

Modular Design of Graph Theory Based Software for Scientific Applications and Education

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Abstract

This work describes a new software design approach in graph theory applications. Sometimes, while using or teaching applications related to this subject, one of the main drawbacks is to define the application-specific graph and easily process and visualize it in a computer. A generic and flexible graph processing and visualization engine is presented. It is focused on a modular scheme, allowing a multidisciplinary framework in a technology-aware platform. We present the power of this tool in computer science courses that include graph algorithms and data structures. However, major potential is achieved within applications in other scientific fields. Since it is well-known that Information Technology (IT) is becoming an essential requirement in most scientific disciplines, we describe the impact of the easy incorporation of the proposed framework in different fields.

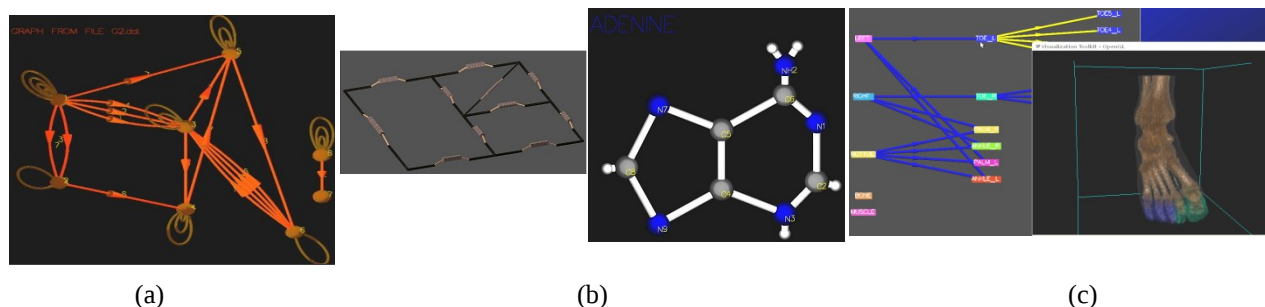


Figure 1: (a) Generic 3D graph visualization tool, (b) Electrical 3D circuit and molecule extensions and (c) Volume navigation extension.

Our proposal starts by building a well-designed and highly modular generic graph processing tool. By applying the Model-View-Controller architecture and the Object Oriented Paradigm (OOP), we implemented the system shown in Figure 1; we used the C++ and OpenGL technology to offer good scalability both in the abstract processing and during the visualization. From this base software described, by exploiting the power of OOP (inheritance, encapsulation...), a robust extension is achieved to match application-specific graph models, such as an electrical circuit or a chemical molecule. The design easily extends to use external tools such as the Volume Visualization Toolkit, as shown by our implementation of an anatomy navigation system guided by a graph model of the medical volume segmentation [APA08].

Despite the fact that IT is becoming an indispensable aid in virtually all fields of knowledge, the incorporation of IT-related

courses in university programs such as Medicine or Chemistry is still very limited in most centers. We consider this application a useful template to be used in courses where application-specific graph models are commonly used, since this framework provides a robust software design methodology and stimulates multidisciplinary team work.

Our proposal is a prototype that we plan to introduce in several scientific courses at the University of Barcelona (Spain) during the next semester. Future projects include the analysis and visualization of virtual social networks and intracellular communication networks, where multiresolution visualization techniques will be an indispensable requisite.

References

[APA08] ABELLAN P., PUIG A., AYALA D.: Focus + context rendering of structured biomedical data. In VCBM'08 (2008), pp. 109-116. 1