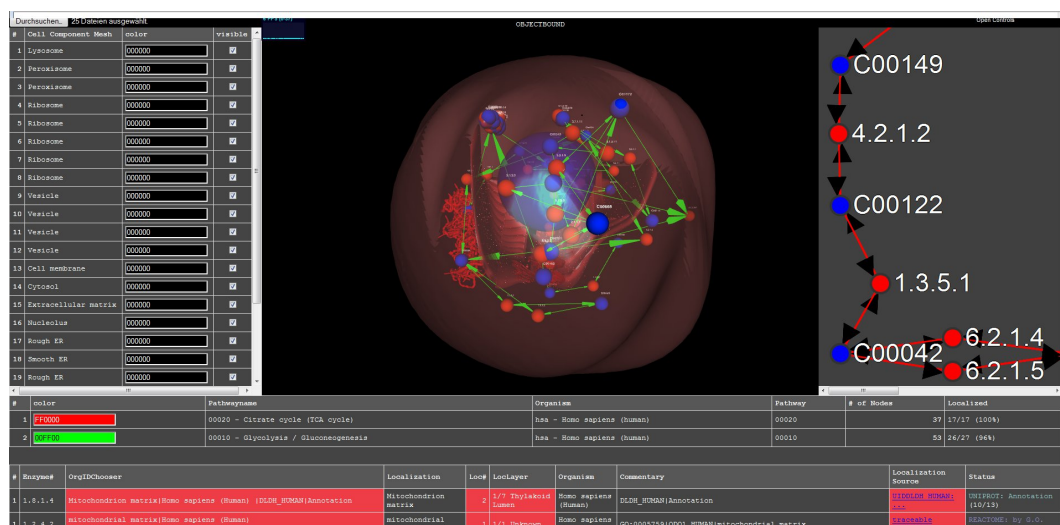

Figure 1: The CmPI WebViewer shows a virtual cell localization scenario correlated with the KEGG citrate cycle and the glycolysis as shown in the browser google Chrome.

3   References

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