

BIOSHAPE: End-User Development for Simulating Biological Systems

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Abstract. The simulation and visualization of biological system models are becoming more and more important, in both clinical and research activities. Many tools help biologists and bioengineers to analyse and to study complex biological phenomena, such as disease spreading, tissue development and neurological reactivity.

We present ongoing work on BIOSHAPE, a bio-inspired 3D simulation tool whose novelty consists of providing a 3D geometry-oriented modelling environment. Unlike most of the other tools, BIOSHAPE development aims to improve usability by taking advantage of End-User Development techniques. While the user can easily understand the basic features of the tool, he is also made capable of extending them at different levels of complexity, for specific simulation purposes.

Keywords: Systems biology, Particle-based models, Simulation of biological systems, Simulation tool.

1 Introduction

Nowadays, systems biology plays an important role in the study and in the development of new improved medical solutions. *In silico* simulation and prediction of pathological phenomena [1], tailoring of medical treatments based on the characteristics of an individual patient ([2], [3]) as well as the research of nanotechnology applications are only some examples. *In silico* experimentation, in particular, permits to execute tests that would be critically expensive if carried out through *in vitro/in vivo* techniques (such as vascular blood diffusion in heart diseases, signal passing in neurological tissue and so on.) It also permits to study phenomena or interactions that do not occur, or occur rarely, in nature.

Since biological processes are inherently complex and computationally expensive, simulation tools often concentrate on the improvement of computational efficiency to gain better outcomes in lesser time. As a result, other important aspects such as the *Human Computer Interaction* (HCI) and the usability are overshadowed and most of these tools tend to push their grain over the user [4].

Recently we proposed BIOSHAPE [5], a bio-inspired simulation tool with a 3D geometry-oriented modelling environment. Unlike other bio-tools, BIOSHAPE

allows biologist and bio-engineers to represent biological processes by taking into account properties such as: *proximity, spacial separation, migration, molecular diffusion* and so on. In this work we demonstrate how End-User Development approaches (EUD) [6] can be successfully applied to BIOSHAPE in order to improve its usability and flexibility.

The paper is organised as follows: Section 2 provides a general description of the tool. Section 3 shows our strategies to simplify and to improve user application tasks. Section 4 summarises and traces ongoing and future work.

2 BIOSHAPE

BIOSHAPE¹ is a spatial 3D simulator that provides a particle-based, geometry-oriented modelling environment. Every element can be treated as a particle, *an entity*, with a specific shape, perception capabilities and a personalised motion law. Entities move and interact into the simulated space, *the simulation environment*; a two-phase collision detection algorithm [7] guarantees that colliding entities that cannot bind will repulse each other according to their motion laws.

BIOSHAPE represents small entities that do not interfere with the collision detection, but affect the simulated process, as gradients over the simulation environment, the *grouped entity*. For instance, a grouped entity can represent water molecules, ions or other particles usually abundant in any biological phenomena.

Entities and simulation environments are represented as *XML datasets*. A typical dataset contains all the information about the entities (e.g. type, position, velocity) and the environment (e.g. dimension, type and number of entities, gradient of grouped entities). We refer the reader to [5] for a complete description of BIOSHAPE's architecture.

3 EUD: simulation power to the user

In this section we describe the ideas that are currently under development in BIOSHAPE. Following the "*gentle slope*" approach ([8], [6]), the tool will provide the user with three levels of EUD activities of increasing complexity.

First level - customization. At this level the user with a little knowledge of the tool can create her/his own basic simulation. Two main aspects are defined: the simulation environment and the entities which move and interact. The default environments expose basic behaviours such as: finite bordering (the simulation is *closed* in the simulated space), purity/semi-purity (default sets of sliders for grouped entities - water, potassium and so on - or no grouped entities at all, depending on the selected default environment). The user is provided with a set of default entities with basic shapes, mainly cones, cylinders, cubes and prisms. They provide some degree of control over basic aspects such as velocity, speed rotation, etc. Both environments and entities can be *annotated* so that the user can incorporate domain-specific information. For instance, a simple sphere entity can be annotated to describe it as a metabolite as well as a cell of a tissue.

¹ The BIOSHAPE Project - <http://cosy.cs.unicam.it/bioshape/>

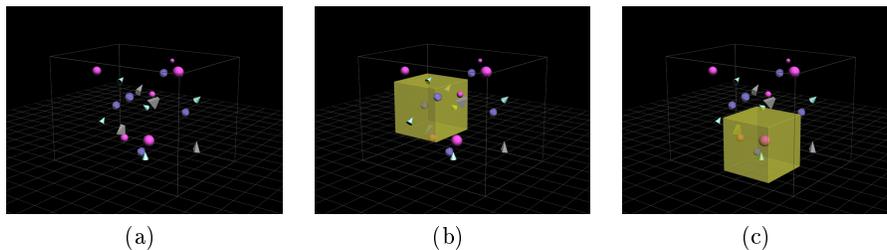


Fig. 1. (a) Simulation environment, (b) enriched with a single diffusion box, (c) displacement of the diffusion box

Second level - integration. The user can *glue* together default entities to create new complex ones not available in the default library. By defining a series of anchor points or anchor surfaces on the component entities, he can create *ad hoc* entities for its own simulations. Sliders and annotations are again used to specify the properties about the new complex entities, just defined. The same strategy is applied to environments that can be glued together. “*Diffusion boxes*” are used to intuitively add grouped entities to the environment through coloured box. Boxes can be dragged in order to define the diffusion area while the density is described by the *intensity* of the colour. At any time, the user has a direct outlook of all the grouped entities and of their position in the space (see figure 1).

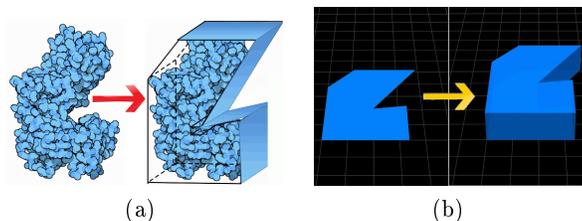


Fig. 2. (a) Hexokinase enzyme approximation to an entity and (b) Hexokinase generation through inflation

Third level - extension. At this level the user can generate his own environments and entities in order to create a very specific simulation. The entities creation phase can be carried out through the “inflatable icons” approach [9]: the user can draw a simple 2D form and then *inflate* it in order to create a 3D form (see figure 2). Inflation can be applied with different strengths to different portions of the 2D/3D entity to create particularly complex entities.

Also simulation environments can be generated through inflation. Moreover, the environments can be further characterised by defining specific behaviours of the walls w.r.t. contained entities. For instance, the user can specify that a type of entity can pass through a wall and *disappear* from the simulation (the so called “open boundaries”) or *reappear* on another wall. This flexibility allows to simu-

late particular case studies such as the section of a vein, in which a simulation wall “produces” entities (e.g. erythrocytes) and another “dissolves” them.

4 Conclusions and future work

In this short paper, we have presented the ongoing work on BIOSHAPE tool and we have shown how EUD techniques can be successfully applied to improve important aspects such as usability and flexibility.

The gentle slope technique guarantees that the user is not overcome with tool grain. Instead, it provides the user with the right means to gradually understand tool potentialities and to exploit them. Users can easily specify models with a high degree of personalisation (e.g. how entities interact, collide with other entities or with the defined boundaries) or they can create their own simulation assets. As a side effect, developers are set free from implementing all the possible simulation scenarios which would be difficult if not impossible.

Currently, a first version of the tool is under development. It includes some basic components - a cubic simulation environment, the distributed collision detection algorithm, the node coordination logic for distributed computation - and the first of the tree level presented. The second and third levels are also scheduled and we plan to integrate them in the next releases of BIOSHAPE.

References

1. Grupe, A., Germer, S., Usuka, J., Aud, D., Belknap, J.K., Klein, R.F., Ahluwalia, M.K., Higuchi, R., Peltz, G.: In silico mapping of complex disease-related traits in mice. *Science* **292** (2001) 1915–8
2. Manos, S., Zasada, S., Coveney, P.V.: Life or death decision-making: the medical case for large-scale, on-demand grid computing. *CTWatch Quarterly* **4** (2008) 1–8
3. Taylor, C.A., Draney, M.T., Ku, J.P., Parker, D., Steele, B.N., Wang, K., Zarins, C.K.: Biomedical paper predictive medicine: Computational techniques in therapeutic decision-making. *Computer Aided Surgery* **4** (1999) 231–247
4. Dix, A., Finlay, J.E., Abowd, G.D., Beale, R.: *Human-Computer Interaction* (3rd Edition). 3 edn. Prentice Hall (2003)
5. Buti, F., Cacciagrano, D., Corradini, F., Merelli, E., Tesei, L.: Bioshape: a spatial shape-based scale-independent simulation environment for biological systems. *Procedia CS* **1** (2010) 827–835
6. Lieberman, H., Paternò, F., Klann, M., Wulf, V.: End-User Development: An Emerging Paradigm. In Lieberman, H., Paternò, F., Wulf, V., eds.: *End User Development*. Volume 9 of *Human-Computer Interaction Series*. Springer Netherlands, Dordrecht (2006) 1–8
7. Mirtich, B.: V-clip: Fast and robust polyhedral collision detection. *ACM Trans. Graph.* **17** (1998) 177–208
8. Mørch, A. In: *Three Levels of End-User Tailoring: Customization, Integration, and Extension*. MIT Press, Cambridge, MA, USA (1997) 51–76
9. Repenning, A.: Inflatable icons: Diffusion-based interactive extrusion of 2d images into 3d models. *J. Graphics Tools* **10** (2005) 1–15