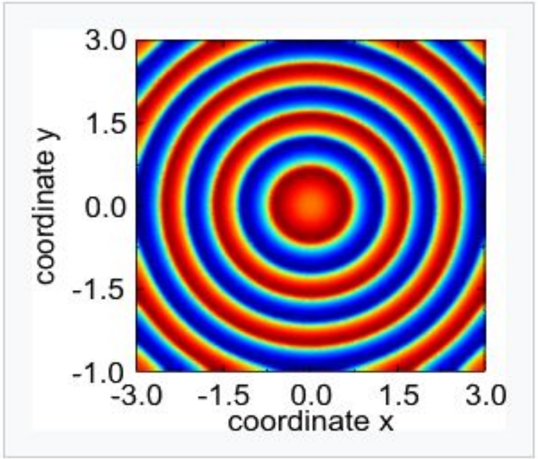
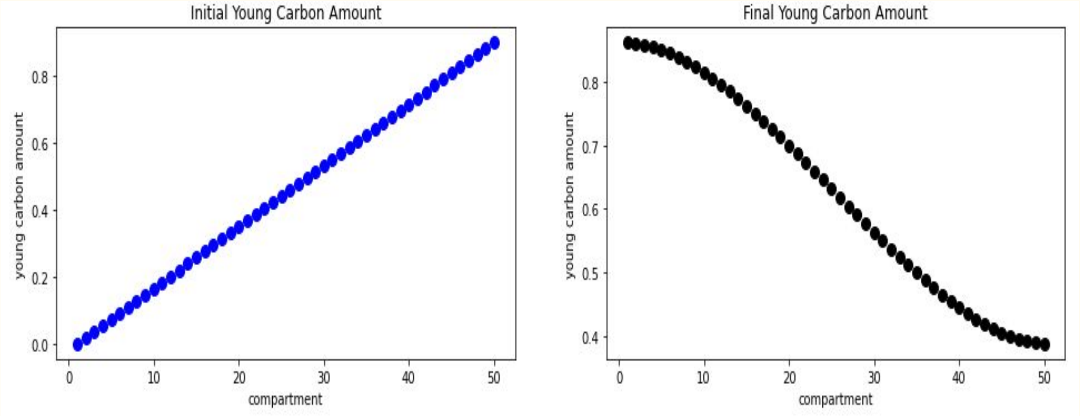
Diffusion Models of Pattern Formation

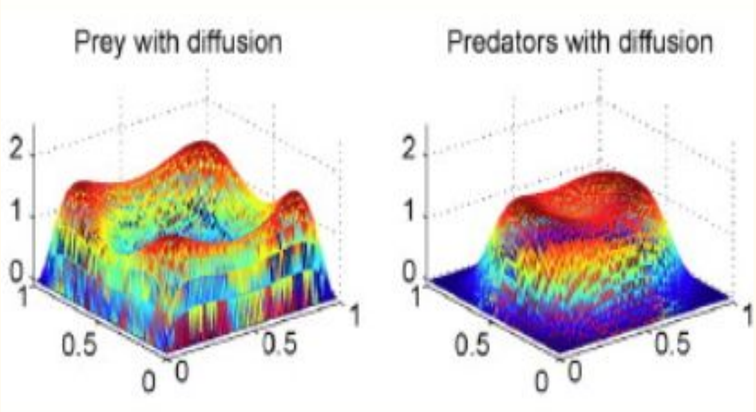
Luke Vaughan

Diffusion in Mathematical Ecology

- Study past/present movement, predict future movement
- Two-dimensional diffusion: “bird’s-eye view”
- Zoology examples: muskrats and insect larvae
- Environmental science example: carbon dynamics
- Reaction-diffusion systems







Two-Dimensional Diffusion Equation Derivation

- Displacement of one particle
- Probability density function (PDF): $\phi(x, y, t)$
- Time $t + \Delta t$: PDF is the mean of $\phi(\xi, \eta, t)$ over all points in the circle of radius ϵ centered at (x, y)
- Mean value theorem for integrals
- Convert to polar coordinates

$$f(c) = \frac{1}{b-a} \int_a^b f(x)dx$$

$$\phi(x, y, t + \Delta t) = \frac{1}{2\pi} \int_0^{2\pi} \phi(\xi, \eta, t)d\theta$$

LHS & RHS: report Taylor expansions

$$\phi(x, y, t + \Delta t) = \frac{1}{2\pi} \int_0^{2\pi} \phi(x + \epsilon\cos\theta, y + \epsilon\sin\theta, t)d\theta$$

Two-Dimensional Diffusion Equation Derivation (cont.)

LHS: $\phi(x,y,t+\Delta t) = \phi + \frac{\partial \phi}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 \phi}{\partial t^2}(\Delta t)^2 + \ldots$

RHS: $\frac{1}{2\pi}\int_0^{2\pi}\left[\phi + \frac{\partial \phi}{\partial x}\epsilon\cos\theta + \frac{\partial \phi}{\partial y}\epsilon\sin\theta + \frac{1}{2}\frac{\partial^2 \phi}{\partial x^2}(\epsilon\cos\theta)^2 + \frac{\partial^2 \phi}{\partial x \partial y}(\epsilon\cos\theta)(\epsilon\sin\theta) + \frac{1}{2}\frac{\partial^2 \phi}{\partial y^2}(\epsilon\sin\theta)^2 + \ldots\right]d\theta$

RHS simplifies: $\int_0^{2\pi}\cos\theta d\theta = \int_0^{2\pi}\sin\theta d\theta = \int_0^{2\pi}\cos\theta\sin\theta d\theta = 0$ and

$\int_0^{2\pi}\cos^2\theta d\theta = \int_0^{2\pi}\sin^2\theta d\theta = \pi$

LHS = RHS: $\phi + \frac{\partial \phi}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 \phi}{\partial t^2}(\Delta t)^2 + \ldots = \phi + \frac{\epsilon^2}{4}\nabla^2\phi + \ldots$

$\frac{\partial \phi}{\partial t} + \frac{1}{2}\frac{\partial^2 \phi}{\partial t^2}\Delta t + \ldots = \frac{\epsilon^2}{4\Delta t}\nabla^2\phi + \ldots$

Take $\lim\limits_{\Delta t \to 0}$: $\boxed{\frac{\partial \phi}{\partial t} = D\nabla^2\phi}$

Diffusion Pattern 1: Muskrats

- Spread rapidly in Central Europe in the early 1900s
- Hunters wanted fur
- Government officials saw the spread as a serious problem to be addressed
- Movement patterns needed to be analyzed

Diffusion Pattern 1: Muskrats (cont.)

- Transition from single-particle to multiple-particle PDF
- Proportion of muskrats at a certain time/place: $\Phi(r,\theta,t) = \frac{1}{4\pi Dt}\exp\left(\frac{-r^2}{4Dt}\right)$
- Let $4D = a^2$
- Integrate θ out: obtain proportion of population on boundary of circle
- Integrate r out: obtain proportion depending only on time: denote as p_t

$$\Phi(t) = \int_0^{2\pi}\int_{R_t}^{\infty} \frac{1}{\pi a^2 t}\exp\left(\frac{-r^2}{a^2 t}\right) r\,dr\,d\theta = \ldots = \exp\left(\frac{-R_t^2}{a^2 t}\right) = p_t$$

- Proportion of population expected to be farther than a distance of R_t away from center of diffusion given by p_t
- One member farther than R_t: set $p_t = \frac{1}{N}$

$$\Rightarrow \frac{1}{N} = e^{-R_t^2/a^2 t} \Rightarrow \ldots \Rightarrow R_t^2 = a^2 t\, \underline{\ln N}$$

$$N_t = N_0 e^{ct}$$

$$\Rightarrow \ldots \Rightarrow \underline{\ln N_t = ct}$$

Diffusion Pattern 1: Muskrats (cont.)

- Radius squared proportional to time squared
- Linear relationship: square root of area and time
- Approximations for contours: “pond ripple pattern”

$$\boxed{R_t^2 = a^2 c\, t^2}$$

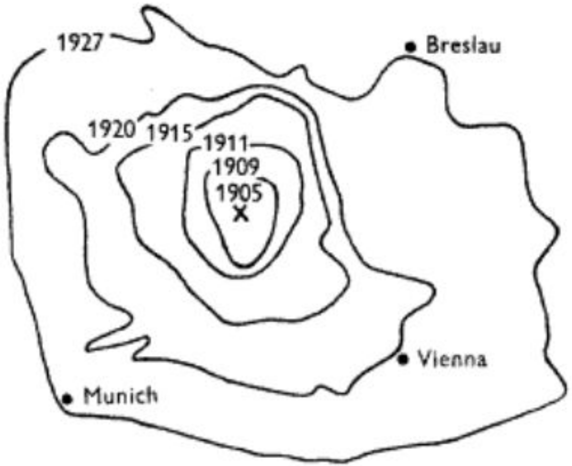


Fig. 1

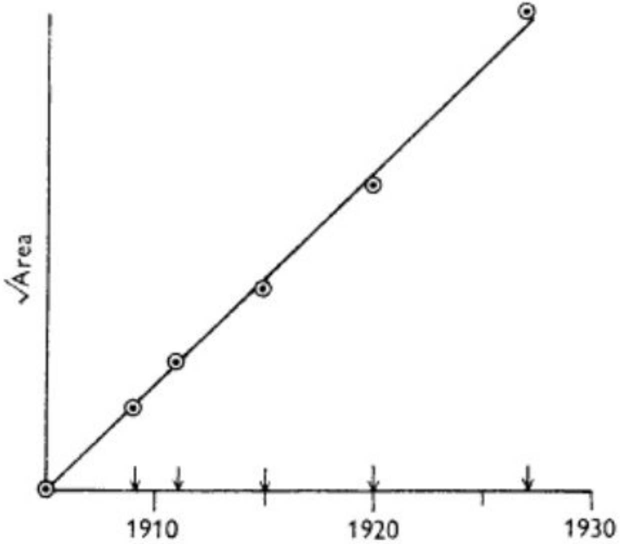


Fig. 2

Diffusion Pattern 2: Insect Larvae

- Proportion function: $\Phi(r,t)dr = \frac{2r}{a^2t}\exp\left(\frac{-r^2}{a^2t}\right)dr$
- Travel times are random variables with PDF $f(t) = \lambda e^{-\lambda t}$ (exponential probability distribution)
- Distribution of distances: $g(r)dr = \left[\int_0^\infty \Phi(r,t)f(t)dt\right]dr$

  Compare to Strauss: $\int_{-\infty}^{\infty} S(x,t)\phi(x)dx \to \phi(0)$
- Rewrite integral expression

$$g(r)dr = \left[\int_0^\infty \frac{2r\lambda}{a^2t}\exp\left(-\lambda t - \frac{r^2}{a^2t}\right)dt\right]dr$$

$$\text{Let } \rho = \frac{2r\sqrt{\lambda}}{a} \Rightarrow d\rho = \frac{2\sqrt{\lambda}}{a}dr$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$h(\rho)d\rho = \rho\left[\frac{1}{2}\int_0^\infty \exp\left(-\lambda t - \frac{\rho^2}{4\lambda t}\right)\frac{dt}{t}\right]d\rho$$

Diffusion Pattern 2: Insect Larvae (cont.)

$$\text{Let } \lambda t = \tau \Rightarrow dt = \frac{d\tau}{\lambda} \Rightarrow dt = \frac{d\tau}{\tau/t} \Rightarrow \frac{dt}{t} = \frac{d\tau}{\tau}$$

$$h(\rho)d\rho = \rho\left[\frac{1}{2}\int_0^\infty \exp\left(-\tau - \frac{\rho^2}{4\tau}\right)\frac{d\tau}{\tau}\right]d\rho$$

$$K_v(z) = \frac{1}{2}\left(\frac{1}{2}z\right)^v \int_0^\infty \exp\left(-t - \frac{z^2}{4t}\right)\frac{dt}{t^{v+1}}$$

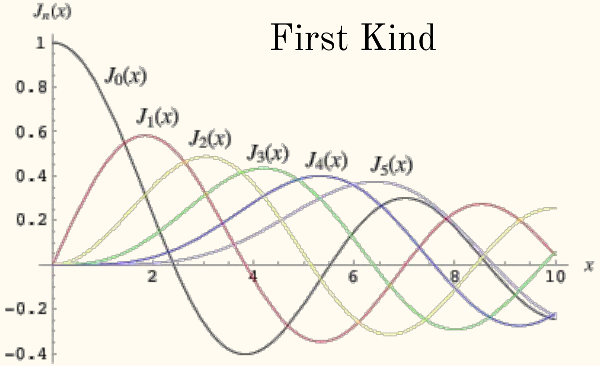
(DLMF: list of integral expressions for various Bessel functions)

Choose $v = 0$

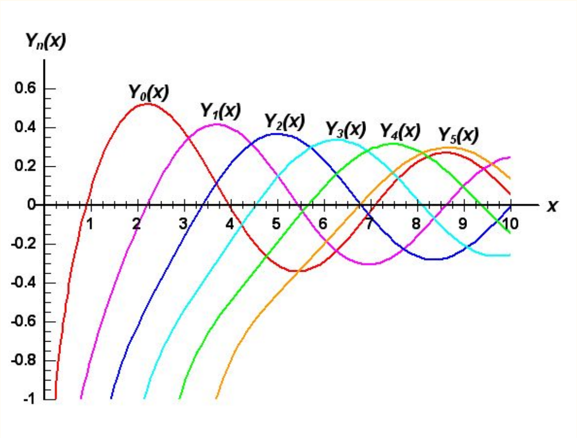
Distribution of distances: $\boxed{h(\rho) = \rho K_0(\rho)}$

where $K_0(\rho)$ is a “modified” Bessel function of the second kind

First Kind

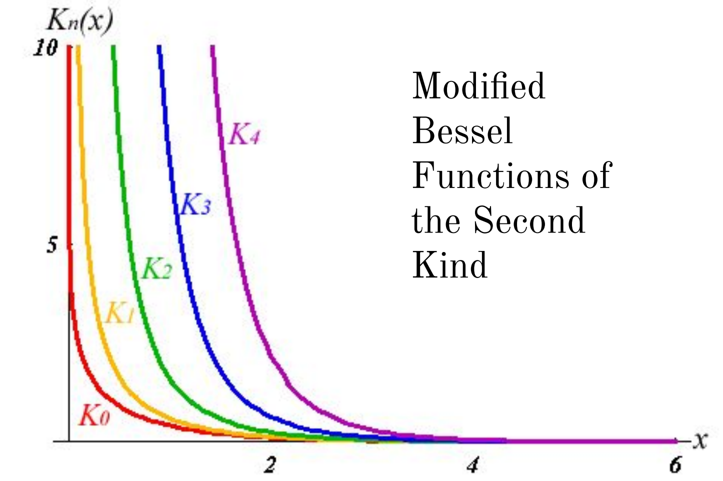


Second Kind



Diffusion Pattern 2: Insect Larvae (cont.)

- Choose $K_0(\rho)$
- Diffusion pattern only depends on radius (pond ripple pattern again)



Modified Bessel Functions of the Second Kind

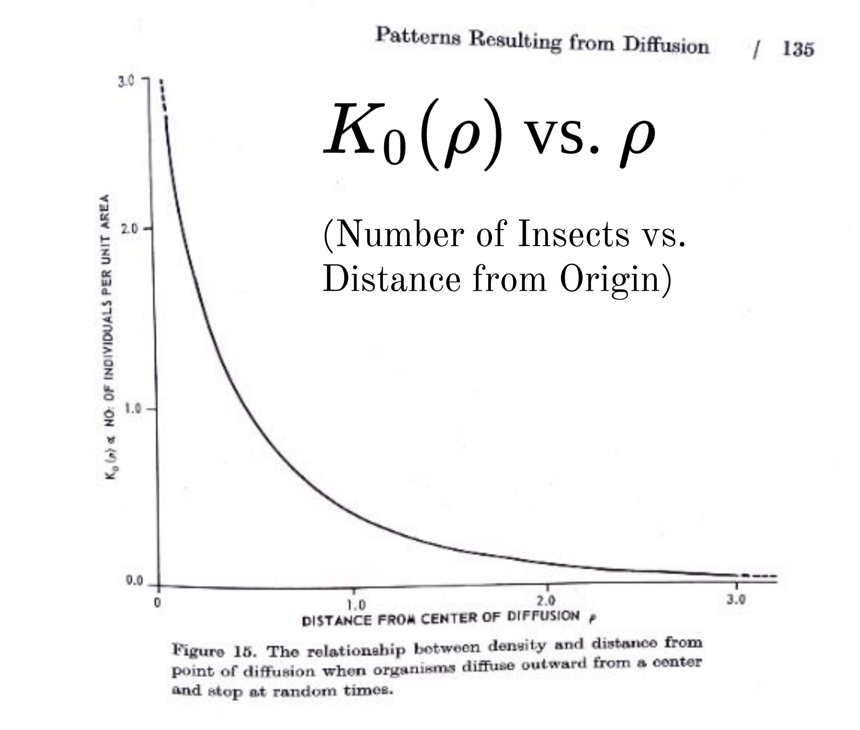
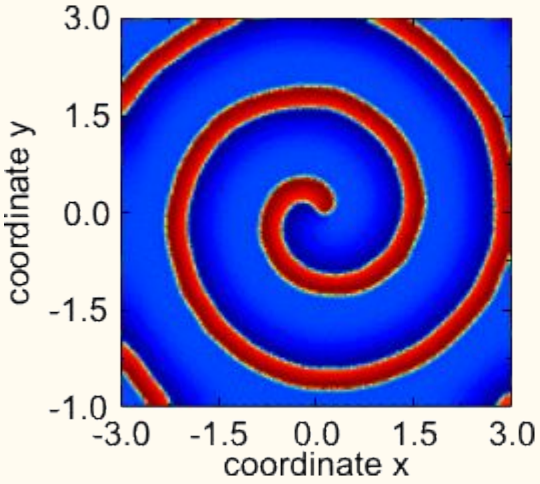


Figure 15. The relationship between density and distance from point of diffusion when organisms diffuse outward from a center and stop at random times.

$K_0(\rho)$ vs. ρ

(Number of Insects vs. Distance from Origin)

Reaction-Diffusion Systems



- Systems of 2 or more PDEs (usually coupled): diffusion equation with “interaction terms” (AKA “reaction terms”)
- General form: $\partial_t \boldsymbol{u} = \boldsymbol{D}\nabla^2 \boldsymbol{u} + \boldsymbol{R}(\boldsymbol{u})$
- Applications in chemistry, biology, environmental science, etc.

Vinyl Alcohol & Ethanal:

$$\begin{cases} u_t = d_u \nabla^2 u + \bar{k}_1 v - \bar{k}_{-1} u - \bar{k}_2 uv \\ v_t = d_v \nabla^2 v + \bar{k}_{-1} u - \bar{k}_1 v - \bar{k}_2 uv \end{cases}$$

Fitzhugh-Nagumo:

$$\begin{cases} u_t = d_u^2 \nabla^2 u + f(u) - \sigma v \\ \tau v_t = d_v^2 \nabla^2 v + u - v \end{cases}$$

Reaction-Diffusion System: One Dimension

- Discretization: one strategy for solving system
- Begin with u: break x up into N compartments
- 1 PDE becomes a system of N ODEs
- Approximate second derivatives with finite differences
- Second-difference matrix S assumes "sealed-end BCs"
- Repeat process for v
- Use a numerical method (such as the Trapezoidal Rule) to plot approximations for solutions

$$\begin{cases} u_t = D_u u_{xx} + a(u,v) \\ v_t = D_v v_{xx} + b(u,v) \end{cases}$$

$$u_{xx} \approx \frac{u(x+\Delta x,t) - 2u(x,t) + u(x-\Delta x,t)}{\Delta x^2}$$

$$S = \begin{pmatrix} -1 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -1 \end{pmatrix}$$

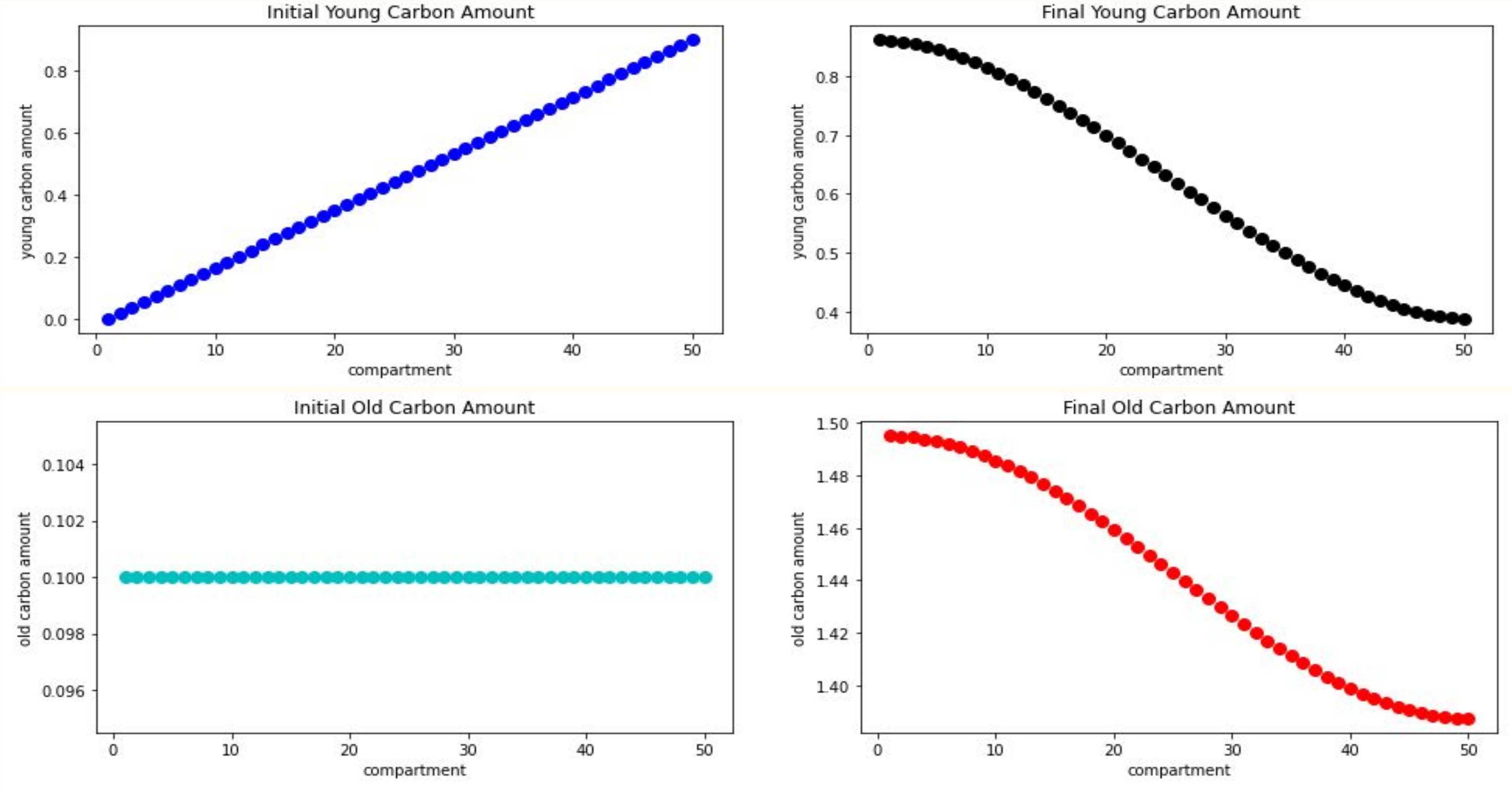
$$\boldsymbol{u}'(t) = \frac{D_u}{\Delta x^2} S\boldsymbol{u}(t) + a\left(\boldsymbol{u}(t), \boldsymbol{v}(t)\right)$$

$$\boldsymbol{v}'(t) = \frac{D_v}{\Delta x^2} S\boldsymbol{v}(t) + b\left(\boldsymbol{u}(t), \boldsymbol{v}(t)\right)$$

Example: carbon dynamics

$$\begin{cases} u_t = D_u u_{xx} + k(x) - \alpha u(x,t) \\ v_t = D_v v_{xx} + \beta u(x,t) - \gamma v(x,t) \end{cases}$$

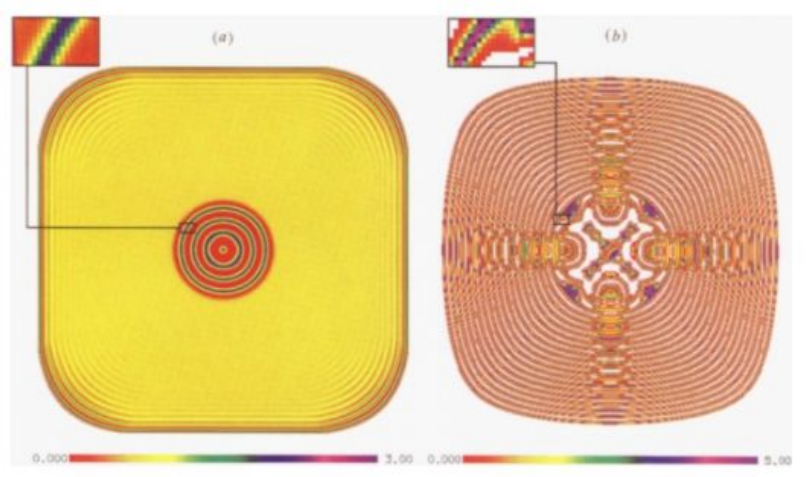
Reaction-Diffusion System: One Dimension (cont.)

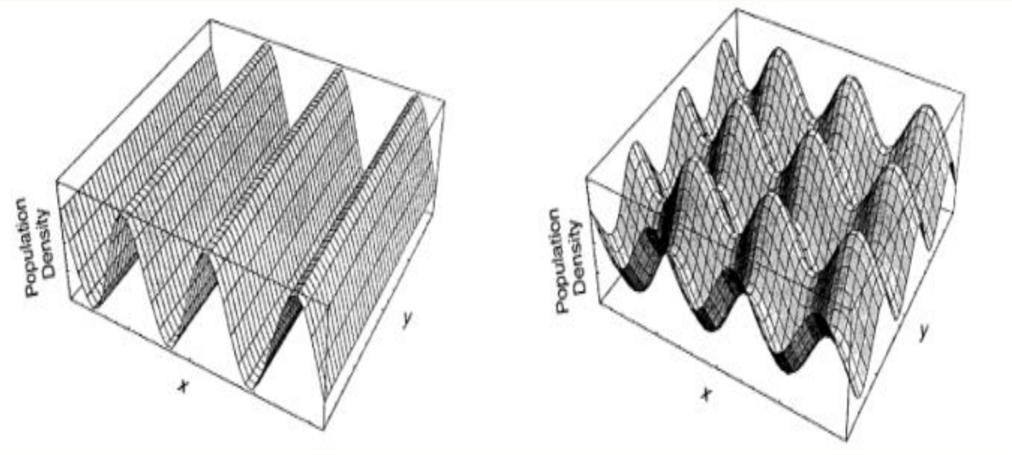


Reaction-Diffusion System: Two Dimensions

- Example: predator-prey model
- Other example of predator-prey interaction: source uses discretization

$$\begin{cases} u_t = f_u(u) - \alpha v g(u) + D_u \nabla^2 u \\ v_t = \beta v g(u) - f_v(v) + D_v \nabla^2 v \end{cases}$$





Conclusions

- The derivation for the two-dimensional diffusion equation gave us a solid foundation on which to move forward, specifically, in the realm of ecology
- For the muskrats, we were able to collapse the diffusion equation down to a simple model of exponential growth (the resulting pattern resembled pond ripples)
- For the insect larvae, rather than trying to solve the diffusion equation directly, we completed an informative analysis of diffusion using statistics, distribution theory, and Bessel functions (again, the resulting pattern resembled pond ripples)
- For reaction-diffusion systems, we scratched the surface of a challenging task: solving systems of PDEs. Discretization serves as an effective strategy for approximating solutions to reaction-diffusion systems in one, two, or perhaps even three dimensions. Studying systems of this type is a stimulating challenge in PDEs research

Sources

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