The BioDynaMo Project
A PLATFORM FOR COMPUTER SIMULATIONS OF BIOLOGICAL DYNAMICS

Leonard Johard · Lukas Breitwieser · Alberto Di Meglio · Marco Manca · Manuel Mazzara · Max Talanov

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Abstract This paper is a brief update on developments in the BioDynaMo project, a new platform for computer simulations for biological research. We will discuss the new capabilities of the simulator, important new concepts simulation methodology as well as its numerous applications to the computational biology and nanoscience communities.

Keywords Computer simulation, Biological development, Biological dynamics, Brain

1 Introduction

The BioDynaMo project aims at a general platform for computer simulations for biological research, and at closing the gap between very specialized applications and highly scalable systems, in order to give life scientists access to the rapidly growing computational resources. Scientific investigations require extensive computer resources, therefore modern platforms have to be executable on hybrid cloud computing systems, allowing for the efficient use of state-of-the-art computing technology.

In this paper we provide an overview of the project development, present the resulting simulator specifications, architecture and suggested applications. We will also provide the reader with a discussion on important topics such as code modernization and software verification and why these are of significance for the objectives of the bionano community.

2 Biological simulations

Biological systems (such as the human brain) comprise an extremely complex organization and heterogeneous interactions across different spatial and temporal scales. In particular, there is a growing interest in the interaction between processes on the molecular level and the emergent large-scale structures and behaviours. This interaction is bidirectional; we can estimate the effect of individual molecules on the overall growth of the tissue as well as make predictions on molecular processes used by cells based on the resulting structures.

This has given rise to a quick adaption of biological simulators as a research tool. We have developed a software architecture that is unique in its ability to handle full-scale simulations of developing cells in biological tissue. The field of computational biology covers a wide range of scientific topics, each producing many different scientific models [Bauer, 2014], [Freund, 2014] and [Izhikevich and Edelman, 2014].

Our particular simulator originated from ideas in the neurodevelopmental simulator Cortex3D, a tool able to grow sophisticated structures based on simple rules that can be defined by the neuroscientists [Zubler and Douglas, 2009]. It has been unique in its ability to move from cellular and molecular development principles into large neural structures aligned with experimental data.

Seeing the promises of this simulator approach, a consortium has been formed around CERN openlab in order to fully realize the potential. This collaboration between computer scientists and biologists has already resulted in several methodological developments for this branch of biological simulations.

The new software will handle generic cell dynamics such as cell motility, cell division, complex spatial
cell structures, communication with molecular gradients, simulated genetic expression and electrophysiology.

3 Modernized Simulator Code

High performance and high scalability are the very prerequisites to address ambitious research questions like modeling neural pathways and the effect of plasticity on structural changes. Like large amounts of research code today, Cortex3D was originally written by domain experts without direct input from computer scientists. Although well-structured, such code needs additional expertise to implement ideas from high-performance computing such as efficient vectorization and parallelization of the code.

Consequently, last years Intel Modern Code Development Challenge was about optimizing the sequential C++ brain simulation code. We showed that several such improvements of the simulation core is able to reduce the initial execution time from 45 hours down to eight and a half minutes. This clearly shows the economic potential of dedicated code modernization efforts.

In addition the BioDynaMo software is being designed to be run large-scale cloud simulations handling up to 10 million nodes. If our new design is indeed able to linearly scale up our initial results, this would allow simulation of substantial tissue such as a full-scale human cortex.

4 Scientific Software Verification

While, historically, the effort of software verification was mostly concerning safety-critical systems in automotive, transportation and aerospace industries – and in general where human lives are at stake – recently attention moved to more traditional, lower stake and off-the-shelf commercial (or not) software.

Computer simulations are not exempt from risks, although the concept of catastrophic has not to be seen in terms of direct, immediate life threats. Biological simulations can run on a single or multiple machines, or on the cloud, and run for a few minutes only or for hours or days. The computational costs, and the financial costs as a consequence can be considerable implying a significant loss in case of errors and need to re-run all or part of the simulation.

The extra effort required by the use of these tools is certainly not for free and comes with increased development costs [Meyer, 2009]. There are several approaches described in literature, and the list here cannot be exhaustive; for instance abstract interpretation [Cousot, 1977] and model checking [Clark, 1999], that seek the automation to formally proving certain conditions of systems.

However, the verification and validation of the software is paramount. The extraordinary risks arising when the correctness and validity of software tools for scientific research are not properly assessed is extensively documented [Eklund, 2016]. BioDynaMo will be one of the first simulators to seriously address the need for verification and redundancy required for reliable simulations of the required scale and complexity.

5 Discussion

The BioDynaMo project is bringing a new generation of simulator technology to the biological community. Our new simulation technology offers exciting new experimental capabilities to test and identify interaction between molecular and larger scales of biological processes. This is of obvious interest to many diverse research groups, with which we would like to connect for fine-tuning of the specification for the greatest possible combined utility for the planned upcoming developments in simulation methodology.

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