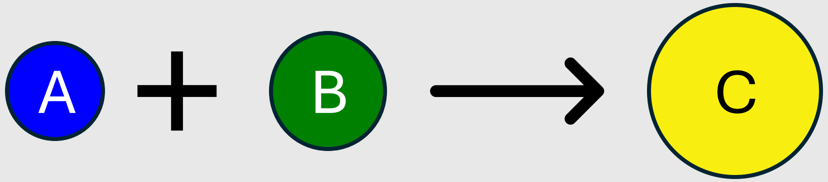
Simulating Continuous Systems Part 2

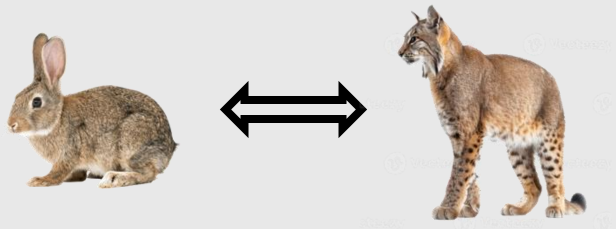
CMSC 326 Simulations

Simulating Continuous Systems

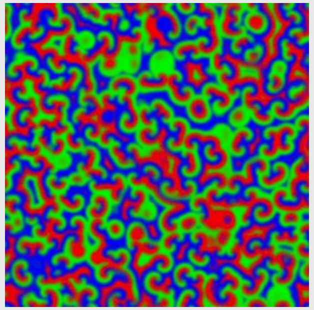
Simple chemical reaction



Rabbit–Lynx “reaction”



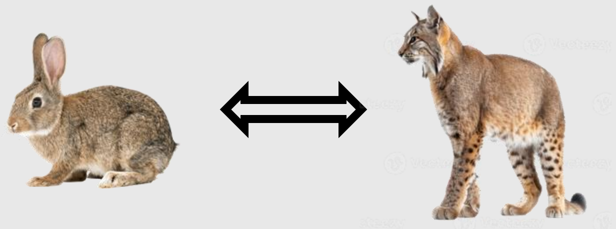
B-Z reaction



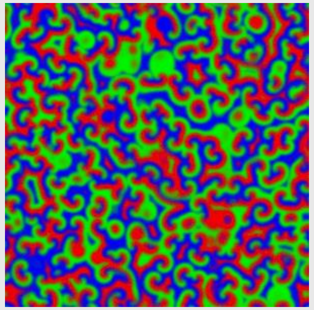
Simulating Continuous Systems

Simple chemical reaction $A + B \longrightarrow C$

Rabbit–Lynx "reaction"



B-Z reaction



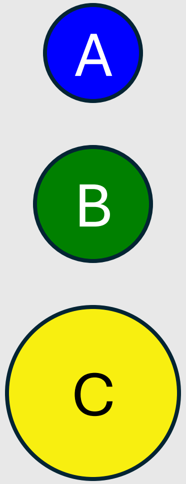
Simulation: Simple Chemical Reaction

Three molecules:

Substance

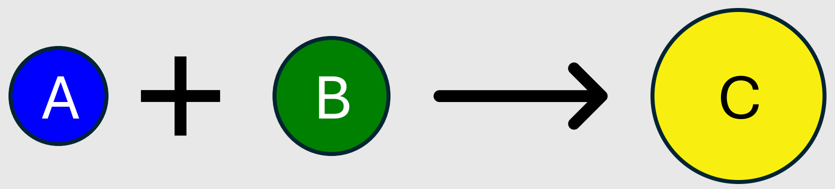
Substance

Substance

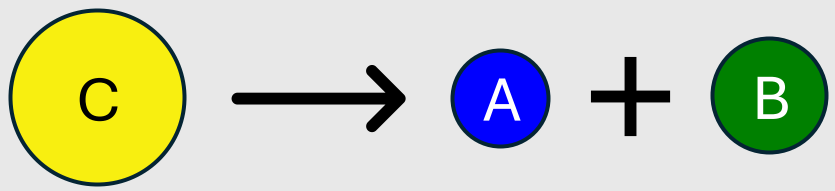


Simulation: Simple Chemical Reaction

Reaction 1:
One molecule of **A** *reacts*
with one molecule of **B**
to produce one molecule of **C**

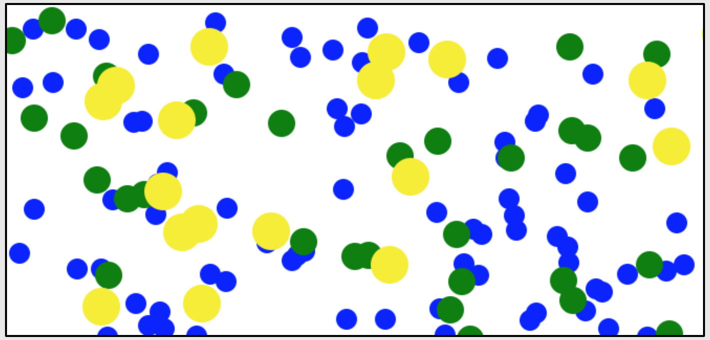


Reaction 2:
A molecule of **C** can *breakdown*
to produce one of each **A** and **B**



Two Simulation Models

Molecules move about randomly in a solution or a gaseous state



At any given instant, exactly one of the two reactions takes place

$$A + B \longrightarrow C$$

$$C \longrightarrow A + B$$

Two Simulation Models

1. We randomly choose the first or second reaction based on the **concentration of molecules**

2. We randomly choose the first or second reaction based on **spatial closeness of molecules**

The Ideal Simulation Model

1. Accurately matches reality
2. Simple to implement, simple to understand
3. Fast execution time computationally
4. As little randomness as possible
5. As few parameters as possible

Deterministic Simulation

A **deterministic simulation** is one in which no randomness is involved in the development of future states of the simulation. Each successive state of the simulation is completely determined by the preceding state.

Consider a Deterministic Model

$A(t)$ = concentration of A molecules at time t

$B(t)$ = concentration of B molecules at time t

$C(t)$ = concentration of C molecules at time t

Focus on A(t)

Consider the concentration a moment later:

$$A(t + s)$$

where $\boldsymbol{s}$ is a small value (like 0.01 seconds)

During $\boldsymbol{s}$, what affects the *concentration* of A?

Focus on A(t)

Let's consider the *change in concentration*:

$$A(t + s) - A(t)$$

Concentration could **decrease** because
A molecules react with B molecules

The *amount of change* depends on $A(t)$ and $B(t)$

Focus on A(t)

Let's consider the *change in concentration*:

$$A(t+s) - A(t)$$

Concentration could **increase** because of C molecules that break down

The *amount of change* depends on $C(t)$

Focus on A(t)

Thus, in that small time S

$A(t+s) - A(t)$ **decreases** in proportion to $A(t)\,B(t)$

$A(t+s) - A(t)$ **increases** in proportion to $C(t)$

The *amount of change* depends on the length of S

- **The more $\boldsymbol{S}$ the more time for reactions**

Putting This All Together

$$A(t+s) - A(t) = \; s\,(C(t) - A(t)\,B(t))$$

Putting This All Together

$$\underbrace{A(t+s) - A(t)}_{\text{The change in concentration of molecule } A \text{ during time } s} = s\,(C(t) - A(t)\,B(t))$$

Putting This All Together

$$A(t+s) - A(t) = s\,(C(t) - A(t)\,B(t))$$

The small moment in time S

Putting This All Together

$$A(t+s) - A(t) = s\,(C(t) - A(t)\,B(t))$$

The same small time period S

Putting This All Together

$$A(t+s) - A(t) = s\,(C(t) - A(t)\,B(t))$$

The small moment in time s

The time s is included because the **longer the time** s, the more reactions occur, and the **more change in concentration** can happen.

Putting This All Together

$$A(t+s) - A(t) = s\,(C(t) - A(t)\,B(t))$$

Concentration of molecule C

Increases the change in concentration of molecule A

Putting This All Together

$$A(t+s) - A(t) = s\,(C(t) - A(t)\,B(t))$$

C $\longrightarrow$ A + B

Concentration of molecule C

Increases the change in concentration of molecule A

Putting This All Together

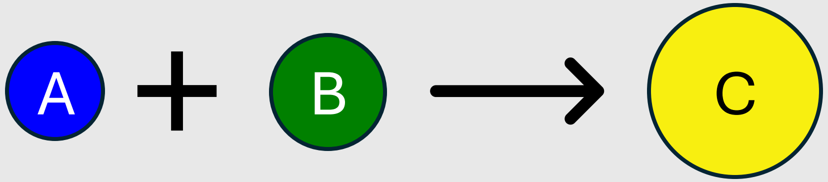
$$A(t+s) - A(t) = s\,(C(t) - \underbrace{A(t)\,B(t)}_{})$$

Concentration of molecule A times concentration of molecule B

Decreases the change in concentration of molecule A

Putting This All Together

$$A(t+s) - A(t) = s\,(C(t) - \underbrace{A(t)\,B(t)})$$



Concentration of molecule A times concentration of molecule B

Decreases the change in concentration of molecule A

By the Same Reasoning

$$B(t+s) - B(t) = \; s\,(C(t) - A(t)\,B(t))$$

Change in Concentration of Molecule C

$C(t+s) - C(t)$ **increases** in proportion to $A(t)\,B(t)$
$C(t+s) - C(t)$ **decreases** in proportion to $C(t)$

Thus,

$$C(t+s) - C(t) = s\,(A(t)\,B(t) - C(t))$$

Change in Concentration of Molecule C

$C(t+s) - C(t)$ **increases** in proportion to $A(t)\,B(t)$

$C(t+s) - C(t)$ **decreases** in proportion to $C(t)$

Thus,

$$C(t+s) - C(t) = s\,\underbrace{(A(t)\,B(t) - C(t))}_{\text{The terms are now reversed}}$$

Change in Concentration of Molecule C

$$C(t+s) - C(t) = s\,(A(t)\,B(t) - C(t))$$

Change in Concentration of Molecule C

$$C(t+s) - \underbrace{C(t)}_{\text{The concentration of molecule } C \text{ at time } t} = s\,(A(t)\,B(t) - C(t))$$

Change in Concentration of Molecule C

$$C(t+s) - C(t) = \; s\,(A(t)\,B(t) - C(t))$$

The concentration of molecule C at time t plus s

The concentration of molecule C at the "next moment in time"

Change in Concentration of Molecule C

$$\underbrace{C(t+s) - C(t)} = s\,(A(t)\,B(t) - C(t))$$

The **change in concentration** of molecule C during time s

Change in Concentration of Molecule C

$$C(t+s) - C(t) = \; s\,(A(t)\,B(t) - C(t))$$

The small moment in time s

The time s is included because the **longer the time** s, the more reactions occur, and the **more change in concentration** can happen.

Change in Concentration of Molecule C

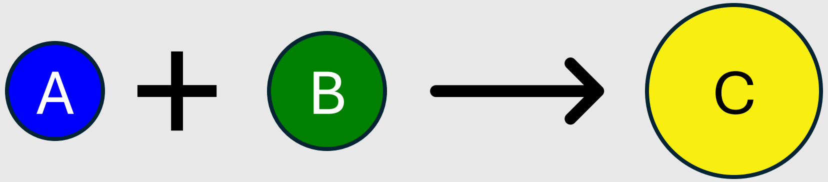
$$C(t+s) - C(t) = s\,(A(t)\,B(t) - C(t))$$

Concentration of molecule A times concentration of molecule B

Increases the change in concentration of molecule C

Change in Concentration of Molecule C

$$C(t+s) - C(t) = s\,\big(\underbrace{A(t)\,B(t)} - C(t)\big)$$



Concentration of molecule A times concentration of molecule B

Increases the change in concentration of molecule C

Change in Concentration of Molecule C

$$C(t+s) - C(t) = s\,(A(t)\,B(t) - \underbrace{C(t)})$$

Concentration of molecule C

Decreases the change in concentration of molecule C

Change in Concentration of Molecule C

$$C(t+s) - C(t) = s\,(A(t)\,B(t) - C(t))$$

C ⟶ A + B

Concentration of molecule C

Decreases the change in concentration of molecule C

A System of Equations

$$A(t+s) - A(t) = s\,(C(t) - A(t)\,B(t))$$

$$B(t+s) - B(t) = s\left(C(t) - A(t)\,B(t)\right)$$

$$C(t+s) - C(t) = s\,(A(t)\,B(t) - C(t))$$

One Important Modification

It may be that the first reaction (A + B → C)
is **more likely** than the second, or the reverse

To adjust, we'll introduce multipliers:

K_{ab} = constant for first reaction (A + B → C)

K_c = constant for second reaction (C → A + B)

A System of Equations

$$A(t+s) - A(t) = s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$

$$B(t+s) - B(t) = s\left(K_c\,C(t) - K_{ab}\,A(t)\,B(t)\right)$$

$$C(t+s) - C(t) = s\,(K_{ab}\,A(t)\,B(t) - K_c\,C(t))$$

A System of Equations

$$A(t+s) - A(t) = s\left(K_c\, C(t) - \boxed{K_{ab}}\, A(t)\, B(t)\right)$$

$$B(t+s) - B(t) = s\left(K_c\, C(t) - \boxed{K_{ab}}\, A(t)\, B(t)\right)$$

$$C(t+s) - C(t) = s\left(\boxed{K_{ab}}\, A(t)\, B(t) - K_c\, C(t)\right)$$

Use a **high value** of the constant K_{ab} to indicate that the first reaction is **more likely**, or happens at a faster rate

A System of Equations

$$A(t+s) - A(t) = s\left(\boxed{K_c}\, C(t) - K_{ab}\, A(t)\, B(t)\right)$$

$$B(t+s) - B(t) = s\left(\boxed{K_c}\, C(t) - K_{ab}\, A(t)\, B(t)\right)$$

$$C(t+s) - C(t) = s\left(K_{ab}\, A(t)\, B(t) - \boxed{K_c}\, C(t)\right)$$

Use a **high value** of the constant K_c to indicate that the second reaction is **more likely**, or happens at a faster rate

A System of Equations

$$A(t+s) - A(t) = s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$

$$B(t+s) - B(t) = s\left(K_c\,C(t) - K_{ab}\,A(t)\,B(t)\right)$$

$$C(t+s) - C(t) = s\,(K_{ab}\,A(t)\,B(t) - K_c\,C(t))$$

A System of Equations

$+\,A(t) \qquad\qquad +\,A(t)$

$$A(t+s) - A(t) = s\,\left(K_c\, C(t) - K_{ab}\, A(t)\, B(t)\right)$$

$+\,B(t) \qquad\qquad +\,B(t)$

$$B(t+s) - B(t) = s\,\left(K_c\, C(t) - K_{ab}\, A(t)\, B(t)\right)$$

$+\,C(t) \qquad\qquad +\,C(t)$

$$C(t+s) - C(t) = s\,\left(K_{ab}\, A(t)\, B(t) - K_c\, C(t)\right)$$

A System of Equations

$$A(t+s) = A(t) + s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$

$$B(t+s) = B(t) + \ s\left(K_c\,C(t) - K_{ab}\,A(t)\,B(t)\right)$$

$$C(t+s) = C(t) + \ s\,(K_{ab}\,A(t)\,B(t) - K_c\,C(t))$$

A System of Equations

Next Value ⟵ Forward ⟵ **Current** Values

$$A(t+s) = A(t) + s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$

$$B(t+s) = B(t) + \; s\left(K_c\,C(t) - K_{ab}\,A(t)\,B(t)\right)$$

$$C(t+s) = C(t) + \; s\,(K_{ab}\,A(t)\,B(t) - K_c\,C(t))$$

We now have a way to **calculate** the changes in concentrations as we go **forward in time**

Calculate the Change in Concentration

Suppose we know the **starting concentrations** at time $t = 0$, that is, we know $A(0)$, $B(0)$ and $C(0)$

Suppose that $s = 0.01, K_{ab} = 1.0, K_c = 0.5$

Calculate the Change in Concentration

We can now compute:

$$A(0+0.01) = A(0) + 0.01\,(0.5\,C(0) - 1.0\,A(0)\,B(0))$$

$$B(0+0.01) = B(0) + 0.01\,(0.5\,C(0) - 1.0\,A(0)\,B(0))$$

$$C(0+0.01) = C(0) + 0.01\,(1.0\,A(0)\,B(0) - 0.5\,C(0))$$

Compute the Change in Concentration

```
# Rate parameters
K_ab = 1.0
K_c = 0.5

# Initial concentration values
A = 0.6
B = 0.3
C = 0.1

# Set our time increment
s = 0.01

# Compute
while t < end_time:
    # Compute the new values at time t + s
    A = A + s * (K_c * C - K_ab * A * B)
    B = B + s * (K_c * C - K_ab * A * B)
    C = C + s * (K_ab * A * B - K_c * C)

    # Change t, and repeat
    t = t + s
```

Compute the Change in Concentration

$$K_{ab} = 1.0$$
$$K_c = 0.5$$

```
# Rate parameters
K_ab = 1.0
K_c = 0.5

# Initial concentration values
A = 0.6
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# Compute
while t < end_time:
    # Compute the new values at time t + s
    A = A + s * (K_c * C - K_ab * A * B)
    B = B + s * (K_c * C - K_ab * A * B)
    C = C + s * (K_ab * A * B - K_c * C)

    # Change t, and repeat
    t = t + s
```

Compute the Change in Concentration

$$A(0)$$
$$B(0)$$
$$C(0)$$

```
# Rate parameters
K_ab = 1.0
K_c = 0.5

# Initial concentration values
A = 0.6
B = 0.3
C = 0.1

# Set our time increment
s = 0.01

# Compute
while t < end_time:
    # Compute the new values at time t + s
    A = A + s * (K_c * C - K_ab * A * B)
    B = B + s * (K_c * C - K_ab * A * B)
    C = C + s * (K_ab * A * B - K_c * C)

    # Change t, and repeat
    t = t + s
```

Compute the Change in Concentration

$$s = 0.01$$

```
# Rate parameters
K_ab = 1.0
K_c = 0.5

# Initial concentration values
A = 0.6
B = 0.3
C = 0.1

# Set our time increment
s = 0.01

# Compute
while t < end_time:
    # Compute the new values at time t + s
    A = A + s * (K_c * C - K_ab * A * B)
    B = B + s * (K_c * C - K_ab * A * B)
    C = C + s * (K_ab * A * B - K_c * C)

    # Change t, and repeat
    t = t + s
```

Compute the Change in Concentration

```
# Rate parameters
K_ab = 1.0
K_c = 0.5

# Initial concentration values
A = 0.6
B = 0.3
C = 0.1

# Set our time increment
s = 0.01

# Compute
while t < end_time:
    # Compute the new values at time t + s
    A = A + s * (K_c * C - K_ab * A * B)
    B = B + s * (K_c * C - K_ab * A * B)
    C = C + s * (K_ab * A * B - K_c * C)

    # Change t, and repeat
    t = t + s
```

Iterate

Compute the Change in Concentration

```python
# Rate parameters
K_ab = 1.0
K_c = 0.5

# Initial concentration values
A = 0.6
B = 0.3
C = 0.1

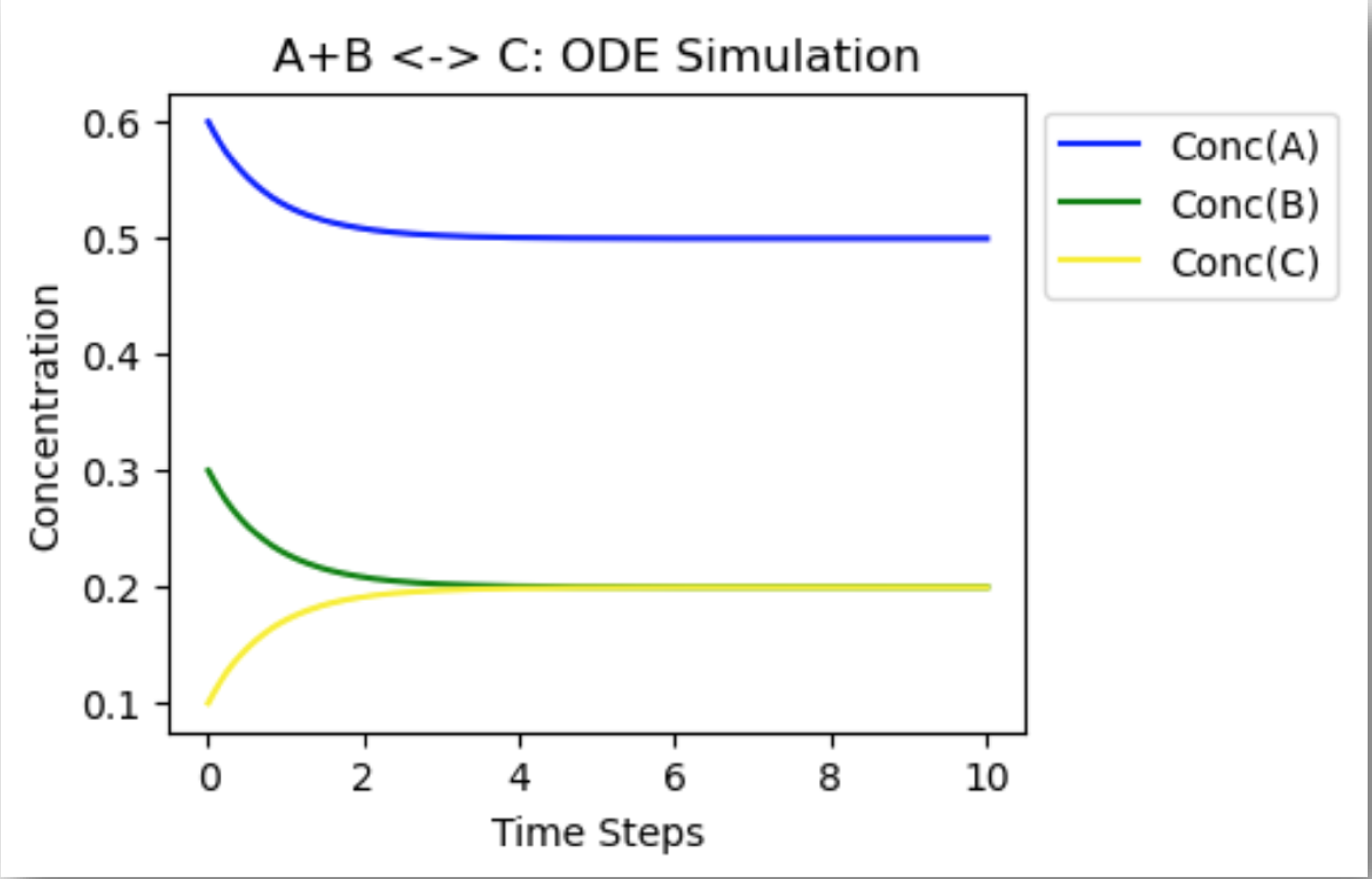
# Set our time increment
s = 0.01

# Compute
while t < end_time:
    # Compute the new values at time t + s
    A = A + s * (K_c * C - K_ab * A * B)
    B = B + s * (K_c * C - K_ab * A * B)
    C = C + s * (K_ab * A * B - K_c * C)

    # Change t, and repeat
    t = t + s
```

$$A(t+s) = A(t) + s\left(K_c\, C(t) - K_{ab}\, A(t)\, B(t)\right)$$
$$B(t+s) = B(t) + s\left(K_c\, C(t) - K_{ab}\, A(t)\, B(t)\right)$$
$$C(t+s) = C(t) + s\left(K_{ab}\, A(t)\, B(t) - K_c\, C(t)\right)$$

Simulation Behavior



What is a Differential Equation?

Recall how we compute the concentrations evolving over time:

$$A(t+s) = A(t) + s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$

$$B(t+s) = B(t) + \ s\left(K_c\,C(t) - K_{ab}\,A(t)\,B(t)\right)$$

$$C(t+s) = C(t) + \ s\,(K_{ab}\,A(t)\,B(t) - K_c\,C(t))$$

What is a Differential Equation?

The form of these equations is:

Next Value

Current Value

Some terms involving the **current** values of some variables

$$A(t+s) = A(t) + s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$

The equations specify an **iterative algorithm** to compute the functions $A(t), B(t), C(t)$

What is a Differential Equation?

The form of these equations is:

Next Value	**Current** Value	Some terms involving the **current** values of some variables

$$A(t+s) = A(t) + s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$

The fact that we compute in the way time evolves makes this a **simulation**

What is a Differential Equation?

Rearrange the terms in this way:

$$\frac{A(t+s) - A(t)}{s} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{B(t+s) - B(t)}{s} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{C(t+s) - C(t)}{s} = K_{ab}\, A(t)\, B(t) - K_c\, C(t)$$

What is a Differential Equation?

Next, consider the limit as $s \to 0$

$$A_s(t) = \frac{A(t+s) - A(t)}{s}$$

What is a Differential Equation?

Next, consider the limit as $s \to 0$

$$A_s(t) = \frac{A(t+s) - A(t)}{s}$$

Then the *sequence of functions* A_s
possibly has a limit as $s \to 0$

That limit is itself a function: $A'(\mathrm{t})$

Called the **derivative** of function $A(t)$

What is a Differential Equation?

If we do this for each of $A(t), B(t), \mathrm{C}(t)$ we get:

$$A'(\mathrm{t}) \;=\; K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$B'(\mathrm{t}) = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$C'(\mathrm{t}) = K_{ab}\, A(t)\, B(t) - K_c\, C(t)$$

What is a Differential Equation?

Sometimes written in slightly different notation as:

$$\frac{dA}{dt} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{dB}{dt} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{dC}{dt} = K_{ab}\, A(t)\, B(t) - K_c\, C(t)$$

What is a Differential Equation?

System of Differential Equations

$$\frac{dA}{dt} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{dB}{dt} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{dC}{dt} = K_{ab}\, A(t)\, B(t) - K_c\, C(t)$$

What is a Differential Equation?

System of Differential Equations

$$\frac{dA}{dt} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{dB}{dt} = K_c\, C(t) - K_{ab}\, A(t)\, B(t)$$

$$\frac{dC}{dt} = K_{ab}\, A(t)\, B(t) - K_c\, C(t)$$

Note: we usually call these *Ordinary Differential Equations* (ODEs) to distinguish them from other kinds (like partial differential equations)

Compute the Change in Concentration

```
# Rate parameters
K_ab = 1.0
K_c = 0.5

# Initial concentration values
A = 0.6
B = 0.3
C = 0.1

# Set our time increment
s = 0.01

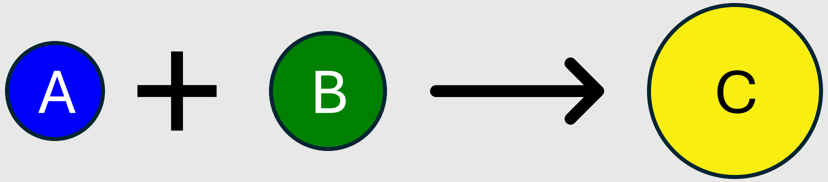
# Compute
while t < end_time:
    # Compute the new values at time t + s
    A = A + s * (K_c * C - K_ab * A * B)
    B = B + s * (K_c * C - K_ab * A * B)
    C = C + s * (K_ab * A * B - K_c * C)

    # Change t, and repeat
    t = t + s
```

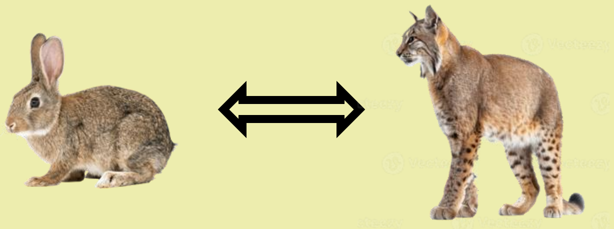
$$A(t+s) = A(t) + s\,(K_c\,C(t) - K_{ab}\,A(t)\,B(t))$$
$$B(t+s) = B(t) + s\,\left(K_c\,C(t) - K_{ab}\,A(t)\,B(t)\right)$$
$$C(t+s) = C(t) + s\,(K_{ab}\,A(t)\,B(t) - K_c\,C(t))$$

Simulating Continuous Systems

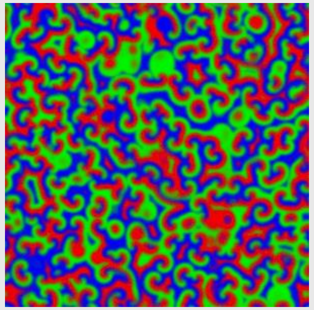
Simple chemical reaction



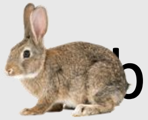
Rabbit–Lynx “reaction”



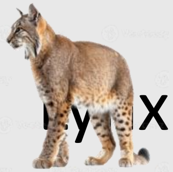
B-Z reaction



Rabbit-Lynx ”Reaction"



Rabbit = prey



Lynx = predator

Although not a chemical reaction,
it almost is (mathematically)

We will model a population of rabbits and lynxes

Rabbit-Lynx ”Reaction"

The environment has sufficient grass for the rabbits to survive

The lynxes, of course, eat the rabbits to thrive

Rabbit-Lynx ”Reaction"

Proportions involved:

1. Rabbits grow at a certain rate

2. Rabbits die at a rate proportional to how many rabbits there are and how many are being devoured by lynxes

3. Lynxes proliferate based on their consumption of rabbits, and die in numbers proportional to the lynx population

Rabbit-Lynx Simulation Model

$X(t)$ = number of rabbits at time t

$Y(t)$ = number of lynxes at time t

Rabbit-Lynx Simulation Model

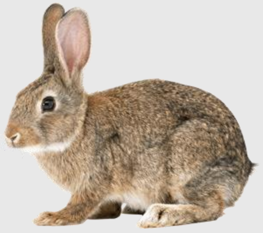
Consider the time interval from t to $t + s$

$X(t + s) - X(t)$ is the change in the number of rabbits

$X(t + s) - X(t)$ will:

- increase from new rabbits born
- decrease from rabbits dying naturally
- decrease from rabbits killed by lynxes
- be proportional to s

Rabbit-Lynx Simulation Model



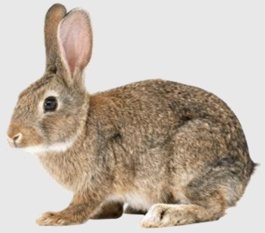
Thus, we can write for the rabbit:

$$X(t+s) - X(t) = s\,(k_1\,X(t) - k_2\,X(t)\,Y(t))$$

Rabbit-Lynx Simulation Model

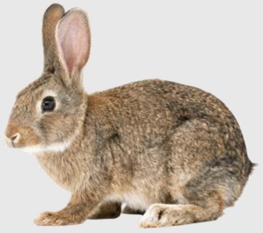
$$\underbrace{X(t+s) - X(t)}_{\text{The }\textbf{change in number}\text{ of rabbits } X \text{ during time } S} = s\,(k_1\, X(t) - k_2\, X(t)\, Y(t))$$

Rabbit-Lynx Simulation Model



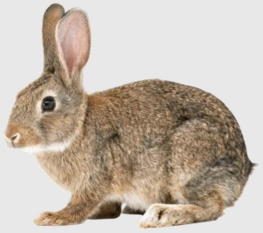
$$X(t+s) - X(t) = \underbrace{s}_{\text{The small moment in time } S} \left(k_1\, X(t) - k_2\, X(t)\, Y(t)\right)$$

Rabbit-Lynx Simulation Model



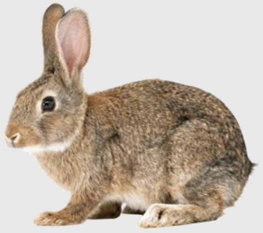
$$X(t+s) - X(t) = s\,(\underbrace{k_1}_{\text{Constant to indicate the likelihood of rabbit birth}}\,X(t) - k_2\,X(t)\,Y(t))$$

Rabbit-Lynx Simulation Model



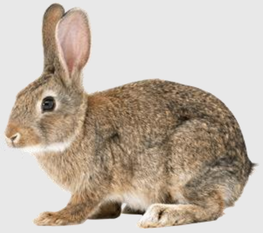
$$X(t+s) - X(t) = s\,(k_1 \underbrace{X(t)}_{\text{Number of rabbits at time } t} - k_2\, X(t)\, Y(t))$$

Rabbit-Lynx Simulation Model



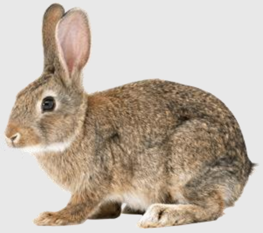
$$X(t+s) - X(t) = s\,(k_1\,X(t) - \underbrace{k_2}_{\text{Constant to indicate the likelihood of lynx eating a rabbit}}\,X(t)\,Y(t))$$

Rabbit-Lynx Simulation Model



$$X(t+s) - X(t) = s\,\big(k_1\, X(t) - k_2\, \underbrace{X(t)\, Y(t)}_{\text{Number or rabbits times the number of lynx at time } t}\big)$$

Rabbit-Lynx Simulation Model



$$X(t+s) - X(t) = s\,(\underbrace{k_1\,X(t)} - k_2\,X(t)\,Y(t))$$

This term **increases** the number of rabbits

Rabbit-Lynx Simulation Model

$$X(t+s) - X(t) = s\,(k_1\,X(t) - \underbrace{k_2\,X(t)\,Y(t))}$$

This term **decreases** the number of rabbits

Rabbit-Lynx Simulation Model

Similarly, the lynx:

$$Y(t+s) - Y(t) = s\,(k_2\,X(t)Y(t) - k_3\,Y(t))$$

Rabbit-Lynx Simulation Model

$$\underbrace{Y(t+s) - Y(t)} = s\,(k_2\,X(t)Y(t) - k_3\,Y(t))$$

The **change in number** of lynx Y during time s

Rabbit-Lynx Simulation Model

$$Y(t+s) - Y(t) = s\,(\underbrace{k_2\,X(t)Y(t)} - k_3\,Y(t))$$

This term **increases** the number of lynx, because the rabbits that are killed are the ones that "generate" the lynxes

Rabbit-Lynx Simulation Model

$$Y(t+s) - Y(t) = s\,\left(k_2\,X(t)Y(t) - \underbrace{k_3\,Y(t)}\right)$$

This term **decreases** the number of lynx due to overcrowding

Rabbit-Lynx Equations

$$X(t+s) - X(t) = s\,(k_1\,X(t) - k_2\,X(t)\,Y(t))$$

$$Y(t+s) - Y(t) = s\,(k_2\,X(t)Y(t) - k_3\,Y(t))$$

Rabbit-Lynx Equations as ODEs

$$X'(t) = k_1\, X(t) - k_2\, X(t)\, Y(t)$$

$$Y'(t) = k_2\, X(t) Y(t) - k_3\, Y(t)$$

Rabbit-Lynx Equations

$$X(t+s) - X(t) = s\,(k_1\,X(t) - k_2\,X(t)\,Y(t))$$

$$Y(t+s) - Y(t) = s\,(k_2\,X(t)Y(t) - k_3\,Y(t))$$

Rabbit-Lynx Equations

$+X(t)$ $\quad$ $+X(t)$

$$X(t+s) - X(t) = s\,(k_1\,X(t) - k_2\,X(t)\,Y(t))$$

$+Y(t)$ $\quad$ $+Y(t)$

$$Y(t+s) - Y(t) = s\,(k_2\,X(t)Y(t) - k_3\,Y(t))$$

Rabbit-Lynx Equations

$$X(t+s) = X(t) + s\,(k_1\,X(t) - k_2\,X(t)\,Y(t))$$

$$Y(t+s) = Y(t) + s\,(k_2\,X(t)Y(t) - k_3\,Y(t))$$

Rabbit-Lynx Equations

Next Value	Forward	**Current** Values

$$X(t+s) = X(t) + \ s\ (k_1\, X(t) - k_2\, X(t)\, Y(t))$$

$$Y(t+s) = Y(t) + s\ (k_2\, X(t) Y(t) - k_3\, Y(t))$$

Rabbit-Lynx Equations

$$X(t+s) = X(t) + \ s\,(k_1\,X(t) - k_2\,X(t)\,Y(t))$$

$$Y(t+s) = Y(t) + s\,(k_2\,X(t)Y(t) - k_3\,Y(t))$$

What do we need to solve this computationally?

Rabbit-Lynx Equations

```
# Model parameters:
k1 = 2.4
k2 = 4.2
k3 = 5.1

# Small amount of time
s = 0.01

# Current time, Initial populations
t = 0.0
X = 1.5
Y = 1.0

# Simulation
while t <= end_time:
    # Rabbit / Lynx "reaction" equations
    X = X + s * (k1 * X - k2 * X * Y)
    Y = Y + s * (k2 * X * Y - k3 * Y)

    # Next time step
    t = t + s
```

Rabbit-Lynx Equations

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Rabbit-Lynx Equations

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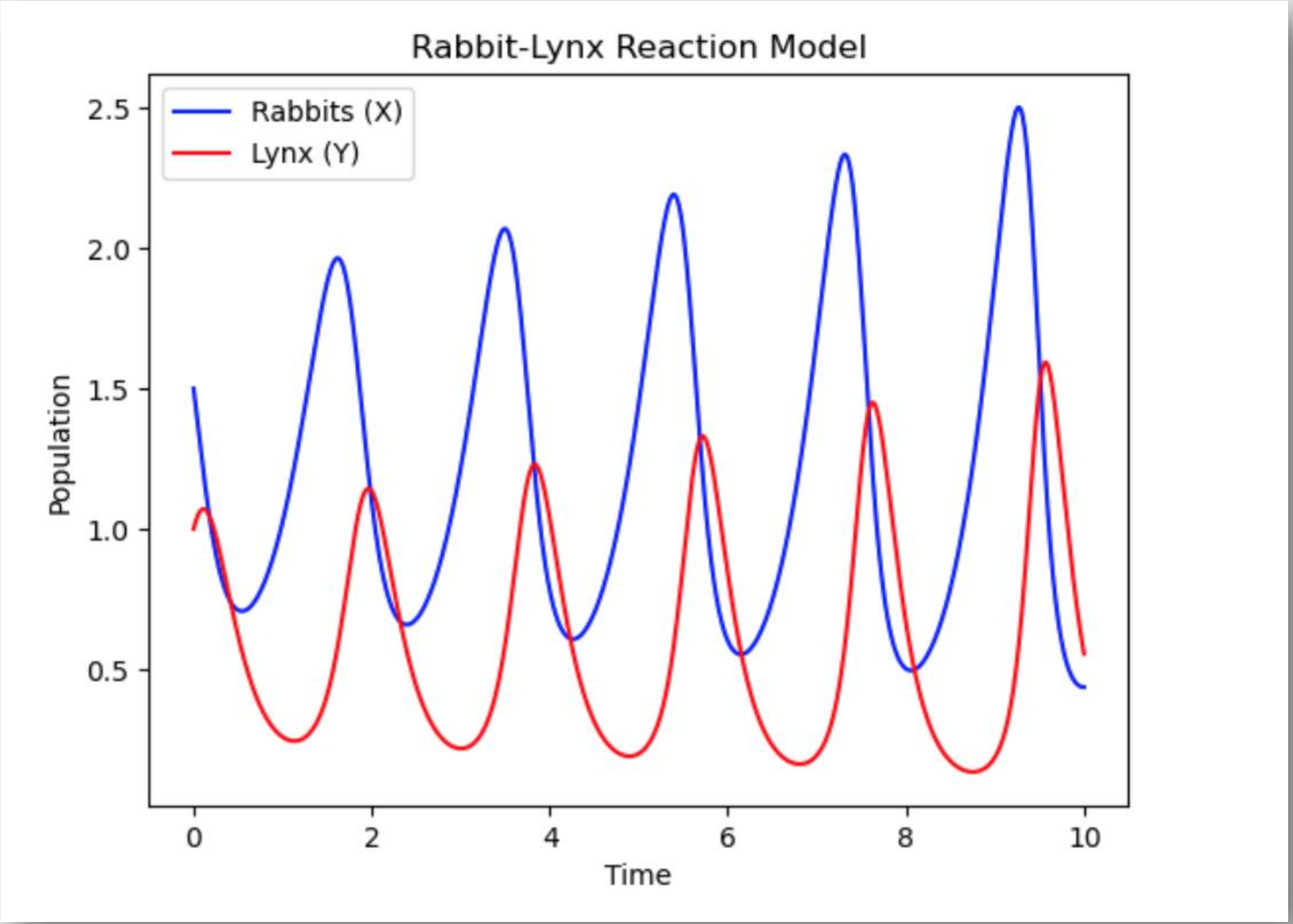
```

Rabbit-Lynx “Reaction”



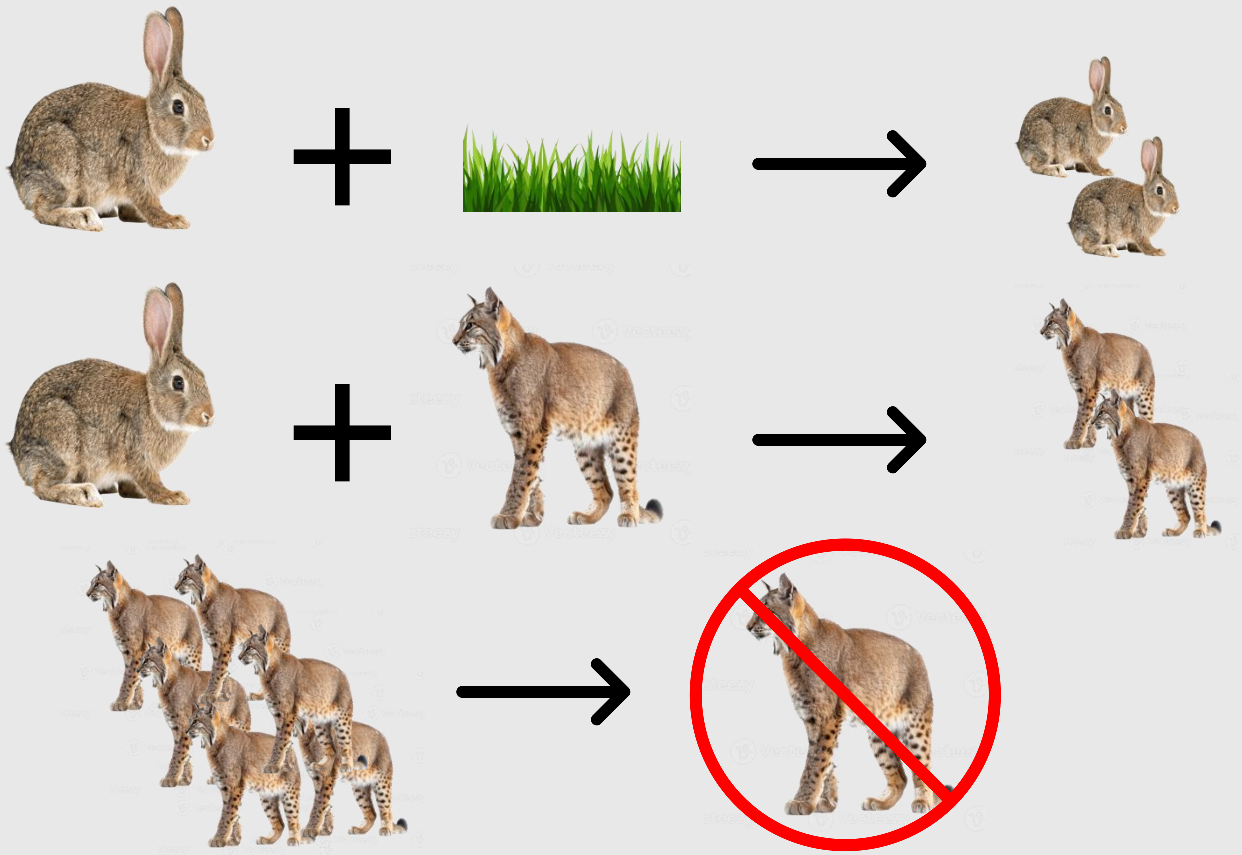
About the Rabbit-Lynx Model

We see that there is a natural oscillation in the populations of rabbits and lynxes:

- The populations don't ever "settle"
- Oscillation is "built in" to the model
- We could hardly have predicted this by staring at the equations or through intuition

About the Rabbit-Lynx Model

Rabbits and lynxes as interacting "molecules", the "reactions" could be written as:

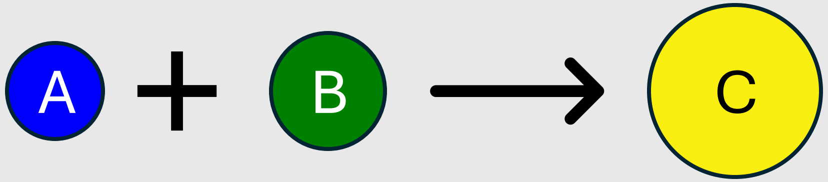


About the Rabbit-Lynx Model

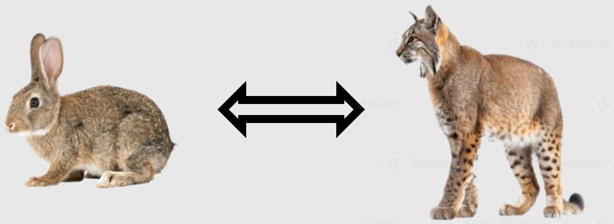
One wonders: Is there a chemical reaction that displays oscillation?

Simulating Continuous Systems

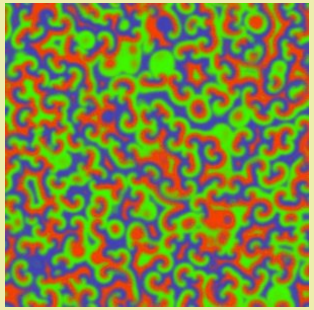
Simple chemical reaction



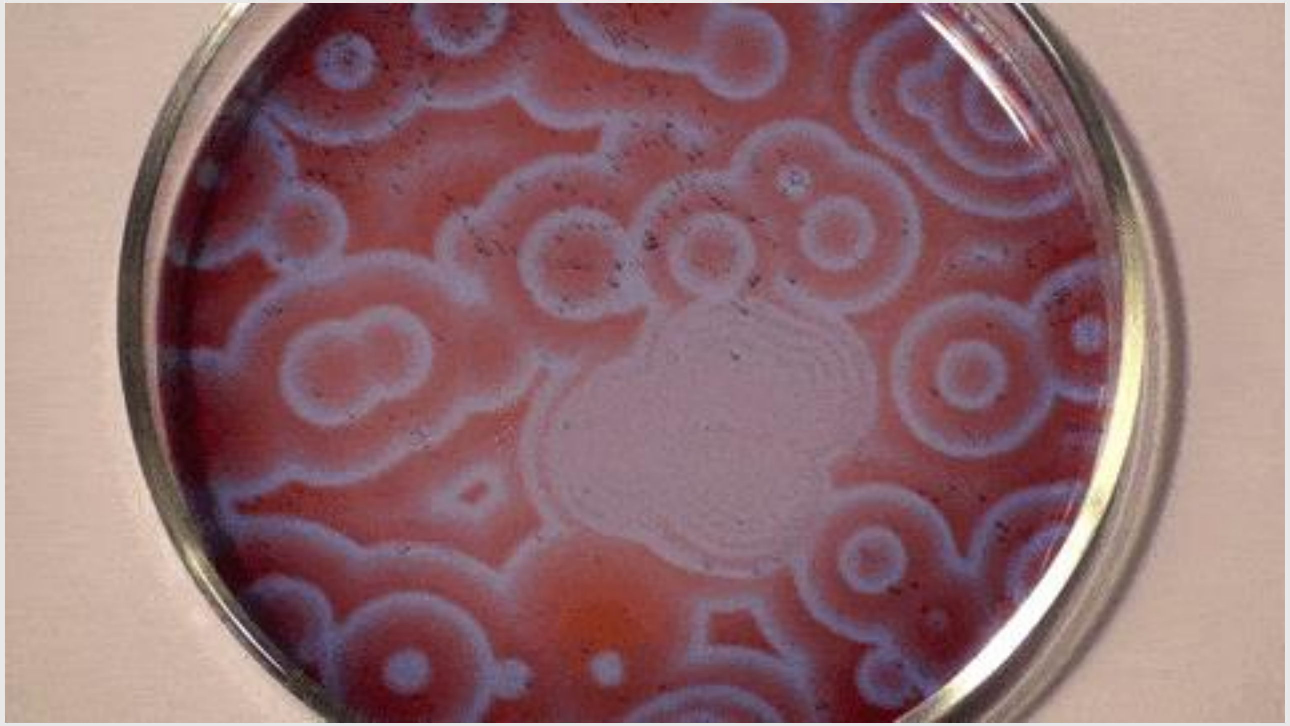
Rabbit–Lynx “reaction”



B-Z reaction



B-Z Reaction



B-Z Reaction

In 1951, the Russian chemist **B**elousov discovered a chemical reaction involving citric acid, acidified bromate, and ceric ions that displayed spectacular oscillations: turning yellow, then colorless, then yellow, in turn.

Belousov couldn't publish his result because nobody believed it!

B-Z Reaction

Later, a student called **Z**habotinsky resurrected the work and convinced others, too late unfortunately for Belousov, who died in 1970 before receiving the prestigious Lenin Prize posthumously in 1980.

B-Z Reaction

The simplified differential equations:

$$X'(t) = q\,Y(t) - X(t)\,Y(t) + X(t)\,(1 - X(t))$$

$$Y'(t) = \frac{1}{e}\,(-q\,Y(t) - X(t)\,Y(t) + f\,Z(t))$$

$$Z'(t) = X(t) - Z(t)$$

Three variables depicting three concentrations

B-Z Reaction