3-D MODELING OF DIFFUSION LIMITED AGGREGATION (DLA) IN HYDRAULICS OF URINE

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Introduction

Diffusion Limited Aggregation (DLA) clusters are aggregates of particles, and the shape of the cluster is controlled by the possibility of particles to associate with other particles. The aggregates typically grow as long as there are particles moving around.

During diffusion of a particle through a solution it is more likely, that it attaches to the outer regions of the cluster. Thus, a solid shape with many dendritic structures, like corals or trees, is generated. The volume is not filled in its entirety, causing many gaps. The premise is that you have particles moving randomly (Brownian motion).

For crystals, we assume that when a particle hits a static structure, it sticks to it. In the most basic implementation, you start with a single fixed particle and add new particles in the manner described above one at a time. The process naturally forms branches structures as the extremities of the growth act to block particles from hitting the interior parts of the static structure.

Background

All biological processes that produce crystals are controlled in a semi solid environment. Hence, diffusion plays a vital role in various chemical compositions, temperature of the body, formation of tissues, tumors, and - more importantly - formation of certain crystals like oxalate crystals and fibrinogen crystals.

Tracking the growth of such a cluster is challenging because the surrounding medium is the controlling parameter for the growth or movement of the particle under investigation.

We started out with simulated tracking of one dimensional (1D) and 2D random movements of particles in the hydraulics of urine (programmed in C++ and openGL). Then we developed 2D DLA crystal simulations in Python.

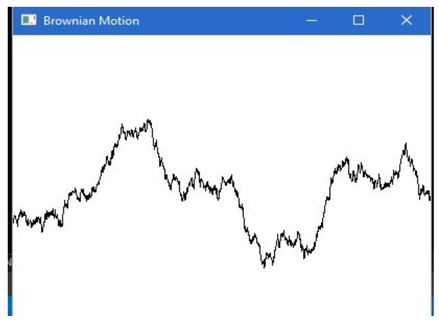
Purpose

The goal of the study is to implement existing simulation algorithms for modeling the hydraulics of urine in the programming languages C++ and openGL. Because of the computational complexity of those more advanced models, existing Python implementations are of limited value for high performance (parallel) computing.

Algorithm

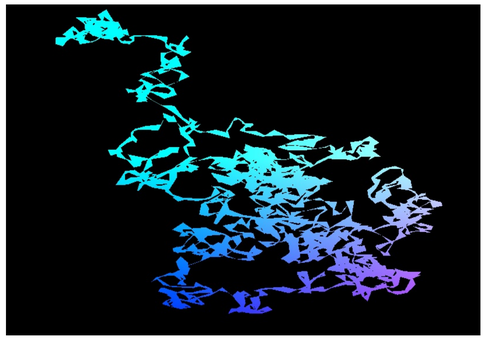
DLA Pseudo Code

```
Create a Blank Screen
Plot a dot in the center of Euclidean space
Repeat for a given number of particles:
    Place particle randomly in the simulation
    Repeat forever:
        If particle is within boundaries:
            If any pixel around particle isn't blank:
                Plot particle
                Break forever loop
            End If
        Else
            Limit particle's coordinates so it is inside the boundary
            Plot particle
            Break forever loop
        End If
        Move particle randomly
    End Loop
End Loop
```

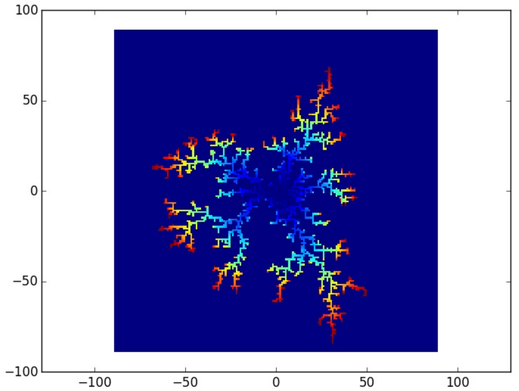


Example of 1D Brownian Motion. The random walk has been plotted for 2000 points.

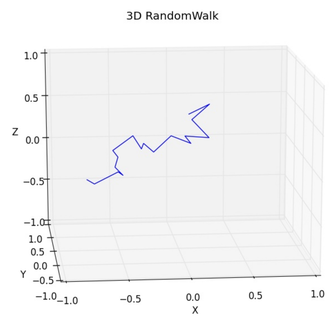
Outcome Illustrations



Example of 2D Brownian motion. Shaders have been introduced to make the tool feasible to scale and translate motion.



Example of 2D Diffusion Limited Aggregation (aggregation plotted for 5000 points).



An animation of a 3D random walk to simulate a particle's trajectory has been developed in Python using the matplotlib library. The intention is to provide a platform to develop 3D Diffusion Limited Aggregation in an animated series.

Discussion and Impact

For this project three dimensional (3D) simulation models have been programmed in C++ and openGL to study DLA clusters and possibly the crystals that are formed in the gout and pseudo gout regions.

Originally, we planned to program DLAs in three dimensions using openGL and C++. This approach proved to be too time consuming to develop a reasonable animation. (High performance computing techniques are required for those models due to their computational complexity.)

Visualizing and modeling complex crystals could help in medical technology to predict the growth of crystals with respect to time. This can help in informing therapy from surgery to drug dosage.

Our study can be extended to analyze any clusters that form in the human body. This ranges from formation of tumor cells to the study of intercellular crystals such as protein clusters.

References:

1. F.L. Braga, M.S. Ribeiro, Diffusion Limited Aggregation: Algorithm optimized revisited Computer Physics Communications 182(2011) 1602-1605.
2. Tamás Viczek, Fractal growth phenomena, World Scientific Publishing Co, 1989, Singapore.
3. T. A. Witten, L. M. Sander: Diffusion-Limited Aggregation, a Kinetic Critical Phenomenon, Phys. Rev. Lett. 47, N 19, 1981
4. https://github.com/nervoussystem retrieved 15 April 2016.

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