

2019-2020

## Proposta para Dissertação de Mestrado em Engenharia Informática

### Title:

*Massive Ray Tracing of Molecules with Millions of Atoms in the Image Space*

### Supervisor:

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### Abstract:

Simulation and rendering of molecules with millions of atoms is a great challenge in molecular graphics, a discipline that combines computer graphics and computational biology. The leading idea is to take advantage of the latest ray tracing techniques in the image space to render molecules with millions of atoms in real-time. Doing so, we will be able to realistically simulate the evolution of molecular conformations over time in the second timescale. We will take advantage of the  $\pi$ -surfaces invented in-house. This project will result in a very useful tool for biologists, chemists, and other scientists who deal with molecular structures, isolated or not, as, for example, in protein docking.

### Objectives

This work is in the cross of computer graphics and biology. The main objective is to develop algorithms for simulation and visualization of massive molecules and their conformations over time.

### Tasks:

This dissertation work will consist of the following tasks:

Task 1. The study of the main concepts behind molecules and their geometric representations.

Task 2. To write a brief survey about the algorithms and tools to visualize and render molecules.

Task 3. To implement an algorithm for ray tracing molecules using distinct geometric representations.

Task 4. To compare the algorithm against a few geometric representations.

Task 5. To write a paper to be submitted to a conference/journal, as well as the write-up of the dissertation.

## Timeline:

	2018					2019				
Task/month	set.	out.	nov.	dez.	jan.	fev.	mar.	abr.	mai.	jun.
<i>Task 1</i>										
<i>Task 2</i>										
<i>Task 3</i>										
<i>Task 4</i>										
<i>Task 5</i>										

## Pre-conditions:

First. The student must have skills in computer graphics.

Second. The student must have a 1<sup>st</sup> year complete with a minimum grade of 14/20.