

# MM Autumn 2025 Mechanistic Modelling Projects

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## General Information

The steps, calculations, results, and code of your projects are to be documented in a report.

The following points have to be done/answered in any case (points with an \* are optional)

1. Classify the PDE
2. Try to find some information about the PDE and describe it shortly
3. Make reasonable assumptions and choices and shortly explain your assumptions and choices:
  - (a) What FD scheme is suited for the problem
  - (b) What BC is suited
  - (c) What IC makes sense
  - (d) Constants in the equations (e.g. diffusion constant, etc.)
4. Discretise the PDE using FD approximations
5. Analyse the step-wise order of the error of the FD approximation
6. Solve the PDE (for time-dependent PDEs, i.e. you observe how it changes after a certain time)
7. Investigate the stability of the scheme (in the case of non-linear PDEs you may simply investigate stability in an experimental fashion)
8. Play around with different values of the coefficients.
9. Visualise the solution(s)
10. \* Solve the PDE using various schemes and compare them
11. \* Make an error estimation for one of the solutions

## Comments

- in some of the equations: The laplace-operator  $\Delta = \nabla^2$  is defined in two dimensions as

$$\nabla^2 = \partial_{xx} + \partial_{yy}$$

, i.e. e.g.

$$\Delta u = u_{xx} + u_{yy}$$

- Tasks with an asterisk \* are optional.
- Integrals turn into sums in a discretised world

# 1 Diffusion-Reaction in Tumor Growth

Description: Model the growth of a tumor in a tissue, considering the effects of diffusion and a reaction term representing the proliferation of cancer cells.

$$\frac{\partial T}{\partial t} = D \nabla^2 T + rT \left(1 - \frac{T}{K}\right) \quad (1)$$

Parameters and Variables:

$$T : \text{Tumor cell density (in cells /cm}^3 \text{)} \quad (2)$$

$$D : \text{Diffusion coefficient} \quad (3)$$

$$r : \text{Proliferation rate} \quad (4)$$

$$K : \text{Carrying capacity} \quad (5)$$

Typical values:  $D = 0.1 - 1 \text{ cm}^2/\text{day}$ ,  $r = 0.01 - 0.1 \text{ day}^{-1}$ ,  $K = 10^4 - 10^6 \text{ cells /cm}^3$

# 2 Cardiac Electrophysiology - FitzHugh-Nagumo Model

Description: Simulate the electrical activity of cardiac cells using the FitzHugh-Nagumo model, representing the dynamics of membrane potential and a recovery variable.

$$\frac{\partial V}{\partial t} = C \nabla^2 V + V(1 - V)(V - a) - W + I_{\text{ext}} \quad (6)$$

$$\frac{\partial W}{\partial t} = \epsilon(V - bW) \quad (7)$$

Parameters and Variables:

$$V : \text{Membrane potential (in Volt)} \quad (8)$$

$$W : \text{Recovery variable (in Volt)} \quad (9)$$

$$C : \text{Diffusion coefficient} \quad (10)$$

$$a, b : \text{Model parameters} \quad (11)$$

$$\epsilon : \text{Time scale separation parameter} \quad (12)$$

$$I_{\text{ext}} : \text{External current} \quad (13)$$

Typical values:  $C = 0.01 - 0.1 \text{ cm}^2/\text{ms}$ ,  $a = 0.1 - 0.5$ ,  $b = 0.1 - 0.5$ ,  $\epsilon = 0.01 - 0.1$ ,  $I_{\text{ext}} = 0.1 - 1 \mu \text{ A}$

# 3 Epidemiological Modeling: SIR Model

Description: Simulate the spread of an infectious disease using the Partial Differential Equation (PDE) version of the Susceptible-Infectious-Recovered (SIR) model. Explore the impact of transmission and recovery rates on the spatial dynamics of the epidemic.

$$\frac{\partial S}{\partial t} = -\beta \cdot \frac{S \cdot I}{N} \quad (14)$$

$$\frac{\partial I}{\partial t} = D_i \nabla^2 I + \beta \cdot \frac{S \cdot I}{N} - \gamma \cdot I \quad (15)$$

$$\frac{\partial R}{\partial t} = \gamma \cdot I \quad (16)$$

Parameters and Variables:

$$S : \text{Susceptible individuals density (individuals /cm}^2 \text{ )} \quad (17)$$

$$I : \text{Infectious individuals density (individuals /cm}^2 \text{ )} \quad (18)$$

$$R : \text{Recovered individuals density (individuals /cm}^2 \text{ )} \quad (19)$$

$$\beta : \text{Transmission rate ( day}^{-1} \text{ )} \quad (20)$$

$$\gamma : \text{Recovery rate ( day}^{-1} \text{ )} \quad (21)$$

$$N : \text{Total population} \quad (22)$$

$$D_i : \text{Diffusion coefficient for } I \text{ ( cm}^2/\text{ day )} \quad (23)$$

Typical values:  $D_s = 0.01 - 0.1 \text{ cm}^2/\text{ day}$ ,  $D_i = 0.01 - 0.1 \text{ cm}^2/\text{ day}$ ,  $\beta = 0.1 - 0.5 \text{ day}^{-1}$ ,  $\gamma = 0.05 - 0.2 \text{ day}^{-1}$ ,  $N = 1000 - 50000$

## 4 Oxygen Distribution in Tissues

Description: Model the distribution of oxygen in tissue, considering diffusion, consumption by cells, and external oxygen supply.

$$\frac{\partial O}{\partial t} = D\nabla^2 O - \mu O + S \quad (24)$$

Parameters and Variables:

$$O : \text{Oxygen concentration} \quad (25)$$

$$D : \text{Diffusion coefficient} \quad (26)$$

$$\mu : \text{Consumption rate by cells} \quad (27)$$

$$S : \text{External oxygen supply} \quad (28)$$

Typical values:  $D = 0.01 - 0.1 \text{ cm}^2/\text{ day}$ ,  $\mu = 0.001 - 0.01 \text{ day}^{-1}$ ,  $S = 1 - 10 \text{ mg}/(\text{cm}^3 \cdot \text{ day})$

## 5 Spatial Prey-Predator Interaction

Description: Model the spatial dynamics of prey and predator populations in an ecosystem, considering the influence of diffusion, local predation, and prey reproduction.

$$\frac{\partial P}{\partial t} = D_p \nabla^2 P + rP \left(1 - \frac{P}{K_p}\right) - \alpha PH \quad (29)$$

$$\frac{\partial H}{\partial t} = D_h \nabla^2 H - \beta PH + \gamma H \quad (30)$$

Parameters and Variables:

$$P : \text{Prey population} \quad (31)$$

$$H : \text{Predator population} \quad (32)$$

$$D_p, D_h : \text{Diffusion coefficients for prey and predator} \quad (33)$$

$$r : \text{Prey reproduction rate} \quad (34)$$

$$K_p : \text{Prey carrying capacity} \quad (35)$$

$$\alpha : \text{Predation rate} \quad (36)$$

$$\beta : \text{Predator death rate due to predation} \quad (37)$$

$$\gamma : \text{Predator birth rate} \quad (38)$$

Typical values:  $D_p = 0.01 - 0.1 \text{ cm}^2/\text{day}$ ,  $D_h = 0.01 - 0.1 \text{ cm}^2/\text{day}$ ,  $r = 0.01 - 0.1 \text{ day}^{-1}$ ,  $K_p = 10^3 - 10^5 \text{ individuals}/\text{cm}^2$ ,  $\alpha = 0.01 - 0.1 \text{ predator individuals/day}$ ,  $\beta = 0.01 - 0.1 \text{ prey individuals/day}$ ,  $\gamma = 0.001 - 0.01 \text{ day}^{-1}$

## 6 The Brusselator Model

The Brusselator model is a classical reaction-diffusion system that describes a special type of chemical reaction between two components. It was proposed by I. Prigogine and co-workers in Brussels, hence its name. You may find a more detailed description under: [https://www.uni-muenster.de/imperia/md/content/physik\\_tp/lectures/ws2016-2017/num\\_methods\\_i/rd.pdf](https://www.uni-muenster.de/imperia/md/content/physik_tp/lectures/ws2016-2017/num_methods_i/rd.pdf) p. 10

$$u_t = D_u \Delta u + a - (b+1)u + u^2v \quad (39)$$

$$v_t = D_v \Delta v + bu - u^2v \quad (40)$$

Parameters and Variables:

$$u : \text{density of first compound} \quad (41)$$

$$v : \text{density of second compound} \quad (42)$$

$$D_u : \text{Diffusion coefficient for first compound} \quad (43)$$

$$D_v : \text{Diffusion coefficient for second compound} \quad (44)$$

$$a : \text{reaction kinetics parameter} \quad (45)$$

$$b : \text{reaction kinetics parameter} \quad (46)$$

Typical values:  $D_u = 5$ ,  $D_v = 12$ ,  $a = 3$ ,  $b = 9$ .

## Reference

Prigogine & Lefever (1968). J. Chem. Phys.

## 7 The spruce budworm model

Description: The spruce budworm model describes the infestation of a spruce or fir tree, native to northern America, by the insect named spruce budworm (*Choristoneura fumiferana*). Every forty years or so, the budworm numbers rise to very high levels, causing heavy damage to the forests. To familiarize yourself with the behavior of a variant of this model, you can check out how it changes under different parameter choices here: [https://mathinsight.org/spruce\\_budworm\\_outbreak\\_model](https://mathinsight.org/spruce_budworm_outbreak_model).

$$\frac{\partial u}{\partial t} = u(1-u) - \frac{1}{R} \frac{u^2}{\epsilon^2 + u^2} + \Delta u$$

Parameters and Variables:

$$u : \text{budworm density} \quad (47)$$

$$R : \text{amount of available foliage to the budworm} \quad (48)$$

$$\epsilon : \text{reaction kinetics parameter, typically small} \quad (49)$$

Typical values:  $R = 10^2$ ,  $\epsilon = 10^{-3}$ .

## 8 Fisher-Kolmogorov-Petrovsky-Piskunoff (FKPP) equation of propagating waves

Description: R. Fisher suggested this model for the spread of a favoured gene in a population. It was generalized and studied for its properties by Kolmogorov, Petrovsky and Piskunoff a bit later. It has been studied for its remarkable properties since the 1930, such as the ability of the solutions to form waves that self-stabilize. You may find a more detailed description under: [https://www.uni-muenster.de/imperia/md/content/physik\\_tp/lectures/ws2016-2017/num\\_methods\\_i/rd.pdf](https://www.uni-muenster.de/imperia/md/content/physik_tp/lectures/ws2016-2017/num_methods_i/rd.pdf), p.75.

$$\frac{\partial u}{\partial t} = ku(1 - u) + D \frac{\partial^2 u}{\partial x^2} \quad (50)$$

Parameters and Variables:

$$u : \text{the frequency of the advantageous mutant gene} \quad (51)$$

$$k : \text{intensity of selection in favor of the advantageous mutant gene} \quad (52)$$

$$D : \text{Diffusion coefficient} \quad (53)$$

$$(54)$$

Typical values:  $D = 1 \text{ km}^2 / \text{day}$ ,  $k = 1 \text{ day}^{-1}$ .

### Reference

Murray, J. D. *Mathematical Biology I & II*. Springer.

## 9 Diffusive Lotka–Volterra Predator–Prey System

Description: The classical predator-prey model by Lotka and Volterra has profoundly influenced ecological modeling, because it showed how coupled time courses of population abundances of predators and prey could emerge from relatively simple nonlinear differential equations. The classical Lotka-Volterra model has drawbacks: there is no spatial information, and the solutions are not structurally stable.

Here, we consider a structural as well as spatial extension of the classical predator–prey model. The structural extension introduces self-limiting growth on the prey. The spatial expansion includes the geographical spread of both prey and predators over an area by diffusion. The dynamics of the Lotka-Volterra are now displayed locally at any given geographical location, but the predators and prey are also thought to spread randomly over the space. Thus, the model describes how prey and predator densities evolve both temporally and spatially. This model has been used to study invasion waves, pattern formation, and spatial coexistence of species.

$$u_t = D_u \nabla^2 u + u(a - bu - cv), \quad (55)$$

$$v_t = D_v \nabla^2 v + v(-d + eu). \quad (56)$$

Parameters and Variables:

- $u(x, y, t)$ : prey density.
- $v(x, y, t)$ : predator density.
- $D_u, D_v$ : diffusion coefficients of prey and predator.
- $a$ : prey intrinsic growth rate.

- $b$ : prey self-limitation coefficient.
- $c$ : predation rate coefficient.
- $d$ : predator natural death rate.
- $e$ : conversion efficiency of consumed prey.

Typical values:

- $D_u \sim 10^{-2}$ ,  $D_v \sim 5 \times 10^{-3}$  (nondimensional), or  $D_u \sim 1 \text{ m}^2/\text{d}$ ,  $D_v \sim 0.5 \text{ m}^2/\text{d}$  (dimensional).
- $a \sim 1 \text{ d}^{-1}$ ,  $d \sim 0.5 \text{ d}^{-1}$ .
- $b, c, e \sim O(1)$  nondimensional.

## Reference

Murray, J. D. *Mathematical Biology I & II*. Springer.

## 10 Rosenzweig–MacArthur Reaction–Diffusion Model

Description: To understand where structural stability in predatory-prey systems originates from, in 1963 Rosenzweig and MacArthur suggested that the way in which predators and prey interact must be changed. Besides adding **logistic prey growth** to the classical **Lotka-Volterra model**, they assumed a **saturating Holling type-II predation term** (Holling had classified all predation interactions with prey into three functional types in the 1950s). This modification allowed for more structurally stable dynamics. Here, we analyze the spatial expansion of this model, where **spatial diffusion allows predator–prey interactions** to take place across heterogeneous landscapes. This model has been used to study the **enrichment paradox and spatial predator–prey waves**.

$$u_t = D_u \nabla^2 u + ru \left(1 - \frac{u}{K}\right) - \frac{\alpha uv}{1 + hu}, \quad (57)$$

$$v_t = D_v \nabla^2 v + \beta \frac{\alpha uv}{1 + hu} - mv. \quad (58)$$

Variables and Parameters:

- $u$  = prey density,  $v$  = predator density.
- $D_u, D_v$  = diffusion coefficients.
- $r$  = prey intrinsic growth rate.
- $K$  = prey carrying capacity.
- $\alpha$  = attack rate.
- $h$  = handling time factor.
- $\beta$  = conversion efficiency.
- $m$  = predator mortality.

Typical Parameter Values:

- $D_u \sim 0.1\text{--}1 \text{ m}^2/\text{d}$ ,  $D_v \sim 0.05\text{--}0.5 \text{ m}^2/\text{d}$ .
- $r \sim 0.1\text{--}1 \text{ d}^{-1}$ ,  $K \sim 10^2\text{--}10^3 \text{ ind}/\text{m}^2$ .
- $\alpha \sim 10^{-3}\text{--}10^{-2} \text{ m}^2/(\text{ind d})$ ,  $h \sim 0.01\text{--}0.1 \text{ ind}^{-1}$ .
- $\beta \sim 0.1\text{--}0.5$ ,  $m \sim 0.01\text{--}0.1 \text{ d}^{-1}$ .

## References

Rosenzweig and MacArthur, 1963, The American Naturalist <https://www.jstor.org/stable/2458702>  
 Grunert et al., 2021, Proceedings of the National Academy Sciences <https://doi.org/10.1073/pnas.2017463118>  
 Cantrell & Cosner (2003). *Spatial Ecology via Reaction–Diffusion Equations*. Wiley.  
 Begon and Townsend (2021), Ecology: From Individuals to Ecosystems

## 11 Competition–Diffusion System

Description: Besides predator-prey models, ecologists are interested in understanding how species compete and interact spatially. The competition - diffusion model represents two competing species with logistic self-limitation and mutual competitive inhibition, that are both subject to spatial dispersal under a diffusion term. This model was used by researchers to study species coexistence, invasion fronts, and competitive exclusion.

$$u_t = D_u \nabla^2 u + u(1 - u - \alpha v), \quad (59)$$

$$v_t = D_v \nabla^2 v + v(1 - v - \beta u). \quad (60)$$

Variables and Parameters

- $u, v$  = densities of species 1 and 2.
- $D_u, D_v$  = diffusion coefficients.
- $\alpha, \beta$  = interspecific competition coefficients.

Typical Parameter Values:

- $D_u \sim 1, D_v \sim 0.5$ –1 (nondimensional).
- $\alpha, \beta \sim 0.5$ –2.

## References

Analyzed mathematically by Pao in 1981: [https://doi.org/10.1016/0022-247X\(81\)90246-8](https://doi.org/10.1016/0022-247X(81)90246-8)  
 Okubo & Levin (2001). *Diffusion and Ecological Problems*. Springer.

## 12 Schnakenberg Model

Description: The formation of patterns on surfaces, such as patterning of the fur of felines, can be analyzed in terms of interacting chemical components that diffuse. Schnakenberg published a paper in 1979 where he presented partial differential equations capable to generate classical Turing patterns (spots, stripes), and that is appropriate to analyze limit cycles. This model was widely used in theoretical developmental biology.

$$u_t = D_u \nabla^2 u + a - u + u^2 v, \quad (61)$$

$$v_t = D_v \nabla^2 v + b - u^2 v. \quad (62)$$

Variables and Parameters

- $u$  = activator,  $v$  = inhibitor.
- $a, b$  = feed parameters.
- $D_u, D_v$  = diffusion coefficients.

Typical Parameter Values:

- $a \sim 0.1\text{--}1$ ,  $b \sim 0.1\text{--}2$ .
- $D_u > 1$ ,  $D_v \sim 10\text{--}100$ .

## Reference

Schnakenberg (1979). J. Theor. Biol. ; [https://doi.org/10.1016/0022-5193\(79\)90042-0](https://doi.org/10.1016/0022-5193(79)90042-0)

## 13 Replicator–Mutator equation in 2D Trait Space

Description: The theory of evolution by natural selection is modelled differently mathematically depending on context. The replicator-mutator equation assumes that selection acts on continuous-traits,  $\theta$ , and describes an evolutionary dynamics that combines selection and mutation. In this model, mutation acts as diffusion in trait space  $\theta$ , spreading out the distribution of the population with certain traits,  $q(\theta, t)$ . Selection, however, acts as channeling force, pushing the trait distribution towards higher fitness values. Together, these two processes give rise to a PDE over trait distributions. This equation is used in adaptive dynamics, evolutionary ecology, and quantitative genetics.

Let  $\theta = (\theta_1, \theta_2)$ :

$$q_t = q(\theta, t)(f(\theta, q) - \bar{f}(q)) + D\Delta_\theta q(\theta, t), \quad (63)$$

with normalization  $\int q(\theta, t) d\theta = 1$ .

Variables and Parameters:

- $q(\theta, t)$  is the trait distribution density at time  $t$ .
- $f(\theta, q) = \alpha \theta_1 + \theta_2$  is the fitness function.
- $\bar{f}(q) = \int q(\theta, t)f(\theta)d\theta$  is the mean fitness of the population.
- $D$  = mutation diffusion coefficient.

Typical Parameter Values:

- $D \sim 10^{-3}\text{--}10^{-1}$  (trait<sup>2</sup>/generation).
- $f$  is typically nondimensional.