Using Conceptual Graphs to embed expert knowledge in VR Interactions: Application to Structural Biology

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Abstract. To manage expert knowledge in VR interactions, we propose a software architecture based on semantic representation with Conceptual Graphs. We applied it on structural biology analysis. We define three semantic layers. The first layer embeds basic and specific domain knowledge (objects of interest). The second one describes the available tools in the application (visual representations). The third layer contains facts coming from VR interactions. Operations such as merging, projection, specialization and generalization allow us to build pattern conceptual graphs. They are translated using application specific wrapper into command interpretable by our targeted application. One goal is to release experts from the technical aspects of commands, and allow them to use their field terminology as vocal commands, in order to concentrate on the exploration task.

Keywords: Virtual Reality, Interactions, Knowledge Representation and Reasoning

1. Introduction

Virtual exploration of data helps in understanding complex phenomena by providing immersion and interaction means to users. A software tool (that we call "actuator") often specific to the domain is used to manage the data and the interactions. Our goal is to remove the cognitive load of using this tool (e.g. remembering an exact syntactic command) and to allow the users to communicate naturally with it. It requires a transformation process from the user command, expressed for example in natural language, to the command that the actuator can apply. This translation is based on knowledge representation and reasoning (KR&R) techniques so that the system can infer the task, from the entities of interest and the operations to be applied on them.

KR&R techniques are used in Virtual Reality (VR) since last couple of decades to incorporate intelligence [1], mostly towards building a machine understandable view of virtual environments (VE), which is not only suitable for processing by software agents but also for a relevant presentation to human users. For example, Gutierrez et al. [2] and Latoschik [3] proposed the use of KR in developing multimodal interactions. Several approaches have been proposed to build full semantic worlds using graph-based KR [4][5][6]. Recently, Dennemont et al. [7] used conceptual graphs (CG) and logical programing to provide context-aware interactions with non-semantic VE. They show that CG offers a good tradeoff for expressivity, understandability, efficient reasoning mechanism and natural language mapping.

In this work we focus on knowledge management in VE, to facilitate users' natural commands with complex tools. We applied our solution to structural biology analysis.

2. Proposed solution

We propose a CG-based approach to transform the user command into the actuator command (Fig. 1). We use the library Cogitant and its interface CoGui. An ontology is defined and a knowledge base is built containing facts encoding content and context information. An identification module receives the user command, deduces keywords and tries to map them onto the ontology, resulting in concepts and individuals. A unified reasoning procedure is applied on the CG. The object inference module infers the virtual objects of interest while the command inference module infers the requested operation. Results are comprehendible commands for the software.

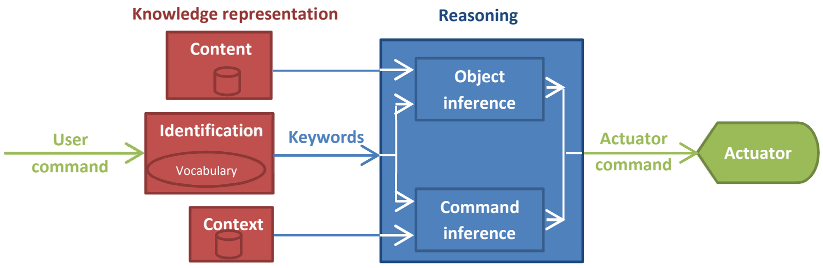


Figure 1: User command transformation process.

2.1 Representation

Knowledge representation includes a vocabulary (containing concepts, relations, and individuals), and a knowledge base containing facts in the form of CG.

Content knowledge is domain specific. It includes information about the entities of

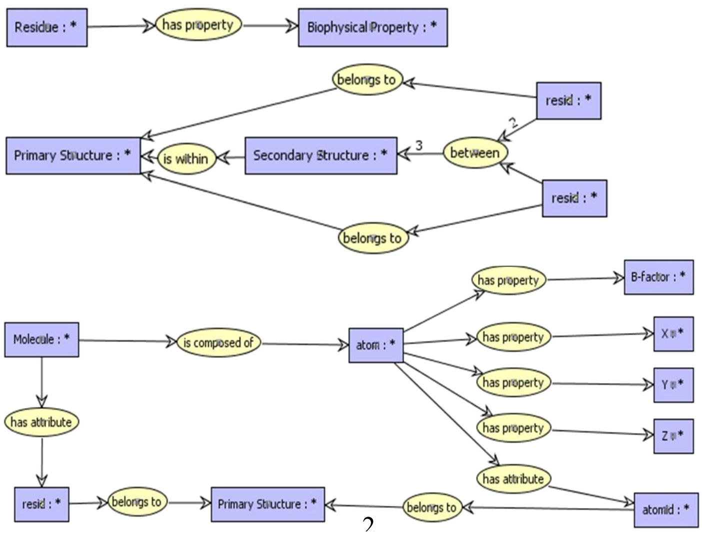


Figure 2: Content general facts.

interests, their attributes and their relationships with each other. For our purpose, content corresponds to protein composition and structure: atom, residue, primary structure, biophysical properties, etc. Content knowledge is stored using general facts (Fig. 2). The specialized facts are generated with a parser from a protein *.pdb* file.

Context knowledge concerns all the environment specific information considered relevant to the interaction with the domain entities. Such knowledge can encompass wide range of information i.e., nature of environment and user, interaction devices etc. We are concerned about the actuator related knowledge. During the interaction, its role is to apply the operations requested by the user to the scene content. Our chosen actuator for molecular visualization is PyMOL. Context knowledge is stored in general facts representing the available commands (*show*, *color*, etc.). They are specialized manually using the list of corresponding parameters: color names and available visual representations (lines, cartoon, etc.).

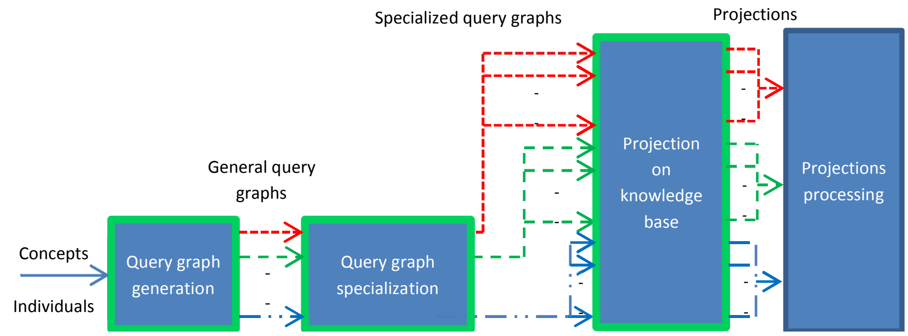


Figure 3: Object and command inference (green modules have the same implementation).

2.2 Reasoning and results

We propose a unified reasoning process for each of the inference modules (object and command) (Fig. 3). To extract the information from the knowledge base, we generate query graphs using the general graphs. Once specialized, queries are applied on the knowledge base to get the projections. Projections are processed to get the desired output (here a PyMOL command).

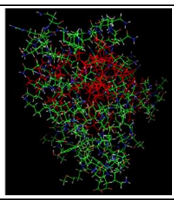
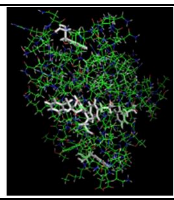
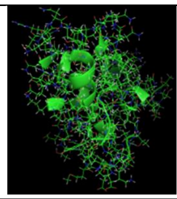
User Command (*keywords*)	*color hydrophobic residue primary structure A red*	*color PHE molecules white*	*show hydrophobic residues positive structure E cartoon*
Generated Command	color red, resn ILE+LEU+GLY in chain A	color white, resn PHE	show cartoon, resn LEU + ILE + PHE + SEC+ CYS + TYR + ALA +THR + LYS + MET+ GLY+TRP + ARG + VAL + HIS in chain E
PyMOL rendering			

Figure 4: Examples of generated commands and representations from user keywords.

Fig. 4 lists some examples of user commands, their corresponding generated PyMOL commands and the effective visualization. The third sample shows that user command is particularly simplified compared to its PyMOL equivalent.

3. Conclusion and future works

To manage expert knowledge in VR interactions, we propose a three-layers architecture based on semantic representation with Conceptual Graphs. We applied it on structural biology analysis. The first layer embeds specific domain knowledge (objects of interest). The second one describes the available tools in the actuator (visual representations). The third layer contains facts coming from VR interactions. Operations such as merging, projection, specialization and generalization allow us to build pattern conceptual graphs. They are translated using application specific wrapper into command interpretable by our targeted application. This approach has several advantages. First, verbal commands can be expressed only by keyword terms coming from molecular visualization and structural biology field, independently to the targeted application syntax. Using expert terminology as vocal commands releases the users from technical aspects and allows them to concentrate only on the exploration task. Secondly, the process is independent of the molecular visualization application, so can be applied on various applications of the same or different fields. In the short term improvements concern the flexibility of the identification process (e.g. allow the use of synonyms and handle logical expressions) and extensions are made to handle multiuser and multimodal commands.

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