University of Ljubljana
Faculty of Computer and
Information Science

FRI Advanced Computer Graphics course 2023
Project report

Generating Organic Structures with Reaction-Diffusion

Tim Vučina

Abstract

This report investigates computational modeling and visualization of Turing pattern-inspired reaction-diffusion systems. Despite yielding some promising results, the study encountered challenges such as grid resolution limitations and instability of generated structures. Potential improvements, including integrating environmental factors, branching parameter enhancements, and algorithmic advancements like adaptive grid refinement are suggested. This multidisciplinary study signifies the potential for further research in this advancing computational field.

Keywords

Reaction-Diffusion Systems, Computational Modeling, Turing Pattern Formation

Advisors: Žiga Lesar

1. Introduction

Reaction-diffusion systems, mathematical models representing the process through which chemical reactions propagate, have become a cornerstone in the field of computational modeling. Originally utilized to illustrate natural processes, such as patterns formation on animal skins or the growth of coral, these systems have found an extended application in a variety of computational graphics and simulations due to their ability to generate diverse and organic structures [1]. However, the primary focus of computational models has largely been limited to 2D systems, with 3D models remaining a largely untapped field.

For this project, the original assignment tasked us with converting 2D textures generated by reaction-diffusion into 3D geometrical representations through methods such as extrusion. This process, although intriguing, appeared less challenging than the alternative approach that we decided to undertake. Instead, we resolved to explore the process of directly generating 3D structures based on a 3D reaction-diffusion model. This route, albeit more complex, was selected due to the appeal of the novel challenges it presented, and the potential rewards of developing a comprehensive solution.

Our final product, a functional add-on for the Blender 3D software, generates intricate, organic structures. Despite the inherent intricacy of simulating reaction-diffusion in a 3D environment, and the accompanying computational power required, the add-on effectively models reaction-diffusion and uses the results to create complex structures.

Despite its potential utility in fields such as 3D modeling, biology, and computer graphics, there is a surprising lack of similar 3D based reaction-diffusion models available. Our research unveiled only a handful of attempts at similar programs [2], highlighting a need for more exploration within this area.

In essence, reaction-diffusion systems are mathematical models that simulate how substances react and diffuse in space over time. This process creates intricate, organic, and diverse patterns that can be utilized in a plethora of computational and graphical applications. The intent of this project is to delve into the application of these systems in a 3D context, a less-explored but promising area of study.

2. Reaction-Diffusion

2.1 Theory

The fundamental theory of reaction-diffusion systems was initially introduced by (who would have guessed it) the British mathematician and logician Alan Turing [3]. It models two key processes: a reaction in which substances are transformed into each other, and diffusion which spreads the substances in space.

The most common reaction-diffusion system, known as the Gray-Scott model, is governed by the following equations:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F(1-u) \tag{1}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (F+k)v \tag{2}$$

In these equations, u and v are the concentrations of two chemical species. $\nabla^2 u$ and $\nabla^2 v$ represent the Laplacian, which is the diffusion of u and v respectively. D_u and D_v are the rates of diffusion of u and v, while F is the feed rate, and k is the kill rate.

In this model, u and v react to produce more v. v is then transformed back into u with the rate controlled by F and k. Different parameters and initial conditions can produce a wide variety of patterns.

2.2 2D vs 3D

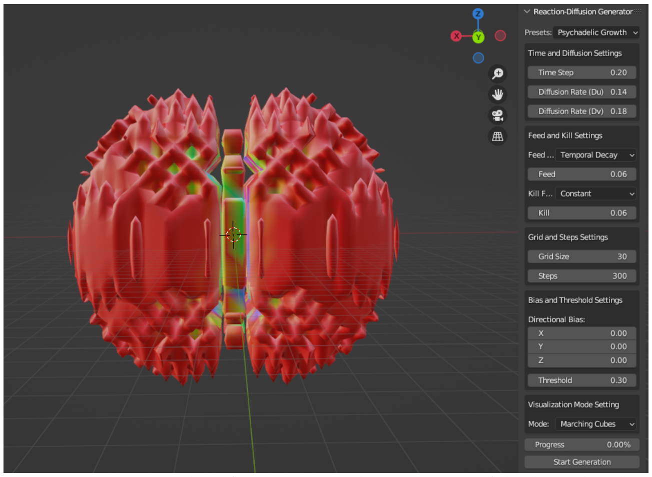
The predominant usage of reaction-diffusion systems in computational graphics and simulations focuses on two-dimensional environments. These 2D systems, while effective in generating intricate and diverse patterns, offer a relatively simplified representation of diffusion and reaction processes.

The extension from 2D to 3D reaction-diffusion systems introduces an additional dimension of complexity. In 3D environments, diffusion and reactions occur in a volumetric space, expanding the spatial interactions and creating a richer set of patterns. However, the increase in computational load is substantial as the volume of the processed data scales cubically with the size of the domain.

While this complexity introduces challenges in computation time and resources, it also provides more realistic models for many natural phenomena. Furthermore, the 3D structures generated could potentially offer novel insights and tools in the fields of computer graphics, biology, and materials science, among others.

3. Implementation

Our implementation involves creating a Blender add-on for simulating 3D reaction-diffusion. We focused on experimentation, trying out various techniques to gain control over the model's behavior and better understand the complexities of 3D reaction-diffusion.



Reaction-Diffusion Generator

Presets: Psychadelic Growth

Time and Diffusion Settings

Time Step 0.20

Diffusion Rate (Du) 0.14

Diffusion Rate (Dv) 0.18

Feed and Kill Settings

Feed ... Temporal Decay

Feed 0.06

Kill F... Constant

Kill 0.06

Grid and Steps Settings

Grid Size 30

Steps 300

Bias and Threshold Settings

Directional Bias:

X 0.00

Y 0.00

Z 0.00

Threshold 0.30

Visualization Mode Setting

Mode: Marching Cubes

Progress 0.00%

Figure 1. Example of a generated structure with the Blender add-on

3.1 Blender add-on

The Blender add-on was designed to be user-friendly and flexible, with adjustable parameters for tuning the simulation. The core functionality revolves around the update of chemical concentrations u and v and the Laplacian computation, a critical component of the Gray-Scott model.

We introduce bias into the system to direct the growth. This bias is added to the u concentrations before using it for updating concentrations. Moreover, the add-on includes the ability to compute new feed rate F and kill rate k values, which are fundamental parameters in the Gray-Scott equations.

In addition to these features, the Blender add-on provides a diverse range of options for customization, reflecting the multiplicity of outcomes possible with reaction-diffusion systems. Among these are a set of predefined presets, which allow for the rapid generation of complex forms reminiscent of natural structures, such as coral, a wasp nest, or a brain.

Furthermore, the add-on allows for a wide variety of parameter adjustments. For instance, users can manipulate the time step (dt), diffusion rates (Du, Dv), feed and kill rates (F, k), and introduce a directional bias into the system. The feed and kill rates can be determined by a constant value, a spatial gradient, a temporal decay function, or a spatiotemporal wave function.

These features enhance the adaptability of the model to different circumstances, providing a customizable and flexible tool for exploring the Gray-Scott model. The grid size (N) and the number of simulation steps (steps) are also adjustable, allowing users to control the scale and duration of the simulation.

3.2 Visualizations

Visualisation of the reaction-diffusion system is implemented through the construction of three-dimensional meshes from the generated grid of values. Three different methods are utilized: Metaball (MBALL), Voxel, and Marching Cubes (MC), each offering a unique visual interpretation of the system.

The function `create_mesh_from_grid` serves as the primary interface for mesh creation. It handles thresholding, checks validity of the input grid, and delegates the creation of meshes to the appropriate methods depending on the mode specified.

The `create_mesh_MBALL` function forms a Metaball object, utilizing metaball elements to represent each point in the grid that exceeds a given threshold. The position and radius of each element is determined based on the grid coordinates and their corresponding value. The Metaball object is then converted into a mesh.

In the `create_mesh_VOXEL` function, the voxel technique is utilized. For each grid coordinate with a value surpassing the threshold, a cube is created and positioned correspondingly. This results in a voxelated representation of the grid.

The `create_mesh_MC` function utilizes the Marching Cubes algorithm to obtain a smooth, continuous surface representation of the grid values. This is a more computationally intensive approach but can provide a higher fidelity visualization. This method first creates vertices and faces based on the algorithm, and then applies these to a new mesh.

Subsequently, the `apply_vertex_colors` function is used to apply vertex colors to the created meshes, and the `add_vertex_color_material` function assigns a material that uses these vertex colors. These two functions together enable the application of a color gradient to the visual representation, providing a more discernible distinction between different value regions.

Lastly, the `animate_object` function is used to animate the visibility of the mesh objects across frames. This facilitates the creation of an animation sequence which illustrates the progression of the reaction-diffusion system over time.

These visualization techniques provide an essential tool for the intuitive interpretation of the reaction-diffusion system, allowing for the identification of patterns and emergent structures.

3.3 Methods

A set of methods are provided to facilitate various operations during the execution of the simulation. The Laplacian operation, which calculates the diffusion of the chemicals, is performed using a 3D convolution with a specially designed kernel.

We initialize the grid with certain mean and standard deviations for u and v, and the values of v are set to 1 at the center to kick start the reaction. A bias grid is created based on the provided bias direction and magnitude, which can be used to guide the formation of patterns.

Another key feature of our implementation is the capability to modify the parameters U and V concentrations in accordance with time and spatial coordinates. This is facilitated by the inclusion of a set of functions each designed to provide a unique variation of the parameters over time and space.

The `compute_constant` function, as the name suggests, simply returns the initial parameter, which implies a constant distribution of the substances over time and space.

The `compute_spatial_gradient` function facilitates spatial variance. It calculates the Euclidean distance from the center of the grid for each cell, scales this to a value between 0 and 1, and uses this gradient to adjust the initial parameter. Thus, the parameters increase based on the distance from the center, allowing for a radial gradient in the parameters.

The `compute_temporal_decay` function applies temporal variance by reducing the parameter over time, following an exponential decay model. This results in parameters that decrease as time passes, introducing a temporal decay effect.

Lastly, the `compute_spatiotemporal_wave` function allows for both spatial and temporal variance. It computes a wave pattern over time and space by taking into account the distance from the center and the time variable. This function results in parameters that change following a sinusoidal wave pattern over both time and space.

These features provide additional control over the reaction-diffusion system, allowing for a more diverse range of patterns and behaviors.

3.4 Experimentation

During the development of this add-on, we experimented with several techniques to gain more control over the behavior of the model and understand the nuances of simulating reaction-diffusion in 3D.

Some of these experiments included adding gradients of substances, employing different initialization techniques, introducing agents that move along the gradients of substances, and simulating light sources. Despite these efforts, the attempts were not included in the final version of the Blender add-on as they often made the system less predictable and more difficult to control.

Additionally, the task of extrapolating 2D parameters such as the Laplacian kernels for convolution into 3D proved to be challenging. Nonetheless, these explorations helped in enriching our understanding of 3D reaction-diffusion systems.

4. Results

4.1 Difficulties

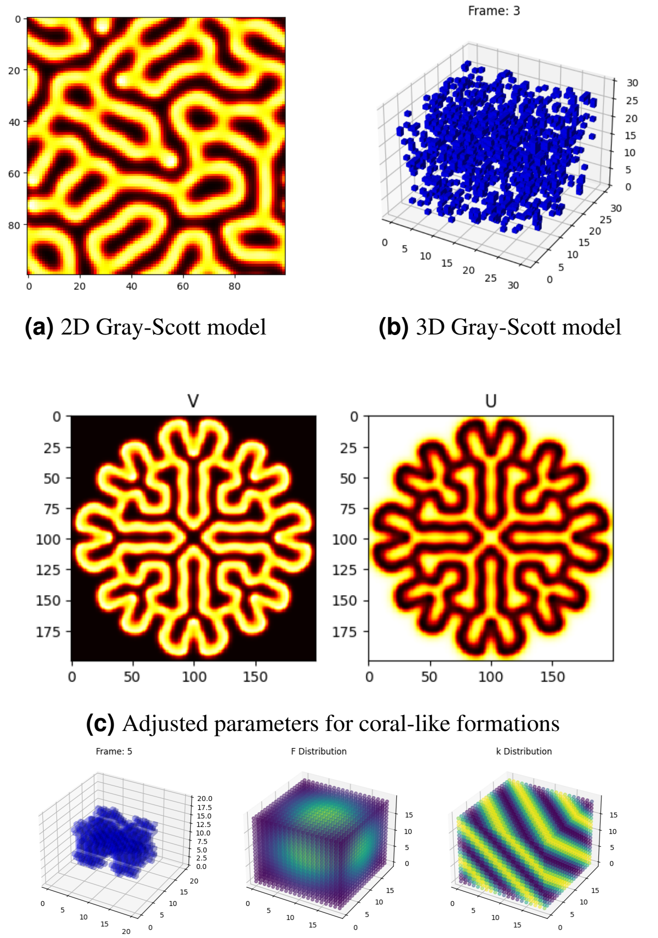
While the visualization of the reaction-diffusion system provided some intriguing results, the process was not without its challenges. One major difficulty was associated with the resolution of the generated grid. High grid resolution is necessary to capture the intricate details of the structures formed by the reaction-diffusion system, yet rendering at such resolutions was a challenge due to computational limitations.

Another significant issue was the instability of the generated structures. They often displayed unpredictable behaviours, such as flickering and disappearance over time steps. This instability is indicative of the inherent challenges of modeling complex biological and chemical systems. It was found that the reaction-diffusion system would occasionally converge into a state where concentrations of the morphogens became zero across the entire grid, resulting in the apparent disappearance of structures.

4.2 Possible Improvements

There are several potential improvements that could be made to the reaction-diffusion system to yield more consistent and realistic results. The incorporation of additional environmental factors such as light intensity, wind speed, gravity, surface area, and object weight into the mathematical model could provide a more holistic representation of the system. These factors would introduce additional complexity and variability, potentially leading to more diverse and realistic structures.

Another avenue for improvement lies in enhancing the branching parameter of the system. By allowing for more controlled and intricate branching patterns, the model could



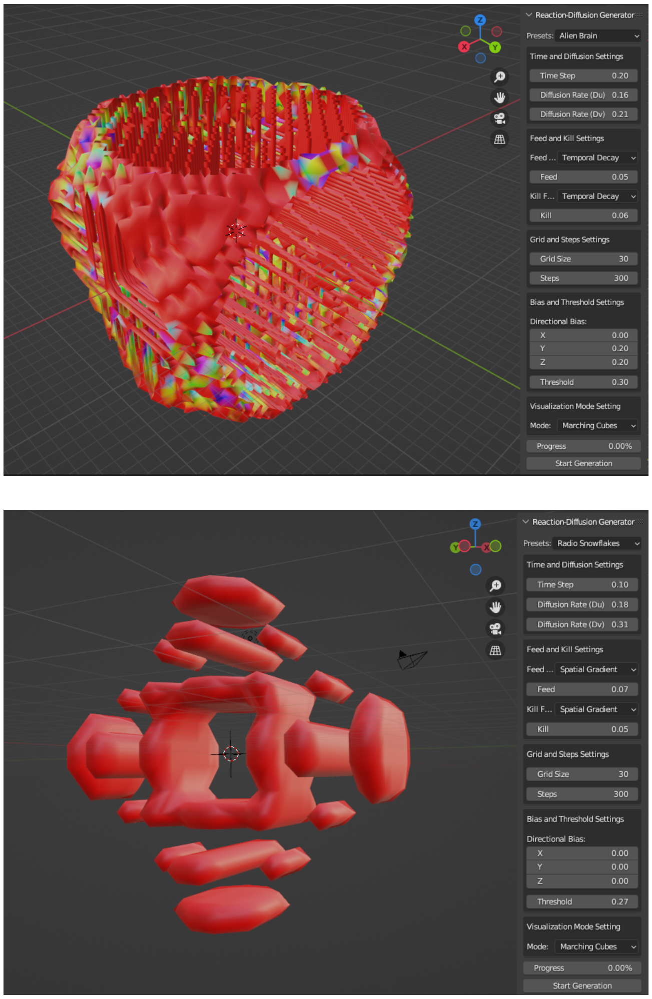
(a) 2D Gray-Scott model

(b) 3D Gray-Scott model

(c) Adjusted parameters for coral-like formations

(d) 3D extrapolation of the coral parameters with added spatial and temporal dependent concentrations

Figure 2. Examples of experimentation results



Reaction-Diffusion Generator
Presets: Alien Brain
Time and Diffusion Settings
Time Step 0.20
Diffusion Rate (Du) 0.16
Diffusion Rate (Dv) 0.21
Feed and Kill Settings
Feed ... Temporal Decay
Feed 0.05
Kill F... Temporal Decay
Kill 0.06
Grid and Steps Settings
Grid Size 30
Steps 300
Bias and Threshold Settings
Directional Bias:
X 0.00
Y 0.20
Z 0.20
Threshold 0.30
Visualization Mode Setting
Mode: Marching Cubes
Progress 0.00%
Start Generation

Reaction-Diffusion Generator
Presets: Radio Snowflakes
Time and Diffusion Settings
Time Step 0.10
Diffusion Rate (Du) 0.18
Diffusion Rate (Dv) 0.31
Feed and Kill Settings
Feed ... Spatial Gradient
Feed 0.07
Kill F... Spatial Gradient
Kill 0.05
Grid and Steps Settings
Grid Size 30
Steps 300
Bias and Threshold Settings
Directional Bias:
X 0.00
Y 0.00
Z 0.00
Threshold 0.27
Visualization Mode Setting
Mode: Marching Cubes
Progress 0.00%
Start Generation

Figure 3. Examples of interesting generated structures

produce structures with greater fidelity to real-world phenomena.

From an algorithmic perspective, introducing adaptive grid refinement could prove beneficial. By locally increasing the resolution of the grid where intricate structures are forming, it might be possible to capture finer details while reducing the overall computational burden.

Finally, utilizing a more advanced numerical method for solving the differential equations, such as a higher-order Runge-Kutta method or an adaptive time stepping approach, could potentially mitigate the instability issues observed in the generated structures.

5. Conclusion

The study of reaction-diffusion systems, through computational modeling and visualization, provides a fascinating lens through which to explore the complex patterns and structures found in nature. While the results obtained in this work were promising, the findings also highlighted the inherent challenges of this endeavor. From the limitations of grid resolution and the instability of generated structures, to the complex interplay of various environmental variables, this work underscores the multifaceted nature of modeling natural systems.

Nevertheless, the potential for improvements and the avenues for further research are abundant. Whether it be through the incorporation of additional environmental factors, enhancement of the branching parameter, or advances in the numerical methods used, the path towards a more refined and accurate model of reaction-diffusion systems is a rich and promising one.

These challenges and the suggested improvements underscore the importance of an interdisciplinary approach, drawing from fields such as computer science, biology, mathematics, and physics. As computational power continues to grow, it is anticipated that the modeling and visualization of reaction-diffusion systems will become increasingly intricate and accurate, thereby enhancing our understanding of these remarkable systems and the natural phenomena they represent.

References

[1] Greg Turk. "Generating textures on arbitrary surfaces using reaction-diffusion". In: *Acm Siggraph Computer Graphics* 25.4 (1991), pp. 289–298.

[2] Greg Cope. *Reaction Diffusion in 3-Dimensions — algosome.com*. https://www.algosome.com/articles/reaction-diffusion-gray-scott-3d.html. [Accessed 26-May-2023].

[3] Alan Mathison Turing. "The chemical basis of morphogenesis". In: *Bulletin of mathematical biology* 52.1-2 (1952), pp. 153–197.