Discussing the use of reaction diffusion equations for the simulation of physical phenomena

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Extended Essay

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Words:

Contents

1 Introduction

Reaction Diffusion equations are a type of equations with a wide range of uses and applications. They allow for the modeling of the iterations between objects throughout space while passing through time. In other words, they track the relationship between things over time as they spread and affect other things. This clearly is not a technical definition but it serves to understand their purpose. It should be evident from the generality of their purpose that their uses are equally universal. As the name implies, they have two 'components' or sections of the equation: the reaction and the diffusion. The reaction serves as the relation between objects and the diffusion is the spacial component. The goal of this paper is to visually and intuitively explain the diffusion and reaction components and to eventually tie them together to show the complex and emergent behavior of Reaction Diffusion systems.

The thing that the Reaction Diffusion takes and manipulates or the 'object' previously referred to is a concentration variable, and the goal is to morph a concentration space. So they pass in a field of values and returns a field or matrix of modified values. One way to think

about the Reaction Diffusion is that there is a reaction that spreads getting more 'fuel' to continue the reaction. The balance between new fuel and using up the fuel is what generates these patterns. Another examples of this sort of reaction is a disease that starts with one person and spreads based off of who touched it and stops when everyone has recovered or died. Given the parameters of the equation there are a variety of intuitive explanations with different levels of accuracy or mathematical formality.

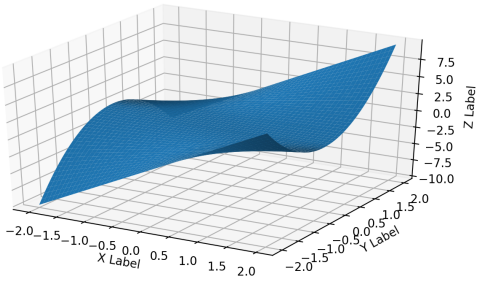
2 Calculus

Reaction diffusion relies on multi-variable calculus, from the partial derivative to the Laplacian operator that governs diffusion. Multi is a natural extension of calculus where instead of focusing on the accumulation or change on 1 axis, that normally being y, it is possible to run the calculus operations for any number of dimensions. This means that if a function has more than 1 input, like for 3D functions, there is a whole new arsenal of tools and methods to analyze these equations. The limit which fundamentally operates the same as in the

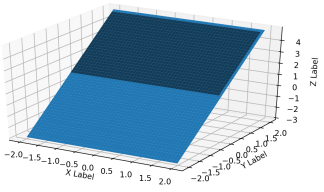
2 dimensional case. If there is a hole in the function it would 'fill in' that hole, and if there is a jump discontinuity the limit is defined for certain directions as it approaches the discontinuity but the limit itself is undefined. Once again, integral and derivative can be derived from the limits as in normal calculus; however, this application will be primarily focusing on partial derivatives and other related operations. Instead derivatives in multivariate partial derivatives are used. These are computed in a similar form to derivatives but the inputs that are not differentiated is treated as a constant. For use in the reaction equations the partial differential equations behave in a similar way to differential equations except they have more inputs, but are still give the rate of change for a given input over a function.

$$\frac{\partial f}{\partial x} = \partial_x f = \lim_{h \to 0} \frac{f(x+h, y) - f(x, y)}{h} \tag{1}$$

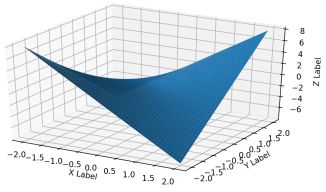
$$\frac{\partial f}{\partial y} = \partial_y f = \lim_{h \to 0} \frac{f(x, y+h) - f(x, y)}{h} \tag{2}$$



(a) $f(x, y) = xy^2 + x$



(b) $\partial_x f(x, y) = y^2 + 1$



(c) $\partial_y f(x, y) = 2xy$

Figure 1: Example functions

Example problem

$$f(x, y) = xy^2 + x$$
$$\partial_x f(x, y) = y^2 + 1$$
$$\partial_y f(x, y) = 2xy$$

Then there are directional derivatives which are similar to the partial derivatives, but instead of being in a component direction like along the x or y direction it would be in the direction of an arbitrary vector $\vec{u}$ with components $< a, b >$. These derivatives can be done

in any number of dimensions (3) but for reaction diffusion formulas shown 2D cases (4) matter more.

$$D_u f(\vec{x}) = \lim_{h \to 0} \frac{f(\vec{x} + hu) - f(\vec{x})}{h} \tag{3}$$

$$D_u f = \lim_{h \to 0} \frac{f(x + ha, y + hb) - f(x, y)}{h} \tag{4}$$

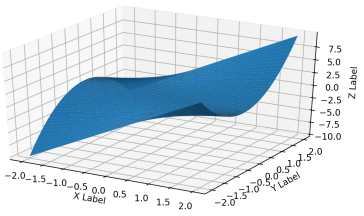
The directional derivative can also be written as a dot products.

$$\begin{aligned} D_u f(x, y) &= a\partial_x f + b\partial_y f \\ &= < \partial_x f, \partial_y f > * < a, b > \\ &= < \partial_x f, \partial_y f > * u \\ &= \nabla f(x, y) * u \end{aligned}$$

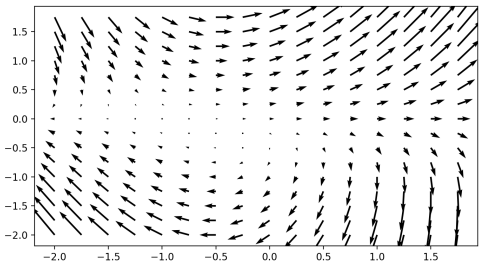
This ∇, or nabla, is the sign for the grad operator. This represents a vector of all of the partial derivatives for all of the function inputs, which is called the gradient. For example in $g(x, y, z)$, the gradient of g is the vector where each component is the partial derivative of g for its inputs x, y, and z. This gradient points in the direction of the 'fastest increase' of the function. So if we had a map of a mountain

range the gradient of the map from a point would be the fastest way to get to the top of the nearest mountain but not necessarily the highest mountain. The gradient is often used for optimization problems since it can go 'the highest' or local maxima in a function of any number of variables. A common abuse of notation is to set ∇ to a value (5)

$$\begin{aligned} \nabla &= < \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} > \\ &= \sum_{i=1}^{n} \vec{e}_i \frac{\partial}{\partial x_i} \end{aligned} \tag{5}$$



(a) $f(x, y) = xy^2 + x$



(b) the gradient vector field: $\nabla * f(x, y)$

So the notation for the gradient makes sense because you would be treating the function f as a scalar and multiplying it with the ∇ vector. This abuse of notation since it would also make sense for the divergence of a vector field. For a vector field the function $\mathbf{F}$ (6) would be a vector function where you could dot product of $\mathbf{F}$ and ∇ (7)

$$\mathbf{F} = P\hat{\imath} + Q\hat{\jmath} + R\hat{k} \tag{6}$$

$$div\,\mathbf{F} = \nabla * \mathbf{F} = \frac{\partial P}{\partial x} + \frac{\partial Q}{\partial y} + \frac{\partial R}{\partial z} \tag{7}$$

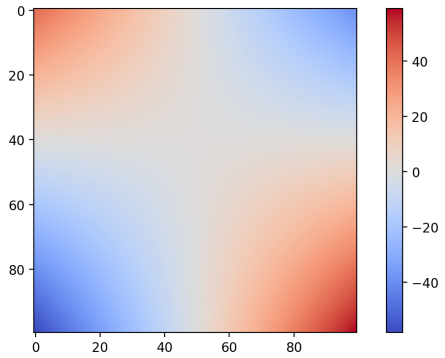


Figure 3: the gradient vector field: $\nabla * f(x, y)$

One can picture a vector field as being a model of fluid flow, where the vector at a point would be the velocity of the fluid. Given this analogy, the divergence is the rate that the fluid speeds up at a point. The divergence if positive when fluid 'speeds up' and negative if it 'slows down'. In a vector field represented by all of the arrows pointing away from the origin and the arrows get larger around a point than the divergence > 0 and if the arrows are smaller or point to the origin than the divergence < 0. Both of these tools are useful but when applied together become what is needed for the diffusion part

of reaction diffusion that being the laplacian. The laplacian (8) is the divergence of the gradient of a function.

$$\begin{aligned} \nabla^2 f &= \nabla * (\nabla f) \\ &= \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \\ &= \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2} \end{aligned} \tag{8}$$

This is called the Laplace operator or the Laplacian of a field because of its relation to Laplace's Equation which has similarities to the heat transfer equation for diffusion. The reason that when put in PDEs they exhibit this diffusion or spreading property is due to their relation to the second derivative in normal calculus. They identify local maxima and minima but in normal calculus where the second derivative is 0 in both cases the laplacian is highly positive in minima and highly negative in maxima. This makes sense because the laplacian is the sum of second partial derivatives for all of the function's inputs. In the case of partial derivative equations (PDEs), the laplacian 'fills in' the minima and 'pushes down' the maxima. This process is what drives osmosis and heat diffusion.

$$\nabla^2 \mathbf{F} = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 0 \tag{9}$$

Equations that satisfies Laplace's Equation (9) are called harmonic functions where at all points the value of the laplacian equals 0

3 Diffusion

Diffusion is the spread of things from high to low densities. A simple example would be heat or osmosis in cells. In general this is seen as spreading out. The mathematical way this is described is through a partial differential equation using the Laplace operator, ∇^2.

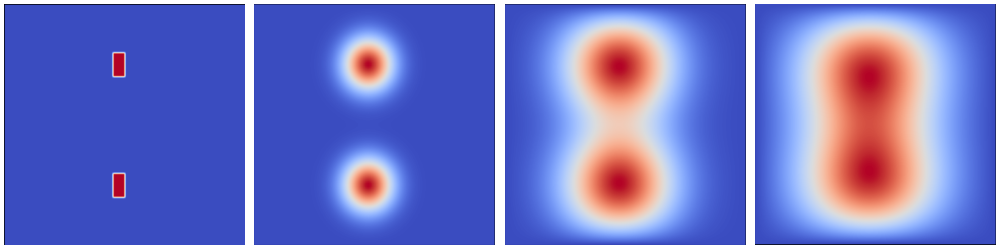
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u \tag{10}$$

$$\frac{\partial u}{\partial t} = \alpha(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}) \tag{11}$$

Equation 10 is a simple partial differential equation that has $u(x, y, z)$ to determine the heat and α as the coefficient of thermal

diffusivity. Because of the Laplace operator, the equation does not need to show its inputs which also allows for a N-dimensional continuation. In 3 dimensions, this equation can be expanded into equation 11.

Figure 4: Heat Diffusion Progression



(a) $n = 0$ (b) $n = 1000$ (c) $n = 5000$ (d) $n = 8000$

Fig. 5 shows the progression from 2 point sources of heat that spread out, diffuse and then eventually merge into a single blob that would continue to spread throughout the plane.

The heat diffusion equation (10) uses the laplacian which "pushes" the local maxima down and the local minima up. Later in the reaction diffusion equations, the laplacian is used to give the equations properties based off their location and physical proximity to other elements. This diffusion component gives reaction diffusion equations their interesting properties since previously converging reactionary systems remain in this possibly unstable equilibrium. The reason for this is

that the reactions, spreading due to diffusion, would encounter more fuel as they go until they eventually 'run out', then generating some homeostasis.

4 Reaction

There things called "reaction systems" that typically contain multiple ordinary or partial differential equations. Where diffusion equations usually have only one variable, reaction systems are often multi-variable. There are many different examples of reaction systems, and this paper is going to focus on the logistic equation and SIR and Lotka-Volterra models.

The most simple and generally recognized ordinary differential equation reaction system, especially relating to population, would be the logistic equation (12) which is a 1 component system that shows the growth and maximum population of an area.

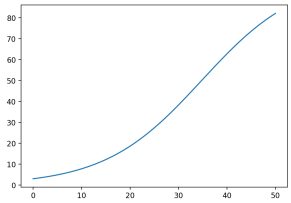
4.1 Logistic Equation

$$\frac{dP}{dt} = rP(1 - \frac{P}{K}) \tag{12}$$

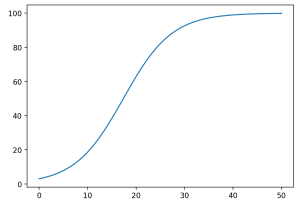
r is the growth rate

K is the carrying capacity

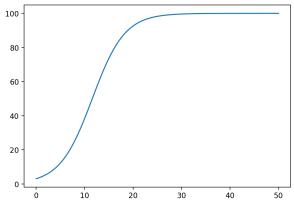
Figure 5: Logistic equation $p_0 = 3$ $k = 100$



(a) $r = 0.1$



(b) $r = 0.2$



(c) $r = 0.3$

This is the equation that describes the S-curve of growth and decay of population growth. rP is the unencumbered growth rate of the population that is clearly proportional to the current population. $1 - \frac{P}{K}$ is the limiting factor for the logistic equation. As your population approaches the carrying capacity the growth slows, so the point they are equal and there is no more growth. If the population increases over the carrying capacity it also pulls the population back into equilibrium This equation was originally generated for describing Malthusian population growth, and was later rediscovered a number of times. An examples of the use of the logistic equation is in modeling of tumor growth (Foryś and Marciniak-Czochra, 2003).

4.2 Lotka-Volterra Model

$$\begin{aligned} \frac{dx}{dt} &= \alpha x - \beta xy \\ \frac{dy}{dt} &= -\gamma y + \delta xy \end{aligned} \tag{13}$$

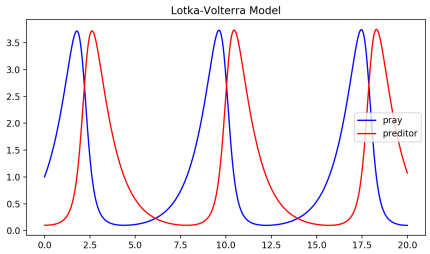
α is the intrinsic rate of pray population growth

β is predation rate coefficient

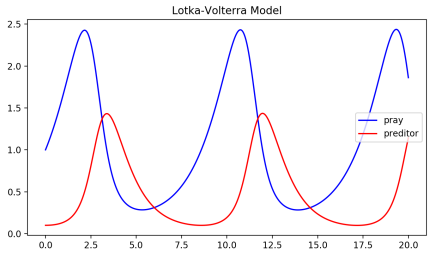
γ is the predator mortality rate.

δ is reproductive rate of the predators per pray eaten

Figure 6: Examples of the Lotka-Volterra Model



(a) $\alpha = \beta = \gamma = \delta = 1$



(b) $\alpha = \frac{2}{3}, \beta = \frac{4}{3}, \gamma = 1, \delta = 1$

Another, and more complex, reaction system is the Lotka-Volterra model (13). This is used to model the populations of predators and pray as they grow and shrink in a cyclical manner, making it a 2 component system, in the case x for prey and y for predators. This is one of the earliest Predator-Pray models based on sound mathematical principles. There are some problems with such a simple model, but the biggest issue is in reality populations reach an equilibrium but this model is cyclic; however, there are also cases were there is a cyclic growth off to infinity becoming unstable (Zhong et al., 1999). These issues mainly come from a lack of gender differences, size effects like overpopulation and resources, and a variety of outside influences. That

is why this is only used to describe specific predator-prey examples like hare and lynx populations. The benefit of such a simple model is the simple explanation. For prey, αx is clearly the unencumbered growth rate and $-\beta xy$ is the rate of predation that is influenced by the size of both the predator and prey populations. The predators explanation is a little more complicated. For predators, the δxy is the increase in predator population given that each predator reproduces at a rate δ per prey eaten; such that, each predator eats all the prey and produces proportional to that. The $-\gamma y$ is simply the mortality rate for the predators.

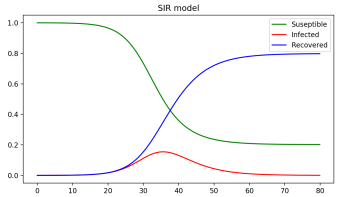
4.3 SIR Model

$$\begin{aligned} \frac{dS}{dt} &= -\beta si \\ \frac{dI}{dt} &= \beta si - \kappa r \\ \frac{dR}{dt} &= \kappa r \end{aligned} \tag{14}$$

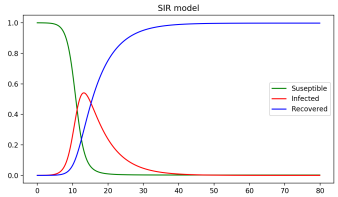
κ is the number of days until recovery

β is the number of days needed to be in contact to spread

Figure 7: Examples of SIR model



(a) $\kappa = \frac{1}{3}, \beta = \frac{1}{2}$



(b) $\kappa = \frac{1}{6}, \beta = 1$

The SIR model (14), or Susceptible-Infected-Recovered Model, is a computational epidemiology and serves as the core of other more advanced models, despite already having 3 components. This model is fairly intuitive. The susceptible equation is similar to the predation in the Lotka-Volterra Model, were the population decreases by the rate of spread times the infected and the susceptible $-\beta si$. That means that if the size of the infected or susceptible populations are low, then there are few new cases of illness. The recovering is simply decreasing by the recovery rate times infected κr. Then, the infected change is equal to the number gained of new infected minus the number lost who recovered $\beta si - \kappa r$. In figure 7a it shows a normal illness if no strong where in a small population similar to a school there is a wave that infect most people but is not an epidemic. Then, figure 7b is an example of an epidemic.

5 Reaction Diffusion

$$\frac{\partial \vec{q}}{\partial t} = -\underline{\underline{\mathbf{D}}}\nabla^2\vec{q} + R(\vec{q}) \tag{15}$$

$\underline{\underline{\mathbf{D}}}$ is a diagonalized weight matrix
$\vec{q}$ is a vector of inputs given a time
$R(\vec{q})$ is a function that takes into account local reactions

Reaction Diffusion is then the merger of diffusion and reaction systems, with emergent properties. The generalized formula (15) works in any number of dimensions and with any number of components. To limit algorithmic complexity, the 1 and 2 dimensional cases will be focused on. The $R(\vec{q})$ is a vector equation that represents the reaction systems described in section 4. To complete the name, the $\underline{\underline{\mathbf{D}}}\nabla^2\vec{q}$ then represents the diffusion for any number of dimensions, exactly like heat diffusion described in section 3.

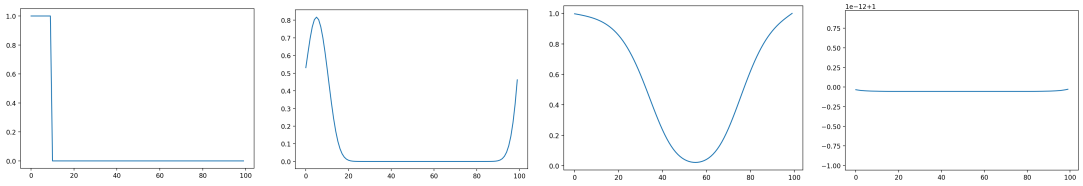
5.1 Fisher's equation

The first reaction diffusion system is Fisher's equation (16) which is a 1 component, 1 dimensional system that represents the wave front switching between equilibrium states, such as a switch of dominate

traits (R.A.Fisher, 1937).

$$\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2} = ur(1-u) \tag{16}$$

Figure 8: Fisher Equation Example



(a) $t = 0$ (b) $t = 50$ (c) $t = 500$ (d) $t = 10000$

The Fisher equation (16) is related to the logistic equation (12) previously described. The logistic equation can be thought of as the $R(\vec{q})$ given in the generalized reaction diffusion equation (15) and the $\frac{\partial^2 u}{\partial t^2}$ is the $-\underline{\underline{\mathbf{D}}}\nabla^2\vec{q}$ of the general form. The fisher equation is not as generalized as the logistic equation since the "carrying capacity" is 1; however, these equations are still useful for illustrating the relation between reaction and reaction-diffusion systems.

5.2 Cahn-Hilliard

$$\begin{aligned} \frac{\partial c}{\partial t} &= D\nabla^2(c^3 - c - \gamma\nabla^2 c) \\ &= D\nabla^2\mu \end{aligned} \tag{17}$$

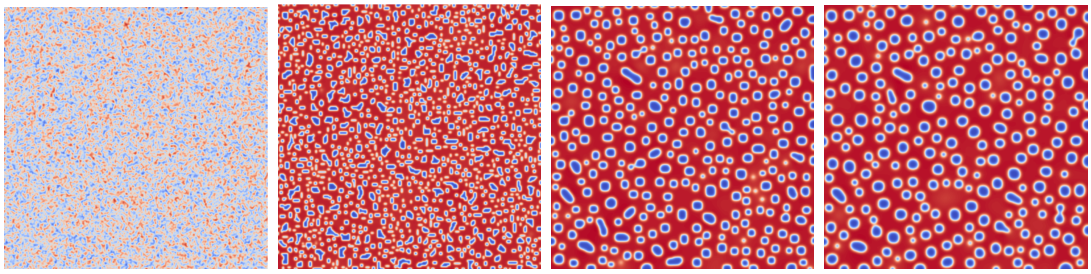
c is the concentration of the liquid

D is the diffusion coefficient

$\sqrt{\gamma}$ is the length of the transition regions between the domain

$\mu = (c^3 - c - \gamma\nabla^2 c)$ is the called the chemical potential

Figure 9: Cahn-Hilliard Examples at $t = 2000$



(a) Initial Seed (b) $\gamma = 0.125$ (c) $\gamma = 0.375$ (d) $\gamma = 0.5$

The Cahn-Hilliard equation (17) is a 1 component, N dimensional system related to phase separation (Cahn and Hilliard, 1958). Where fisher's equation (16) is about the phase transition in 1 dimension, which is a wave, the Cahn-Hilliard equation can be used to describe the phase transition on a plane or any space, $\mathbb{R}^n$. This system can be applied to a multitude of uses, a theme of reaction diffusion equations.

One such use is in high-strength alloys (F. J. Vermolen, 2009). An intuitive way of thinking about this process despite losing some of the generality is thinking about the Cahn-Hilliard equation is as the interaction between insoluble fluids. If the γ in the chemical potential, μ, is high enough as t approaches ∞ the two insoluble fluids completely separate. It is clear that the Cahn-Hilliard equation is very useful for studying emulsions and solutions as shown by Joon Choi and Anderson (2012) and other studies.

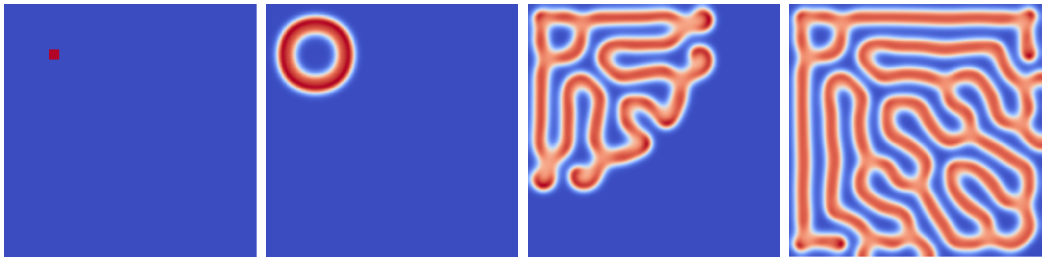
$$\begin{aligned} \frac{\partial a}{\partial t} &= d_a \nabla^2 a - ab^2 + f(1-a) \\ \frac{\partial b}{\partial t} &= d_b \nabla^2 b + ab^2 - (k+f)b \end{aligned} \tag{18}$$

$$\begin{aligned} a + 3b &\rightarrow 3b \\ b &\rightarrow p \end{aligned} \tag{19}$$

d_a is the rate of growth for a
d_b is the rate of growth for b
f is the feed rate also keeps a from exceeding 1
k is the kill rate of b which is scaled by b to prevent it from being less than 0

The Gray-Scott Model the reaction diffusion equation for computational art. Originally it was for a modeling a specific chemical reaction (Gray and Scott, 1984); however, due to its generality and in-

Figure 10: Coral Simulation



(a) $r = 0.1$ (b) $r = 0.2$ (c) $r = 0.3$ (d) $r = 0.3$

teresting patterns it became used for making natural-looking patterns with a seed, example Gray-Scott lamp (Jessica, 2010). The original reaction takes in a and b then produces a, p, byproduct. k is the rate that b turns into the nonreactive p and f is the rate that a is added and the other components are removed. It has also been picked up by computational artists. Its main uses are for modeling patterns in biology. These patterns, also known as Turing patterns, can be used to generate mitosis and spirals to zebrafish patterns. An example of the differences between reaction and reaction diffusion systems is firstly the spatial component and secondly how the patterns change given their environment. In animal Turing patterns, the area and type of skin effects the pigment patterns. For leopards, the patterns for the patches are not homogeneous; around the center of their sides the patches are

normally larger and decrease in size as they go to the paws or face (Liu et al., 2006).

6 Conclusion

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7 Appendix

List of Figures

Listing 1: Surface

```
import numpy as np
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt

# base function
def fun(x, y):
    return x*(y**2) + y

```

```
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
x = y = np.arange(-2.0, 2.0, 0.01)
X, Y = np.meshgrid(x, y)
zs = np.array([dx(x, y) for x, y in zip(np.ravel(X), np.ravel(Y))])
Z = zs.reshape(X.shape)

ax.plot_surface(X, Y, Z)

ax.set_xlabel('X Label')
ax.set_ylabel('Y Label')
ax.set_zlabel('Z Label')

plt.show()
```

Listing 2: Gradient

```
import numpy as np
import matplotlib.pyplot as plt

# The base function
def fun(x, y):
    return x*(y**2) + y

def dy(x, y): return 2*x*y  # Partial derivative on Y
def dx(x, y): return 2*y+1  # Partial derivative on X

# gets input points
x = y = np.arange(-2.0, 2.0, 0.25)
```

```
X, Y = np.meshgrid(x, y)
# Derivatives for each point
Dx = np.array([dx(x, y) for x, y in zip(np.ravel(X), np.ravel(Y))])
Dy = np.array([dy(x, y) for x, y in zip(np.ravel(X), np.ravel(Y))])
Dx = Dx.reshape(X.shape)
Dy = Dy.reshape(Y.shape)
# Vectors given derivatives
Ax = np.array([x + dx for x, dx in zip(np.ravel(X), np.ravel(Dx))])
Ay = np.array([y + dy for y, dy in zip(np.ravel(Y), np.ravel(Dy))])
Ax = Ax.reshape(X.shape)
Ay = Ay.reshape(Y.shape)
# Graph
plt.quiver(X, Y, Ax, Ay, cmap=plt.cm.coolwarm)
plt.show()
```

Listing 3: Divergence

```
import matplotlib.pyplot as plt # graphing library
from numpy import fromfunction # generates matrix

size: int = 100 # size of the matrix

# The base function
def fun(x, y): return x*(y**2) + y

def dy(x, y): return 2*x*y # Partial derivative on Y
def dx(x, y): return 2*y+1 # Partial derivative on X

# Divergence function, sum of the partials
```

```
def div(x, y): return dx(x,y) + dy(x,y)

# transforms the coordinates to get the right domain
def t(x): return (x - (size/2))/10

# Generates a matrix from a functions that is given X and Y
# In this case, the x, y operate like a cartesian plane centered at
    0
# we then plug in our modified coordients into our div function
P = fromfunction(lambda x, y: div(t(x), t(y)), (size, size))

# Graphs the matrix
plt.imshow(P, cmap=plt.cm.coolwarm, interpolation='bilinear')
plt.colorbar() # side colorbar for reference
plt.show()
```

Listing 4: Diffusion

```
import numpy as np
import matplotlib.pyplot as plt

# Simulation constants
alpha = 0.00001  # Laplician multiplier
n = 8000  # number of iterations
s = 100  # size of the matrix
dx = 2/s  # Simulation speed/accuracy

# Matrix initialization
M = np.fill((s, s), 0.0)
```

```
# Hotspot Seeding
M[20:30, 45:50] = 90
M[70:80, 45:50] = 90

# Implementation of the decretized laplacian operator
def laplacian(Z):
    Ztop = Z[0:-2, 1:-1]
    Zleft = Z[1:-1, 0:-2]
    Zbottom = Z[2:, 1:-1]
    Zright = Z[1:-1, 2:]
    Zcenter = Z[1:-1, 1:-1]
    return (Ztop + Zleft + Zbottom + Zright - (4 * Zcenter)) / dx**2

# Iterations through PDE
for _ in range(n):
    Mn = M[1:-1, 1:-1]
    M[1:-1, 1:-1] = Mn + np.multiply(laplacian(M), alpha)

# Graph Data
plt.imshow(M, cmap=plt.cm.coolwarm,
           interpolation='bilinear', extent=[-1, 1, -1, 1])
plt.show()
```

code/logistic.py

```
import matplotlib.pyplot as plt  # Graphing lib

# Model Params
r = 0.3  # growth rate
```

```
k = 100  # carrying capacity
p = 3  # init value

# Simulation params
t = 50  # total time units
dt = 0.01  # the resiprical of the iterations per time
n = int(t/dt)  # number of iterations

# Storing calculated values
y = []  # Output
t = []  # time for graphing

# Solve ODE using Euler's method
for i in range(n):
    p += ((r * p) * (1 - (p/k))) * dt  # logistic equation
    y.append(p)  # records output
    t.append(i*dt)  # records time

# graphs points
plt.plot(t, y)
plt.show()
```

Listing 5: Lotka-Volterra

```
import matplotlib.pyplot as plt

# Model params
alpha = 2/3
beta = 4/3
```

```
gamma = 1
delta = 1

# Simulation constants: descrete time and space
dt = 0.001  # the change in time
n = 20000  # number of iterations

# Seed the space
U = 1  # Population of Pray
V = 0.1  # Population of Preditors
# output Arrays
Uy = []
Vy = []
X = []

# Simulate this ODE with Euler's method
for i in range(n):
    # Gets copies to prevent overwritting
    Uc = U
    Vc = V
    # Generate next time step
    U += (alpha*Uc - beta*Uc*Vc)*dt
    V += (gamma*Uc*Vc - delta*Vc)*dt
    # Record outputs
    Uy.append(U)
    Vy.append(V)
    X.append(i*dt)

```

```
# Graph Data
plt.title("Lotka-Volterra Model")
plt.plot(X, Uy, 'b', label="pray")
plt.plot(X, Vy, 'r', label="preditor")
plt.legend()
plt.show()
```

Listing 6: SIR

```
import matplotlib.pyplot as plt

# Model params
b = 1  # days of contact to spread
k = 1/6  # days to recover

# Simulation params
dt = 0.1  # change in time
n = 800  # number of iterations

# Seeding
s = 1  # suseptible population
i = 1.27E-4  # Infected
r = 0  # Recovered
# To graph and record values
Sy = []
Iy = []
Ry = []
X = []

```

```
# Simulate ODE with Euler's method
for x in range(n):
    # Edge case
    if i <= 0:
        print("Done")
        break
    # copy to prevent overwritting
    Sc = s
    Ic = i
    Rc = r
    # Generate next timestep
    s += (-b * Sc * Ic) * dt
    i += ((b * Sc * Ic) - (k * Ic)) * dt
    r += (k * Ic) * dt
    # Record values
    Sy.append(s)
    Iy.append(i)
    Ry.append(r)
    X.append(x*dt)

# Graph Data
plt.title("SIR model")
plt.plot(X, Sy, 'g', label="Suseptible")
plt.plot(X, Iy, 'r', label="Infected")
plt.plot(X, Ry, 'b', label="Recovered")
plt.legend()
plt.show()
```

Listing 7: Cahn-Hilliard

```
from scipy.ndimage.filters import laplace  # Descrete Laplace
import matplotlib.pyplot as plt  # Graphing
import numpy.random as r  # Matrix Seeding

# Simulation constants
alpha = 0.04  # Diffusion constant
gamma = 0.125  # constant multiplier
n = 2000  # number of iterations
s = 200  # size of the matrix

# Matrix initialization
r.seed(100)
M = r.rand(s, s)

# iterating the Cahn-Hilliard Equation
for _ in range(n):
    G = gamma * laplace(M)  # inner laplace
    Mu = M**3 - M - G  # Mu: chemical potential
    M += laplace(Mu) * alpha  # outer laplace

# Graph Data
plt.imshow(M, cmap=plt.cm.coolwarm, interpolation='bicubic')
plt.axis('off')
plt.show()
```

Listing 8: Gray-Scott

```
from scipy.ndimage.filters import laplace  # Descrete Laplace
import matplotlib.pyplot as plt  # graphing
from numpy import full  # matrix init

# Constants
s = 250  # size of the matrix
Du = 1  # U growth rate
Dv = 0.5  # V growth rate
f = .0545  # feed rate
k = .062  # kill rate


# Simulation Params
t = 5000  # 'time' simulated
dt = .1  # Iterations per time unit
n = int(t/dt)  # total iteration count

fig = plt.figure()

# Matrix Inits
U = full((s, s), 1.0)  # Starts U full of 1
V = full((s, s), 0.0)  # stats V full of 0
V[45:55, 45:55] = 1.0  # Adds a bit to V

# iterate though PDE
for _ in range(n):
    uvv = U * V * V  # prevents write error and clean
    U += ((Du*laplace(U) - uvv + (f * (1 - U))) * dt)  # U solve
```

```
    V += ((Dv*laplace(V) + uvv - (V * (f + k))) * dt)  # V solve

# Graph
plt.imshow(V, cmap=plt.cm.coolwarm)
plt.axis("off")
plt.show()
```