

Temporal

```

import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact_manual, FloatSlider
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display

# ===== Quasi-steady dimer functions =====
def plot_stream(alpha,beta,n,Kd):
    def compute_A2_B2(Atot, Btot, Kd=Kd):
        S = Atot + Btot
        denom_common = Kd + 4.0*S + np.sqrt(Kd**2 + 8.0*S*Kd)
        A2 = 2.0 * Atot**2 / denom_common
        B2 = 2.0 * Btot**2 / denom_common
        return A2, B2

    # ===== Vector field definition =====
    def dAt_dt(Atot, Btot):
        A2, _ = compute_A2_B2(Atot, Btot)
        actA = beta * (A2**n) / (1.0 + A2**n)
        return alpha + actA - Atot

    def dBt_dt(Atot, Btot):
        _, B2 = compute_A2_B2(Atot, Btot)
        actB = beta * (B2**n) / (1.0 + B2**n)
        return alpha + actB - Btot

    # ===== Step 1: Define the grid =====
    start_x, end_x, num_points_x = 0, 50, 1000
    start_y, end_y, num_points_y = 0, 50, 1000
    x, y = np.meshgrid(np.linspace(start_x, end_x, num_points_x),
                        np.linspace(start_y, end_y, num_points_y))

    # ===== Step 2: Compute vector components =====
    u = dAt_dt(x, y) # x-component
    v = dBt_dt(x, y) # y-component

    # ===== Step 3: Compute magnitude for coloring =====
    magnitude = np.sqrt(u**2 + v**2)

    # ===== Step 4: Create the streamline plot =====
    plt.figure(figsize=(8, 6))
    plt.streamplot(x, y, u, v, color=magnitude, cmap='plasma',
                   linewidth=1.5, density=2.5, arrowstyle='->')
    plt.colorbar(label="Vector Magnitude")
    plt.contour(x, y, u, levels=[0], colors='red', linewidths=2, linestyles='--')
    plt.contour(x, y, v, levels=[0], colors='black', linewidths=2, linestyles='--')

    # ===== Step 5: Labels and styling =====
    plt.title("Phase Portrait with Magnitude Coloring")
    plt.xlabel(r"\$[A_{tot}]\$")
    plt.ylabel(r"\$[B_{tot}]\$")
    plt.axis("scaled")
    plt.grid(True)

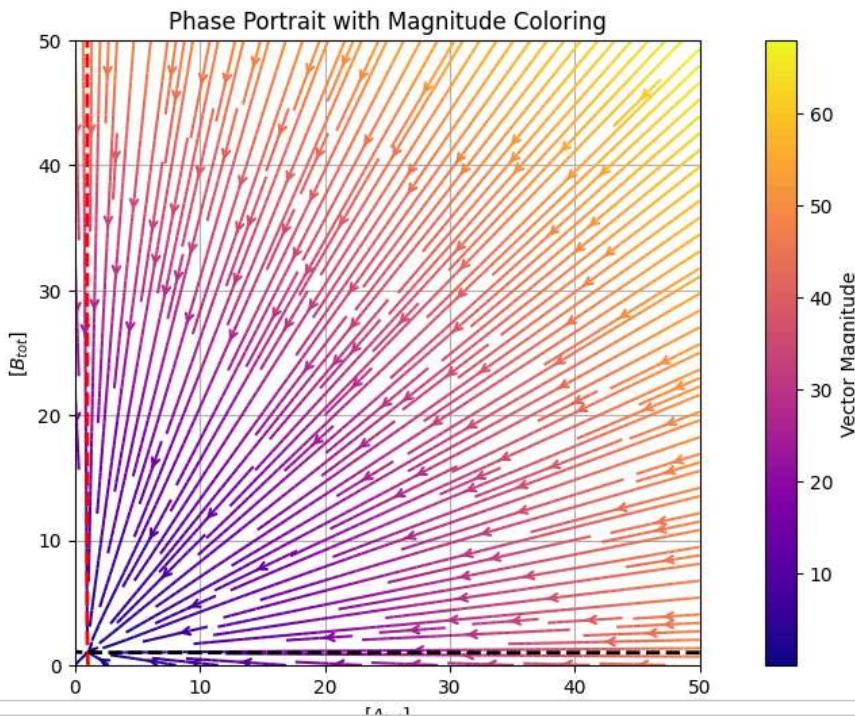
    plt.show()

# ===== Parameters =====
interact_manual(plot_stream,
                alpha = FloatSlider(min=0.1, max=3.0, step=0.1, value=1.0),
                beta = FloatSlider(min=0.5, max=15, step=0.5, value=1.0),
                n = FloatSlider(min=0.5, max=5.0, step=0.5, value=2.0),
                Kd = FloatSlider(min=0.1, max=3.0, step=0.1, value=1.0))

```

alpha	<input type="radio"/>	1.00
beta	<input type="radio"/>	1.00
n	<input type="radio"/>	2.00
Kd	<input type="radio"/>	1.00

Run Interact



```

import sympy as sp

# ===== Symbols =====
A, B = sp.symbols('A B', real=True, nonnegative=True)
alpha, beta, n, Kd = sp.symbols('alpha beta n Kd', positive=True)

# ===== Define A2, B2 symbolically =====
S = A + B
denom_common = Kd + 4*S + sp.sqrt(Kd**2 + 8*S*Kd)
A2 = 2*A**2 / denom_common
B2 = 2*B**2 / denom_common

# ===== Dynamics =====
dA = alpha + beta * (A2**n) / (1 + A2**n) - A
dB = alpha + beta * (B2**n) / (1 + B2**n) - B

# ===== Numerical solve =====
# Substitute parameter values
params = {alpha: 1.0, beta: 5.0, n: 2.0, Kd: 1.0}

# Try solving with an initial guess
sol = sp.nsolve([dA.subs(params), dB.subs(params)], (A, B), (5, 5))
print("Fixed point:", sol)

```

Fixed point: Matrix([[1.16312977452925], [1.16312977452925]])

```

import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact_manual, FloatSlider
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display

# ===== Numba acceleration =====
from numba import njit, prange

@njit(fastmath=True)

```

```

def _compute_A2_B2_elem(Atot, Btot, Kd):
    S = Atot + Btot
    # Denominator shared by both A2 and B2
    denom_common = Kd + 4.0 * S + np.sqrt(Kd * Kd + 8.0 * S * Kd)
    A2 = 2.0 * Atot * Atot / denom_common
    B2 = 2.0 * Btot * Btot / denom_common
    return A2, B2

@njit(parallel=True, fastmath=True)
def _compute_field(x, y, alpha, beta, n, Kd):
    nx, ny = x.shape
    u = np.empty((nx, ny), dtype=np.float64)
    v = np.empty((nx, ny), dtype=np.float64)
    for i in prange(nx):
        for j in range(ny):
            At = x[i, j]
            Bt = y[i, j]
            A2, B2 = _compute_A2_B2_elem(At, Bt, Kd)

            # actA = beta * (A2**n) / (1 + A2**n)
            tA = A2 ** n
            actA = beta * (tA / (1.0 + tA))
            u[i, j] = alpha + actA - At

            # actB = beta * (B2**n) / (1 + B2**n)
            tB = B2 ** n
            actB = beta * (tB / (1.0 + tB))
            v[i, j] = alpha + actB - Bt
    return u, v

@njit(parallel=True, fastmath=True)
def _magnitude(u, v):
    nx, ny = u.shape
    mag = np.empty((nx, ny), dtype=np.float64)
    for i in prange(nx):
        for j in range(ny):
            # hypot for numerical stability
            mag[i, j] = np.hypot(u[i, j], v[i, j])
    return mag

# ===== Quasi-steady dimer functions (Numba-backed) =====
def plot_stream(alpha, beta, n, Kd):
    # ----- Define the grid -----
    start_x, end_x, num_points_x = 0.0, 30.0, 1000
    start_y, end_y, num_points_y = 0.0, 30.0, 1000

    # Note: meshgrid returns (ny, nx) shaped arrays with default indexing='xy'
    x_vals = np.linspace(start_x, end_x, num_points_x, dtype=np.float64)
    y_vals = np.linspace(start_y, end_y, num_points_y, dtype=np.float64)
    x, y = np.meshgrid(x_vals, y_vals) # shape = (ny, nx)

    # ----- Compute vector field with Numba -----
    u, v = _compute_field(x, y, float(alpha), float(beta), float(n), float(Kd))

    # ----- Magnitude for coloring (Numba) -----
    magnitude = _magnitude(u, v)

    # ----- Plot -----
    plt.figure(figsize=(8, 6))
    plt.streamplot(x, y, u, v, color=magnitude, cmap='plasma',
                   linewidth=1.5, density=2.5, arrowstyle='->')
    plt.colorbar(label="Vector Magnitude")

    # Nullclines: u=0 (red), v=0 (black)
    plt.contour(x, y, u, levels=[0], colors='red', linewidths=2, linestyles='--')
    plt.contour(x, y, v, levels=[0], colors='black', linewidths=2, linestyles='--')

    plt.title("Phase Portrait with Magnitude Coloring")
    plt.xlabel(r"\[A_{tot}]\$")
    plt.ylabel(r"\[B_{tot}]\$")
    plt.axis("scaled")
    plt.grid(True)
    plt.show()

# ===== Parameters =====
interact_manual()

```

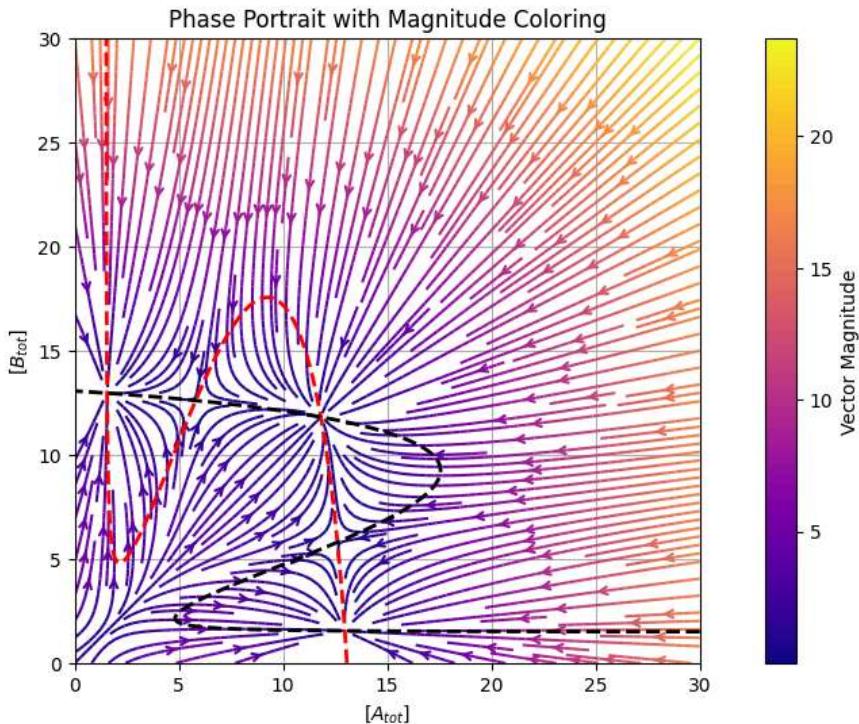
```

    plot_stream,
    alpha = FloatSlider(min=0.1, max=3.0, step=0.1, value=1.0, description='alpha'),
    beta = FloatSlider(min=0.5, max=20, step=0.5, value=1.0, description='beta'),
    n = FloatSlider(min=0.5, max=5.0, step=0.5, value=2.0, description='n'),
    Kd = FloatSlider(min=0.1, max=3.0, step=0.1, value=1.0, description='Kd')
)

```

alpha	<input type="radio"/>	1.50
beta	<input checked="" type="radio"/>	12.00
n	<input type="radio"/>	2.00
Kd	<input type="radio"/>	1.50

Run Interact



```

plot_stream
def plot_stream(alpha, beta, n, Kd)

<no docstring>

```

```

import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact_manual, FloatSlider
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display

# ===== Numba acceleration =====
from numba import njit, prange

@njit(parallel=True, fastmath=True)
def _compute_field(x, y, alpha_A, alpha_B, gamma_A, gamma_B):
    nx, ny = x.shape
    u = np.empty((nx, ny), dtype=np.float64) # dA/dt
    v = np.empty((nx, ny), dtype=np.float64) # dB/dt
    for i in prange(nx):
        for j in range(ny):
            A = x[i, j]
            B = y[i, j]
            # Toggle switch ODEs
            dA = alpha_A / (1.0 + B*B) - gamma_A * A
            dB = alpha_B / (1.0 + A*A) - gamma_B * B
            u[i, j] = dA
            v[i, j] = dB
    return u, v

```

```
@njit(parallel=True, fastmath=True)
def _magnitude(u, v):
    nx, ny = u.shape
    mag = np.empty((nx, ny), dtype=np.float64)
    for i in prange(nx):
        for j in range(ny):
            mag[i, j] = np.hypot(u[i, j], v[i, j])
    return mag

# ===== Toggle switch field plot (Numba-backed) =====
def plot_stream(alpha_A, alpha_B, gamma_A, gamma_B):
    # ----- Define the grid -----
    start_x, end_x, num_points_x = 0.0, 5.0, 500
    start_y, end_y, num_points_y = 0.0, 5.0, 500

    x_vals = np.linspace(start_x, end_x, num_points_x, dtype=np.float64)
    y_vals = np.linspace(start_y, end_y, num_points_y, dtype=np.float64)
    x, y = np.meshgrid(x_vals, y_vals)

    # ----- Compute vector field -----
    u, v = _compute_field(x, y, float(alpha_A), float(alpha_B), float(gamma_A), float(gamma_B))

    # ----- Magnitude for coloring -----
    magnitude = _magnitude(u, v)

    # ----- Plot -----
    plt.figure(figsize=(8, 6))
    plt.streamplot(x, y, u, v, color=magnitude, cmap='plasma',
                   linewidth=1.2, density=2.0, arrowstyle='->')
    plt.colorbar(label="Vector Magnitude")

    # Nullclines: dA/dt=0 (red), dB/dt=0 (black)
    plt.contour(x, y, u, levels=[0], colors='red', linewidths=2, linestyles='--')
    plt.contour(x, y, v, levels=[0], colors='black', linewidths=2, linestyles='--')

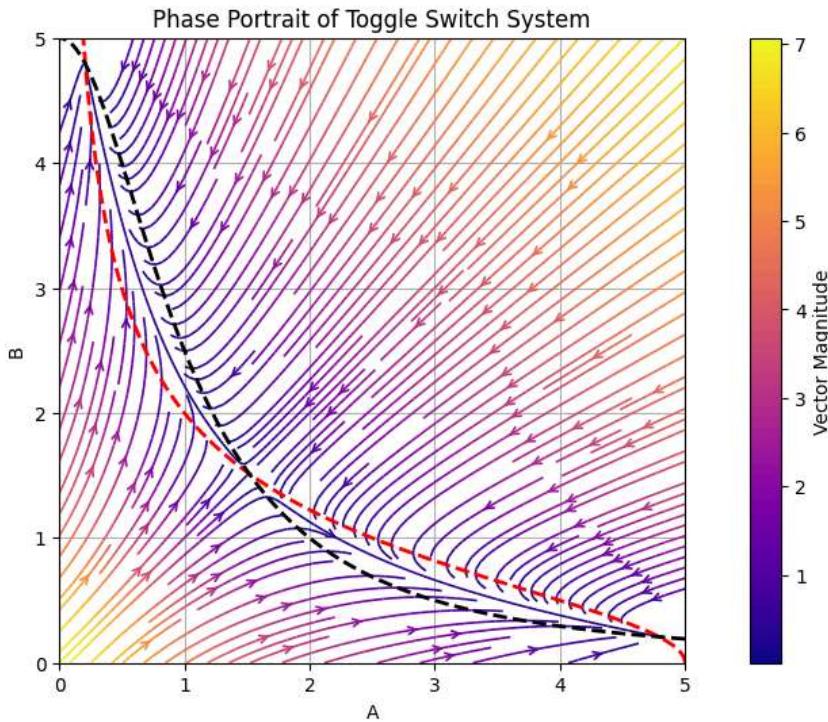
    plt.title("Phase Portrait of Toggle Switch System")
    plt.xlabel("A")
    plt.ylabel("B")
    plt.axis("scaled")
    plt.grid(True)
    plt.show()

# ===== Interactive sliders =====
interact_manual(
    plot_stream,
    alpha_A = FloatSlider(min=0.1, max=5.0, step=0.1, value=2.5, description='alpha_A'),
    alpha_B = FloatSlider(min=0.1, max=5.0, step=0.1, value=1.5, description='alpha_B'),
    gamma_A = FloatSlider(min=0.1, max=3.0, step=0.1, value=1.0, description='gamma_A'),
    gamma_B = FloatSlider(min=0.1, max=3.0, step=0.1, value=1.0, description='gamma_B')
)
```

```

alpha_A      ○ 5.00
alpha_B      ○ 5.00
gamma_A     ○ 1.00
gamma_B     ○ 1.00
Run Interact

```



```

plot_stream
def plot_stream(alpha_A, alpha_B, gamma_A, gamma_B)
<no docstring>

```

Initial Conditions

```

# === MultiFate Reaction-Diffusion (Numba-accelerated, Gray-Scott-style UI) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display

def Square_Initial():
    # ----- Grid & Initial Condition -----
    N = 60

    # Initialize desired fields
    A0 = np.random.uniform(19.0, 20.0, (N, N))
    B0 = np.random.uniform(19.0, 20.0, (N, N))

    # ----- Parameters -----
    Du, Dv = 0.10, 0.05
    alpha, beta, n, Kd = 0.4, 10.0, 1.5, 1.0
    dt = 0.2
    steps = 10000
    save_every = 1    # store frame every 100 steps

    # ----- Numba kernels -----
    from numba import njit, prange

    @njit(fastmath=True)
    def _compute_A2_B2_elem(Atot, Btot, Kd):

```

```

S = Atot + Btot
denom_common = Kd + 4.0 * S + np.sqrt(Kd * Kd + 8.0 * S * Kd)
A2 = 2.0 * Atot * Atot / denom_common
B2 = 2.0 * Btot * Btot / denom_common
return A2, B2

@njit(parallel=True, fastmath=True)
def _step_periodic(A, B, Du, Dv, alpha, beta, n, Kd, dt):
    nx, ny = A.shape
    Anew = np.empty_like(A)
    Bnew = np.empty_like(B)

    for i in prange(nx):
        im = (i - 1) % nx
        ip = (i + 1) % nx
        for j in range(ny):
            jm = (j - 1) % ny
            jp = (j + 1) % ny

            LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
            LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

            A2, B2 = _compute_A2_B2_elem(A[i, j], B[i, j], Kd)

            tA = A2 ** n
            actA = beta * (tA / (1.0 + tA))
            fA = alpha + actA - A[i, j]

            tB = B2 ** n
            actB = beta * (tB / (1.0 + tB))
            fB = alpha + actB - B[i, j]

            Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
            Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

    # Clamp negatives only
    for i in prange(nx):
        for j in range(ny):
            if Anew[i, j] < 0.0:
                Anew[i, j] = 0.0
            if Bnew[i, j] < 0.0:
                Bnew[i, j] = 0.0

    return Anew, Bnew

# ----- Simulation -----
A_temp, B_temp = A0.copy(), B0.copy()
A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt) # JIT warmup

A_list = [A0.copy()]
B_list = [B0.copy()]
for s in range(1, steps + 1):
    A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt)
    if s % save_every == 0:
        A_list.append(A_temp.copy())
        B_list.append(B_temp.copy())

# ----- Viewer -----
from ipywidgets import ToggleButtons

def plot_at_time(idx, species):
    plt.figure(figsize=(8, 6))

    if species == "A":
        data = A_list[idx]
        title = f"A Concentration (frame {idx}, step={idx*save_every})"
    else:
        data = B_list[idx]
        title = f"B Concentration (frame {idx}, step={idx*save_every})"

    img = plt.imshow(data, cmap='inferno', interpolation='bilinear')
    plt.colorbar(img, ax=plt.gca())
    plt.title(title)
    plt.axis('off')
    plt.show()

```

```

# Species toggle
species_toggle = ToggleButtons(
    options=["A", "B"],
    value="A",
    description="Species:",
    button_style="info"
)

# Frame controls
play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100, description="Play")
slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description='Frame')

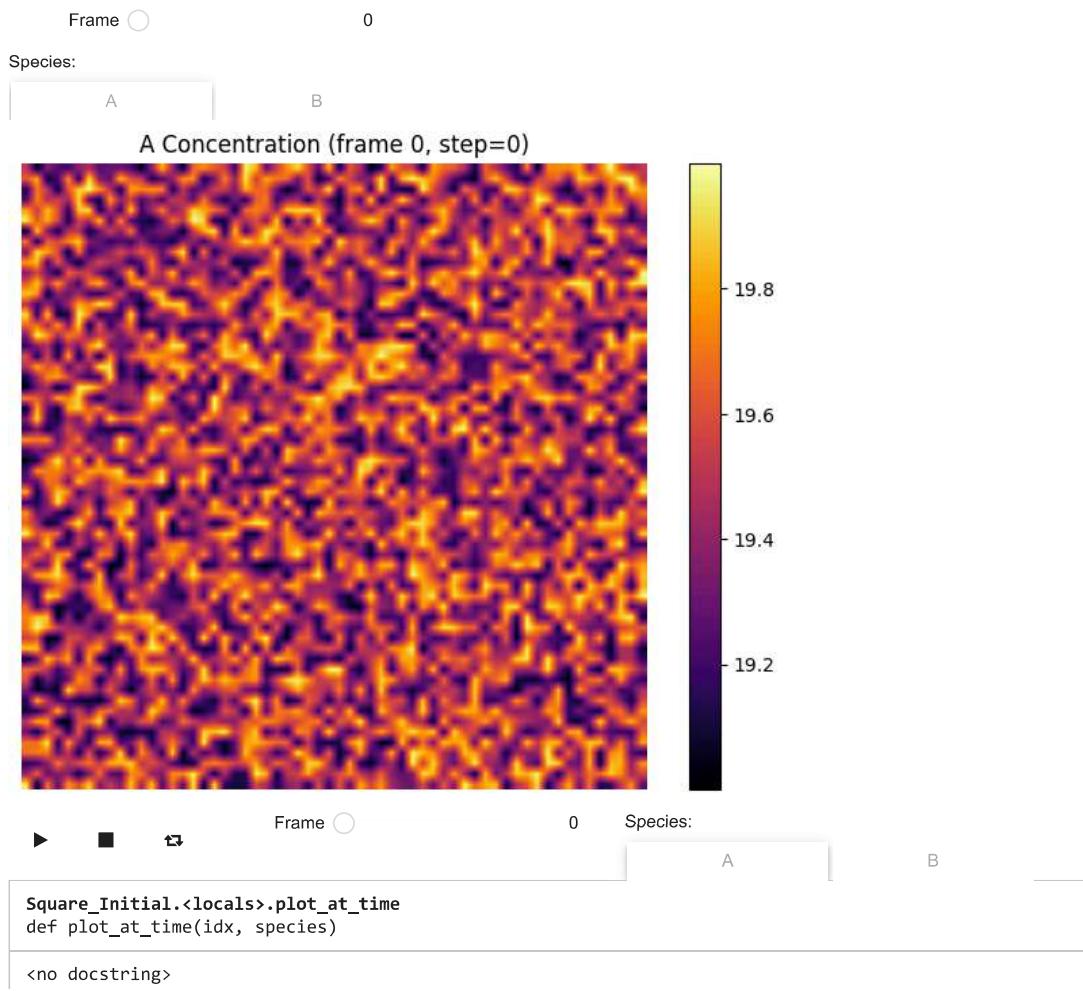
# Layout with toggle button
widgets = HBox([play, slider, species_toggle])
interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)

from ipywidgets import jslink
jslink((play, 'value'), (slider, 'value'))

display(widgets, interact_ui)

Square_Initial()

```



```

# === MultiFate Reaction-Diffusion (Numba-accelerated, Gray-Scott-style UI) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display

def Random_Initial():
    # ----- Grid & Initial Condition -----
    N = 60

```

```

# Initialize desired fields
# ---- Grid setup ----
nx, ny = 60, 60
A0 = np.zeros((nx, ny))
B0 = np.zeros((nx, ny))

num_total = 900
num_set = 300
total_points = nx * ny

# ---- Species A ----
all_indices_A = np.random.choice(total_points, size=num_total, replace=False)
set1_A = all_indices_A[:num_set]
set2_A = all_indices_A[num_set:2*num_set]
set3_A = all_indices_A[2*num_set:3*num_set]

coords1_A = np.array(np.unravel_index(set1_A, (nx, ny))).T
coords2_A = np.array(np.unravel_index(set2_A, (nx, ny))).T
coords3_A = np.array(np.unravel_index(set3_A, (nx, ny))).T

A0[coords1_A[:,0], coords1_A[:,1]] = 9.0
A0[coords2_A[:,0], coords2_A[:,1]] = 0.5
A0[coords3_A[:,0], coords3_A[:,1]] = 9.0

# ---- Species B ----
all_indices_B = np.random.choice(total_points, size=num_total, replace=False)
set1_B = all_indices_B[:num_set]
set2_B = all_indices_B[num_set:2*num_set]
set3_B = all_indices_B[2*num_set:3*num_set]

coords1_B = np.array(np.unravel_index(set1_B, (nx, ny))).T
coords2_B = np.array(np.unravel_index(set2_B, (nx, ny))).T
coords3_B = np.array(np.unravel_index(set3_B, (nx, ny))).T

B0[coords1_B[:,0], coords1_B[:,1]] = 9.0
B0[coords2_B[:,0], coords2_B[:,1]] = 9.0
B0[coords3_B[:,0], coords3_B[:,1]] = 0.5

# ----- Parameters -----
Du, Dv = 0.10, 0.05
alpha, beta, n, Kd = 0.4, 10.0, 1.5, 1.0
dt = 0.2
steps = 10000
save_every = 1 # store frame every 100 steps

# ----- Numba kernels -----
from numba import njit, prange

@njit(fastmath=True)
def _compute_A2_B2_elem(Atot, Btot, Kd):
    S = Atot + Btot
    denom_common = Kd + 4.0 * S + np.sqrt(Kd * Kd + 8.0 * S * Kd)
    A2 = 2.0 * Atot * Atot / denom_common
    B2 = 2.0 * Btot * Btot / denom_common
    return A2, B2

@njit(parallel=True, fastmath=True)
def _step_periodic(A, B, Du, Dv, alpha, beta, n, Kd, dt):
    nx, ny = A.shape
    Anew = np.empty_like(A)
    Bnew = np.empty_like(B)

    for i in prange(nx):
        im = (i - 1) % nx
        ip = (i + 1) % nx
        for j in range(ny):
            jm = (j - 1) % ny
            jp = (j + 1) % ny

            LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
            LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

            A2, B2 = _compute_A2_B2_elem(A[i, j], B[i, j], Kd)

            tA = A2 ** n
            actA = beta * (tA / (1.0 + tA))

```

```

fA = alpha + actA - A[i, j]

tB = B2 ** n
actB = beta * (tB / (1.0 + tB))
fB = alpha + actB - B[i, j]

Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

# Clamp negatives only
for i in prange(nx):
    for j in range(ny):
        if Anew[i, j] < 0.0:
            Anew[i, j] = 0.0
        if Bnew[i, j] < 0.0:
            Bnew[i, j] = 0.0

return Anew, Bnew

# ----- Simulation -----
A_temp, B_temp = A0.copy(), B0.copy()
A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt) # JIT warmup

A_list = [A0.copy()]
B_list = [B0.copy()]
for s in range(1, steps + 1):
    A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt)
    if s % save_every == 0:
        A_list.append(A_temp.copy())
        B_list.append(B_temp.copy())

# ----- Viewer -----
from ipywidgets import ToggleButtons

def plot_at_time(idx, species):
    plt.figure(figsize=(8, 6))

    if species == "A":
        data = A_list[idx]
        title = f"A Concentration (frame {idx}, step={idx*save_every})"
    else:
        data = B_list[idx]
        title = f"B Concentration (frame {idx}, step={idx*save_every})"

    img = plt.imshow(data, cmap='inferno', interpolation='bilinear')
    plt.colorbar(img, ax=plt.gca())
    plt.title(title)
    plt.axis('off')
    plt.show()

# Species toggle
species_toggle = ToggleButtons(
    options=["A", "B"],
    value="A",
    description="Species:",
    button_style="info"
)

# Frame controls
play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100, description="Play")
slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description='Frame')

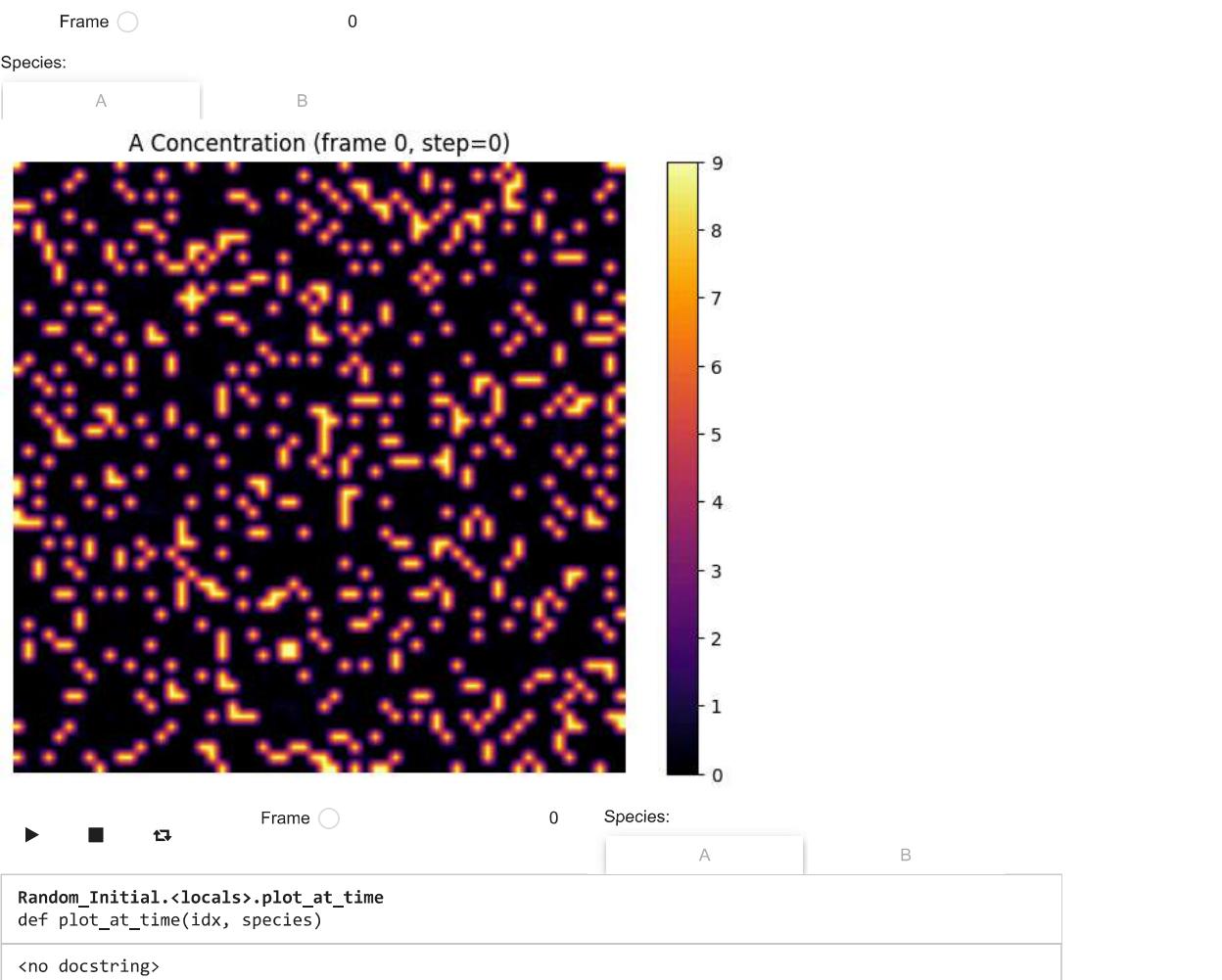
# Layout with toggle button
widgets = HBox([play, slider, species_toggle])
interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)

from ipywidgets import jslink
jslink((play, 'value'), (slider, 'value'))

display(widgets, interact_ui)

Random_Initial()

```



```
# === MultiFate Reaction-Diffusion (Numba-accelerated, Gray-Scott-style UI) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display

def Radial_Initial():
    # ----- Grid & Initial Condition -----
    N = 60

    def radial_gradient_both(N, center=None,
                            A_inner=10.0, A_outer=0.0,
                            B_inner=10.0, B_outer=0.0):
        """Radial gradient initial condition for both A and B."""
        if center is None:
            center = (N//2, N//2)
        ii, jj = np.indices((N, N))
        r = np.sqrt((ii-center[0])**2 + (jj-center[1])**2)
        r = r/r.max() # normalize radius [0,1]

        # Exponential radial interpolation
        A = A_outer + (A_inner - A_outer) * np.exp(-4 * r)
        B = B_outer + (B_inner - B_outer) * np.exp(-4 * r)
        return A, B

    # Use radial gradient instead of random init
    A, B = radial_gradient_both(N,
                                A_inner=15.0, A_outer=1.0,
                                B_inner=15.0, B_outer=1.0)

    # Adding some noise
    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))
```

```

# ----- Parameters -----
Du, Dv = 0.10, 0.05
alpha, beta, n, Kd = 0.4, 10.0, 1.5, 1.0
dt = 0.2
steps = 10000
save_every = 1 # store frame every step

# ----- Numba kernels -----
from numba import njit, prange

@njit(fastmath=True)
def _compute_A2_B2_elem(Atot, Btot, Kd):
    S = Atot + Btot
    denom_common = Kd + 4.0 * S + np.sqrt(Kd * Kd + 8.0 * S * Kd)
    A2 = 2.0 * Atot * Atot / denom_common
    B2 = 2.0 * Btot * Btot / denom_common
    return A2, B2

@njit(parallel=True, fastmath=True)
def _step_periodic(A, B, Du, Dv, alpha, beta, n, Kd, dt):
    nx, ny = A.shape
    Anew = np.empty_like(A)
    Bnew = np.empty_like(B)

    for i in prange(nx):
        im = (i - 1) % nx
        ip = (i + 1) % nx
        for j in range(ny):
            jm = (j - 1) % ny
            jp = (j + 1) % ny

            LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
            LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

            A2, B2 = _compute_A2_B2_elem(A[i, j], B[i, j], Kd)

            tA = A2 ** n
            actA = beta * (tA / (1.0 + tA))
            fA = alpha + actA - A[i, j]

            tB = B2 ** n
            actB = beta * (tB / (1.0 + tB))
            fB = alpha + actB - B[i, j]

            Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
            Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

    # Clamp negatives only
    for i in prange(nx):
        for j in range(ny):
            if Anew[i, j] < 0.0:
                Anew[i, j] = 0.0
            if Bnew[i, j] < 0.0:
                Bnew[i, j] = 0.0

    return Anew, Bnew

# ----- Simulation -----
A_temp, B_temp = A0.copy(), B0.copy()
A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt) # JIT warmup

A_list = [A0.copy()]
B_list = [B0.copy()]
for s in range(1, steps + 1):
    A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt)
    if s % save_every == 0:
        A_list.append(A_temp.copy())
        B_list.append(B_temp.copy())

# ----- Viewer -----
from ipywidgets import ToggleButtons

def plot_at_time(idx, species):
    plt.figure(figsize=(8, 6))

```

```

if species == "A":
    data = A_list[idx]
    title = f"A Concentration (frame {idx}, step={idx*save_every})"
else:
    data = B_list[idx]
    title = f"B Concentration (frame {idx}, step={idx*save_every})"

img = plt.imshow(data, cmap='inferno', interpolation='bilinear')
plt.colorbar(img, ax=plt.gca())
plt.title(title)
plt.axis('off')
plt.show()

# Species toggle
species_toggle = ToggleButtons(
    options=["A", "B"],
    value="A",
    description="Species:",
    button_style="info"
)

# Frame controls
play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100, description="Play")
slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description='Frame')

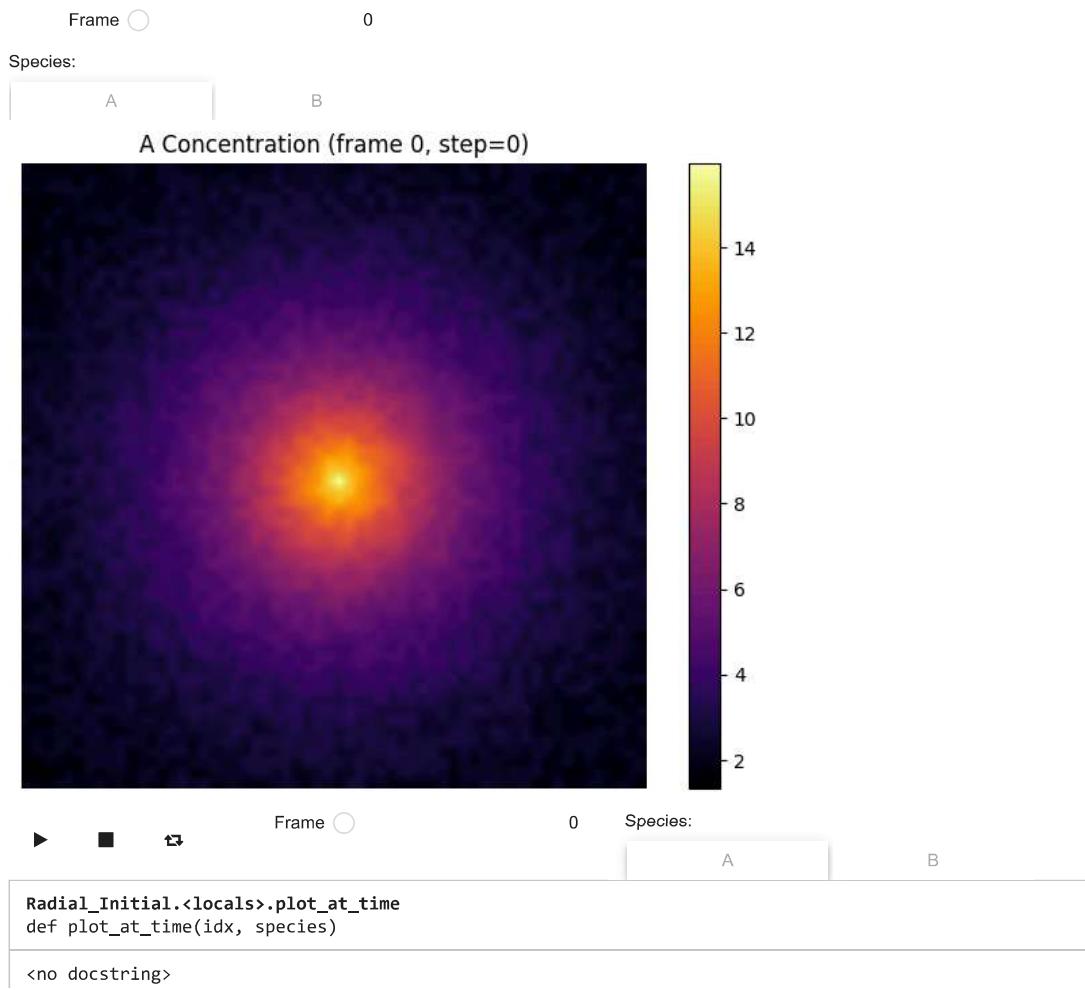
# Layout with toggle button
widgets = HBox([play, slider, species_toggle])
interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)

from ipywidgets import jslink
jslink((play, 'value'), (slider, 'value'))

display(widgets, interact_ui)

Radial_Initial()

```



```
# === MultiFate Reaction-Diffusion (Numba-accelerated, Gray-Scott-style UI) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display

def MultiGaussian_Initial():
    # ----- Grid & Initial Condition -----
    N = 60

    def multi_gaussian(N, centers, A_inner=10, B_inner=10):
        A = np.zeros((N, N))
        B = np.zeros((N, N))
        for cx, cy in centers:
            rr, cc = np.indices((N, N))
            dist2 = (rr-cx)**2 + (cc-cy)**2
            A += A_inner * np.exp(-dist2/(2*5.0**2))
            B += B_inner * np.exp(-dist2/(2*5.0**2))
        return A, B

    A, B = multi_gaussian(N, [(20, 20), (45, 45), (55, 20)])

    # Adding some noise
    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))

    # ----- Parameters -----
    Du, Dv = 0.10, 0.05
    alpha, beta, n, Kd = 0.4, 10.0, 1.5, 1.0
    dt = 0.2
    steps = 10000
    save_every = 1  # store frame every step

    # ----- Numba kernels -----
    from numba import njit, prange

    @njit(fastmath=True)
    def _compute_A2_B2_elem(Atot, Btot, Kd):
        S = Atot + Btot
        denom_common = Kd + 4.0 * S + np.sqrt(Kd * Kd + 8.0 * S * Kd)
        A2 = 2.0 * Atot * Atot / denom_common
        B2 = 2.0 * Btot * Btot / denom_common
        return A2, B2

    @njit(parallel=True, fastmath=True)
    def _step_periodic(A, B, Du, Dv, alpha, beta, n, Kd, dt):
        nx, ny = A.shape
        Anew = np.empty_like(A)
        Bnew = np.empty_like(B)

        for i in prange(nx):
            im = (i - 1) % nx
            ip = (i + 1) % nx
            for j in range(ny):
                jm = (j - 1) % ny
                jp = (j + 1) % ny

                LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
                LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

                A2, B2 = _compute_A2_B2_elem(A[i, j], B[i, j], Kd)

                tA = A2 ** n
                actA = beta * (tA / (1.0 + tA))
                fA = alpha + actA - A[i, j]

                tB = B2 ** n
                actB = beta * (tB / (1.0 + tB))
                fB = alpha + actB - B[i, j]

                Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
                Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

        # Clamp negatives only
        Anew[Anew < 0] = 0
        Bnew[Bnew < 0] = 0

        return Anew, Bnew

    return _step_periodic

```

```

for i in prange(nx):
    for j in range(ny):
        if Anew[i, j] < 0.0:
            Anew[i, j] = 0.0
        if Bnew[i, j] < 0.0:
            Bnew[i, j] = 0.0

return Anew, Bnew

# ----- Simulation -----
A_temp, B_temp = A0.copy(), B0.copy()
A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt) # JIT warmup

A_list = [A0.copy()]
B_list = [B0.copy()]
for s in range(1, steps + 1):
    A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt)
    if s % save_every == 0:
        A_list.append(A_temp.copy())
        B_list.append(B_temp.copy())

# ----- Viewer -----
from ipywidgets import ToggleButtons

def plot_at_time(idx, species):
    plt.figure(figsize=(8, 6))

    if species == "A":
        data = A_list[idx]
        title = f"A Concentration (frame {idx}, step={idx*save_every})"
    else:
        data = B_list[idx]
        title = f"B Concentration (frame {idx}, step={idx*save_every})"

    img = plt.imshow(data, cmap='inferno', interpolation='bilinear')
    plt.colorbar(img, ax=plt.gca())
    plt.title(title)
    plt.axis('off')
    plt.show()

# Species toggle
species_toggle = ToggleButtons(
    options=["A", "B"],
    value="A",
    description="Species:",
    button_style="info"
)

# Frame controls
play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100, description="Play")
slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description='Frame')

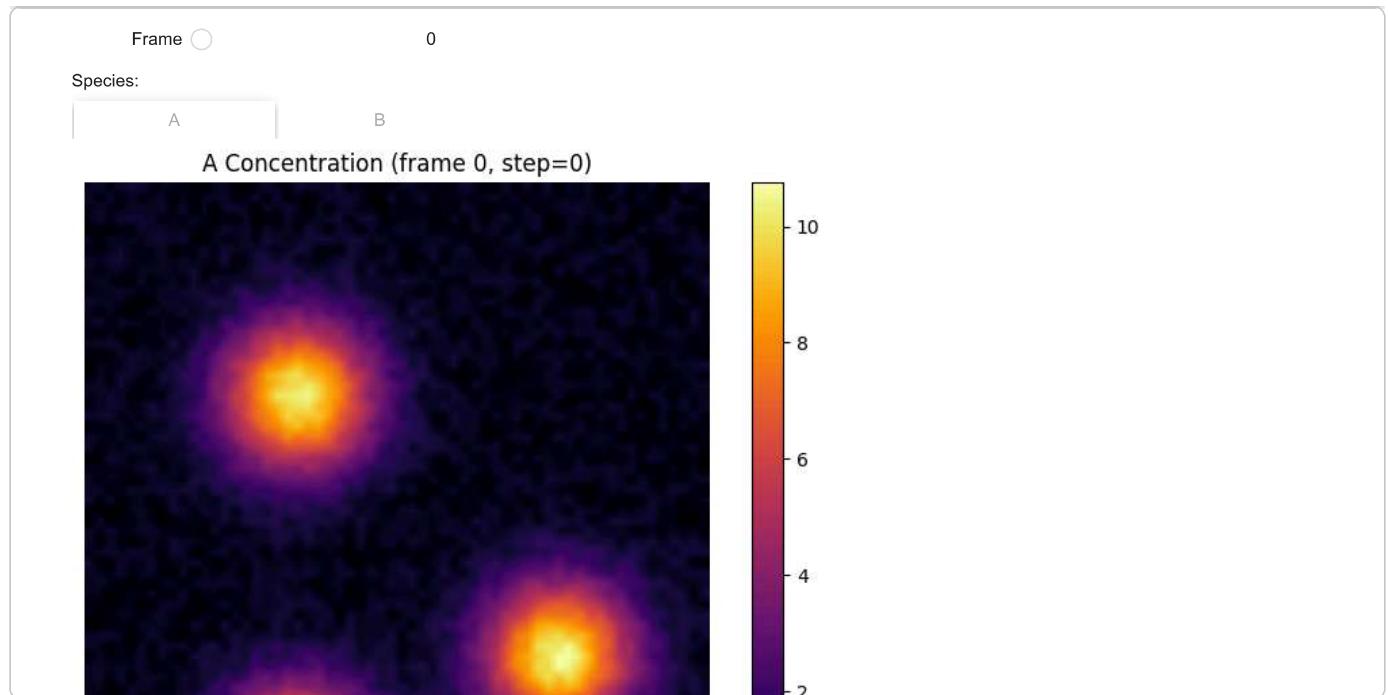
# Layout with toggle button
widgets = HBox([play, slider, species_toggle])
interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)

from ipywidgets import jslink
jslink((play, 'value'), (slider, 'value'))

display(widgets, interact_ui)

MultiGaussian_Initial()

```



MultiFate 2

PBC

Frame 0Species: A B

```
# === MultiFate Reaction-Diffusion (Numba-accelerated, Gray-Scott-style UI) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox, Dropdown, ToggleButtons, jslink
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display
from numba import njit, prange

def Initial():
    # ----- Grid -----
    N = 60

    # ----- Initial Conditions -----
def square(N):
    """Uniform random high values for both species."""
    A0 = np.random.uniform(19.0, 20.0, (N, N))
    B0 = np.random.uniform(19.0, 20.0, (N, N))

    return A0, B0

def random_300(N):
    """Place three sets (300 each) of special values for A and B at random coordinates."""
    nx, ny = N, N
    A0 = np.zeros((nx, ny))
    B0 = np.zeros((nx, ny))

    num_total = 900
    num_set = 300
    total_points = nx * ny

    # Species A
    all_indices_A = np.random.choice(total_points, size=num_total, replace=False)
    for k, val in enumerate([9.0, 0.5, 9.0]):
        part = all_indices_A[k * num_set:(k + 1) * num_set]
        coords = np.array(np.unravel_index(part, (nx, ny))).T
        A0[coords[:, 0], coords[:, 1]] = val

    # Species B
    all_indices_B = np.random.choice(total_points, size=num_total, replace=False)
    for k, val in enumerate([9.0, 9.0, 0.5]):
```

```

        part = all_indices_B[k * num_set:(k + 1) * num_set]
        coords = np.array(np.unravel_index(part, (nx, ny))).T
        B0[coords[:, 0], coords[:, 1]] = val

    return A0, B0

def radial_gradient_both(N, center=None,
                        A_inner=10.0, A_outer=1.0,
                        B_inner=10.0, B_outer=1.0):
    if center is None:
        center = (N // 2, N // 2)
    ii, jj = np.indices((N, N))
    r = np.sqrt((ii - center[0]) ** 2 + (jj - center[1]) ** 2)
    r = r / r.max()

    A = A_outer + (A_inner - A_outer) * np.exp(-4 * r)
    B = B_outer + (B_inner - B_outer) * np.exp(-4 * r)

    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))

    return A0, B0

def multi_gaussian(N, centers=[(30, 30), (15, 45), (45, 15)], A_inner=10, B_inner=10):
    A = np.zeros((N, N))
    B = np.zeros((N, N))
    rr, cc = np.indices((N, N))
    for cx, cy in centers:
        dist2 = (rr - cx) ** 2 + (cc - cy) ** 2
        A += A_inner * np.exp(-dist2 / (2 * 5.0 ** 2))
        B += B_inner * np.exp(-dist2 / (2 * 5.0 ** 2))

    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))

    return A0, B0

def sinusoidal_initial(N=60, noise_strength=0.1):
    """
    Sinusoidal checkerboard initial condition with small noise.
    Returns A0, B0 fields on an N×N grid.
    """
    # Grid in [0, 2π]
    x = np.linspace(0, 2*np.pi, N)
    y = np.linspace(0, 2*np.pi, N)
    X, Y = np.meshgrid(x, y)

    # Sinusoidal pattern
    pattern = np.sin(X) * np.sin(Y)

    # Scale into ~[19,20] for consistency with your code
    A = 19.0 + (pattern + 1) / 2
    B = 19.0 + (pattern + 1) / 2

    # Add small uniform noise
    A0 = A + noise_strength * (np.random.rand(N, N) - 0.5)
    B0 = B + noise_strength * (np.random.rand(N, N) - 0.5)

    return A0, B0

# Dictionary to access IC functions
ic_options = {
    "Radial Gradient": radial_gradient_both,
    "Random 300": random_300,
    "Multi Gaussian Peaks": multi_gaussian,
    "Square": square,
    "Sinusoidal": sinusoidal_initial
}

# ----- Parameters -----
Du, Dv = 0.10, 0.05
alpha, beta, n, Kd = 0.40, 10.0, 1.5, 1.0
dt = 0.2
steps = 10000 # reduce for faster demo
save_every = 1

```

```

# ----- Numba kernels -----
@njit(fastmath=True)
def _compute_A2_B2_elem(Atot, Btot, Kd):
    S = Atot + Btot
    denom_common = Kd + 4.0 * S + np.sqrt(Kd * Kd + 8.0 * S * Kd)
    A2 = 2.0 * Atot * Atot / denom_common
    B2 = 2.0 * Btot * Btot / denom_common
    return A2, B2

@njit(parallel=True, fastmath=True)
def _step_periodic(A, B, Du, Dv, alpha, beta, n, Kd, dt):
    nx, ny = A.shape
    Anew = np.empty_like(A)
    Bnew = np.empty_like(B)
    for i in prange(nx):
        im = (i - 1) % nx
        ip = (i + 1) % nx
        for j in range(ny):
            jm = (j - 1) % ny
            jp = (j + 1) % ny

            LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
            LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

            A2, B2 = _compute_A2_B2_elem(A[i, j], B[i, j], Kd)

            tA = A2 ** n
            actA = beta * (tA / (1.0 + tA))
            fA = alpha + actA - A[i, j]

            tB = B2 ** n
            actB = beta * (tB / (1.0 + tB))
            fB = alpha + actB - B[i, j]

            Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
            Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

    for i in prange(nx):
        for j in range(ny):
            if Anew[i, j] < 0.0:
                Anew[i, j] = 0.0
            if Bnew[i, j] < 0.0:
                Bnew[i, j] = 0.0

    return Anew, Bnew

# ----- Simulation Runner -----
def run_sim(initial_condition):
    # Get initial condition by passing N to the selected IC function
    A0, B0 = ic_options[initial_condition](N)
    A_temp, B_temp = A0.copy(), B0.copy()
    A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt) # warmup

    # Run simulation
    A_list = [A0.copy()]
    B_list = [B0.copy()]
    for s in range(1, steps + 1):
        A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt)
        if s % save_every == 0:
            A_list.append(A_temp.copy())
            B_list.append(B_temp.copy())

    # Plotting function
    def plot_at_time(idx, species):
        plt.figure(figsize=(5, 5), dpi=150)
        if species == "A":
            data = A_list[idx]
            title = f"A Concentration (t={idx * save_every * dt:.2f})"
        else:
            data = B_list[idx]
            title = f"B Concentration (t={idx * save_every * dt:.2f})"
        img = plt.imshow(data, cmap='inferno', origin='lower', interpolation='bilinear')
        plt.colorbar(img)
        plt.title(title)
        plt.axis('off')
        plt.show()

    return A_list, B_list

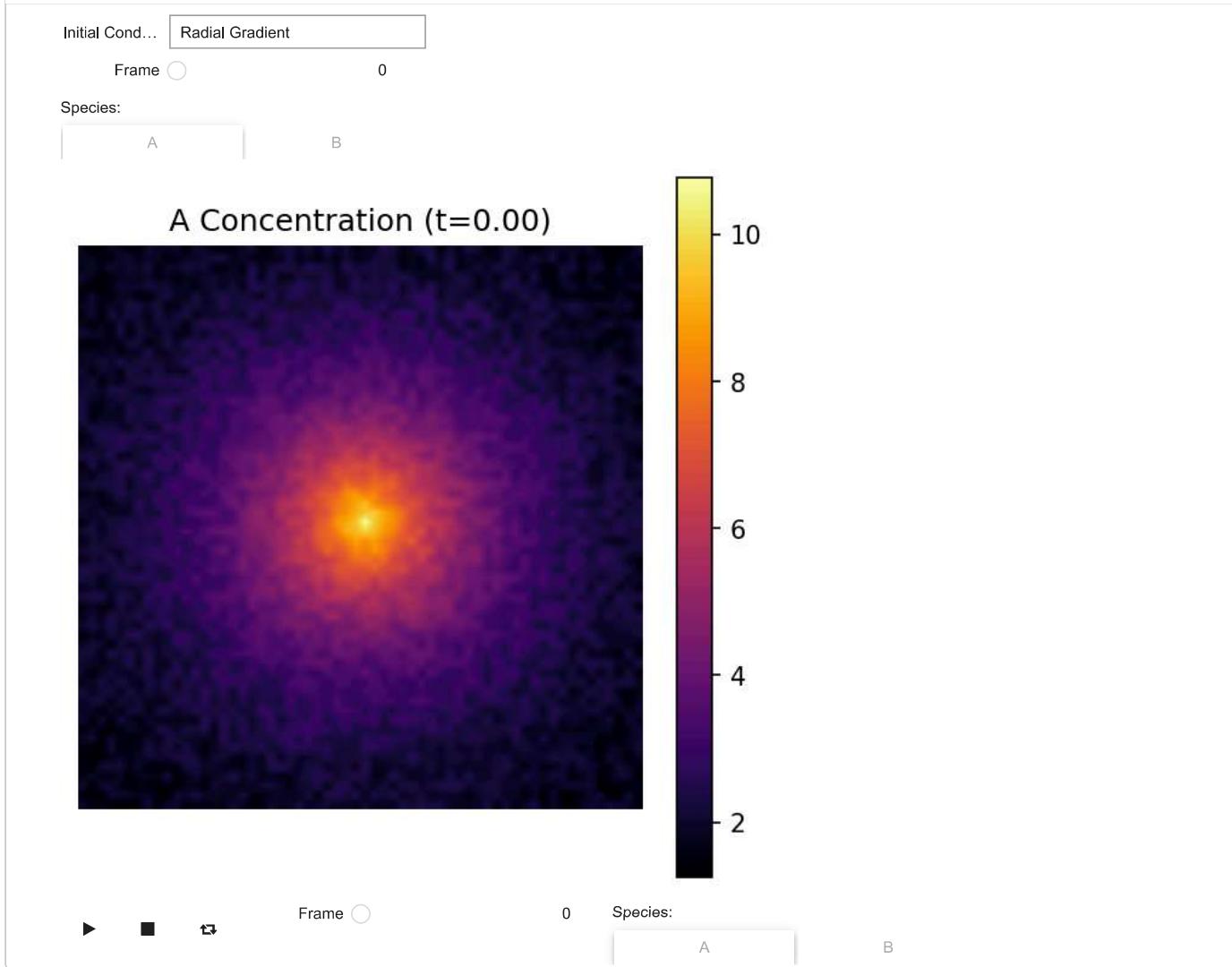
```

```
# Controls
species_toggle = ToggleButtons(options=["A", "B"], value="A", description="Species:", button_style="info")
play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100)
slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description="Frame")
jslink((play, 'value'), (slider, 'value'))

widgets = HBox([play, slider, species_toggle])
interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)
display(widgets, interact_ui)

# ----- Dropdown for IC -----
ic_dropdown = Dropdown(options=list(ic_options.keys()), value="Radial Gradient", description="Initial Condition:")
interact(run_sim, initial_condition=ic_dropdown)

Initial()
```



NBC

```
# === MultiFate Reaction-Diffusion (Numba-accelerated, Gray-Scott-style UI) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox, Dropdown, ToggleButtons, jslink
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display
from numba import njit, prange

def Initial_N():
    # ----- Grid -----
    N = 60
```

```

# ----- Initial Conditions -----
def square(N):
    """Uniform random high values for both species."""
    A0 = np.random.uniform(19.0, 20.0, (N, N))
    B0 = np.random.uniform(19.0, 20.0, (N, N))

    return A0, B0

def random_300(N):
    """Place three sets (300 each) of special values for A and B at random coordinates."""
    nx, ny = N, N
    A0 = np.zeros((nx, ny))
    B0 = np.zeros((nx, ny))

    num_total = 900
    num_set = 300
    total_points = nx * ny

    # Species A
    all_indices_A = np.random.choice(total_points, size=num_total, replace=False)
    for k, val in enumerate([9.0, 0.5, 9.0]):
        part = all_indices_A[k * num_set:(k + 1) * num_set]
        coords = np.array(np.unravel_index(part, (nx, ny))).T
        A0[coords[:, 0], coords[:, 1]] = val

    # Species B
    all_indices_B = np.random.choice(total_points, size=num_total, replace=False)
    for k, val in enumerate([9.0, 9.0, 0.5]):
        part = all_indices_B[k * num_set:(k + 1) * num_set]
        coords = np.array(np.unravel_index(part, (nx, ny))).T
        B0[coords[:, 0], coords[:, 1]] = val

    return A0, B0

def radial_gradient_both(N, center=None,
                        A_inner=10.0, A_outer=1.0,
                        B_inner=10.0, B_outer=1.0):
    if center is None:
        center = (N // 2, N // 2)
    ii, jj = np.indices((N, N))
    r = np.sqrt((ii - center[0]) ** 2 + (jj - center[1]) ** 2)
    r = r / r.max()

    A = A_outer + (A_inner - A_outer) * np.exp(-4 * r)
    B = B_outer + (B_inner - B_outer) * np.exp(-4 * r)

    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))

    return A0, B0

def multi_gaussian(N, centers=[(30, 30), (15, 45), (45, 15)], A_inner=10, B_inner=10):
    A = np.zeros((N, N))
    B = np.zeros((N, N))
    rr, cc = np.indices((N, N))
    for cx, cy in centers:
        dist2 = (rr - cx) ** 2 + (cc - cy) ** 2
        A += A_inner * np.exp(-dist2 / (2 * 5.0 ** 2))
        B += B_inner * np.exp(-dist2 / (2 * 5.0 ** 2))

    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))

    return A0, B0

def sinusoidal_initial(N=60, noise_strength=0.1):
    """
    Sinusoidal checkerboard initial condition with small noise.
    Returns A0, B0 fields on an NxN grid.
    """
    # Grid in [0, 2π]
    x = np.linspace(0, 2*np.pi, N)
    y = np.linspace(0, 2*np.pi, N)
    X, Y = np.meshgrid(x, y)

    # Sinusoidal pattern

```

```

pattern = np.sin(X) * np.sin(Y)

# Scale into ~[19,20] for consistency with your code
A = 19.0 + (pattern + 1) / 2
B = 19.0 + (pattern + 1) / 2

# Add small uniform noise
A0 = A + noise_strength * (np.random.rand(N, N) - 0.5)
B0 = B + noise_strength * (np.random.rand(N, N) - 0.5)

return A0, B0

```

Dictionary to access IC functions

```

ic_options = {
    "Radial Gradient": radial_gradient_both,
    "Random 300": random_300,
    "Multi Gaussian Peaks": multi_gaussian,
    "Square": square,
    "Sinusoidal": sinusoidal_initial
}

```

----- Parameters -----

```

Du, Dv = 0.01, 0.01
alpha, beta, n, Kd = 0.40, 10.0, 1.50, 1.0
dt = 0.2
steps = 10000 # reduce for faster demo
save_every = 1

```

----- Numba kernels -----

```

@njit(fastmath=True)
def _compute_A2_B2_elem(Atot, Btot, Kd):
    S = Atot + Btot
    denom_common = Kd + 4.0 * S + np.sqrt(Kd * Kd + 8.0 * S * Kd)
    A2 = 2.0 * Atot * Atot / denom_common
    B2 = 2.0 * Btot * Btot / denom_common
    return A2, B2

@njit(parallel=True, fastmath=True)
def _step_neumann(A, B, Du, Dv, alpha, beta, n, Kd, dt):
    nx, ny = A.shape
    Anew = np.empty_like(A)
    Bnew = np.empty_like(B)
    for i in prange(nx):
        im = max(i - 1, 0)
        ip = min(i + 1, nx - 1)
        for j in range(ny):
            jm = max(j - 1, 0)
            jp = min(j + 1, ny - 1)

            LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
            LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

            A2, B2 = _compute_A2_B2_elem(A[i, j], B[i, j], Kd)

            tA = A2 ** n
            actA = beta * (tA / (1.0 + tA))
            fA = alpha + actA - A[i, j]

            tB = B2 ** n
            actB = beta * (tB / (1.0 + tB))
            fB = alpha + actB - B[i, j]

            Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
            Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

    # Clamp negative concentrations
    for i in prange(nx):
        for j in range(ny):
            if Anew[i, j] < 0.0:
                Anew[i, j] = 0.0
            if Bnew[i, j] < 0.0:
                Bnew[i, j] = 0.0

    return Anew, Bnew

```

```

# ----- Simulation Runner -----
def run_sim(initial_condition):
    # Get initial condition by passing N to the selected IC function
    A0, B0 = ic_options[initial_condition](N)
    A_temp, B_temp = A0.copy(), B0.copy()
    A_temp, B_temp = _step_neumann(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt) # warmup

    # Run simulation
    A_list = [A0.copy()]
    B_list = [B0.copy()]
    for s in range(1, steps + 1):
        A_temp, B_temp = _step_neumann(A_temp, B_temp, Du, Dv, alpha, beta, n, Kd, dt)
        if s % save_every == 0:
            A_list.append(A_temp.copy())
            B_list.append(B_temp.copy())

    # Plotting function
    def plot_at_time(idx, species):
        plt.figure(figsize=(5, 5), dpi=150)
        if species == "A":
            data = A_list[idx]
            title = f"A Concentration (t={idx * save_every * dt:.2f})"
        else:
            data = B_list[idx]
            title = f"B Concentration (t={idx * save_every * dt:.2f})"
        img = plt.imshow(data, cmap='inferno', origin='lower', interpolation='bilinear')
        plt.colorbar(img)
        plt.title(title)
        plt.axis('off')
        plt.show()

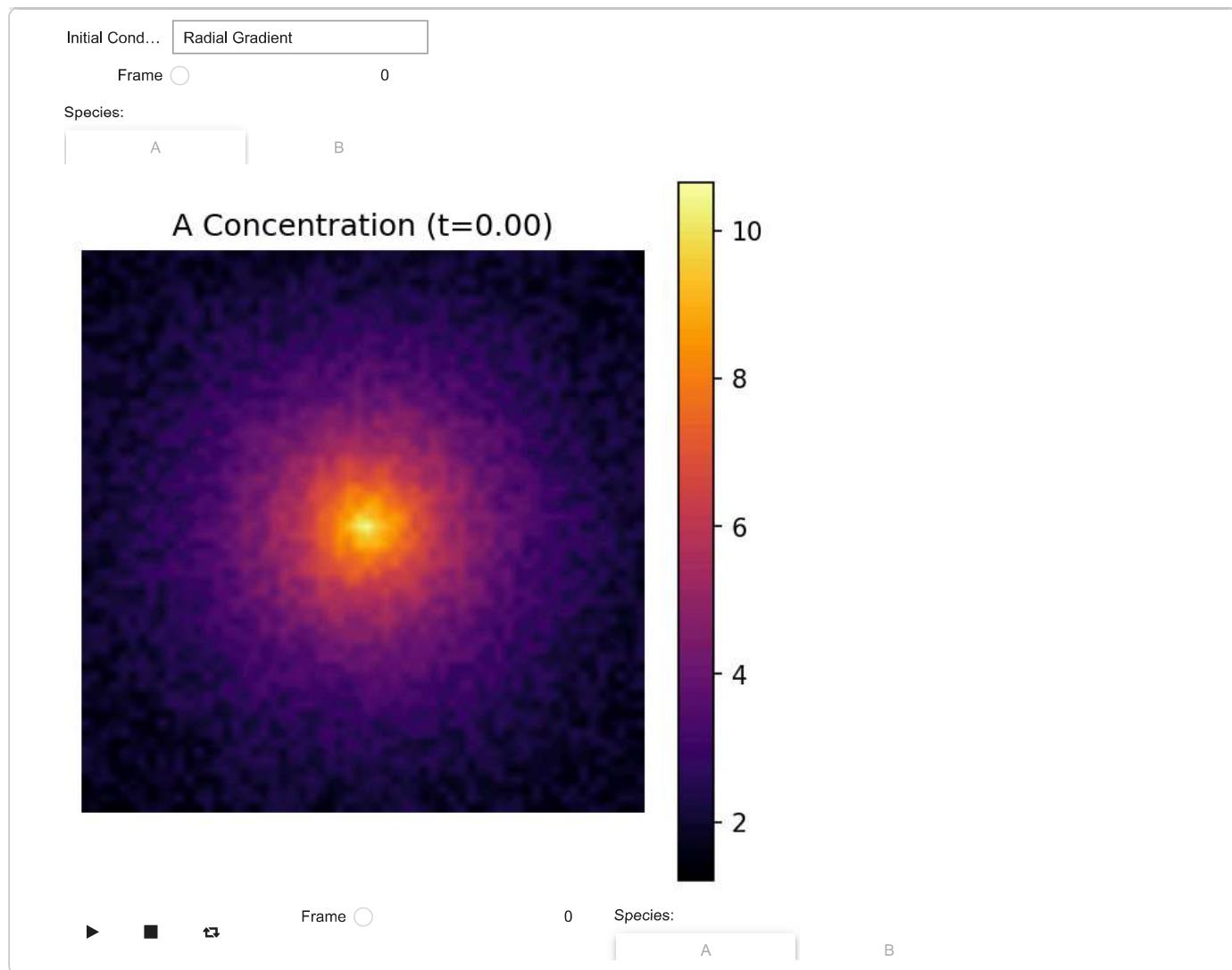
    # Controls
    species_toggle = ToggleButtons(options=["A", "B"], value="A", description="Species:", button_style="info")
    play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100)
    slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description="Frame")
    jslink((play, 'value'), (slider, 'value'))

    widgets = HBox([play, slider, species_toggle])
    interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)
    display(widgets, interact_ui)

# ----- Dropdown for IC -----
ic_dropdown = Dropdown(options=list(ic_options.keys()), value="Radial Gradient", description="Initial Condition:")
interact(run_sim, initial_condition=ic_dropdown)

Initial_N()

```



▼ Toggle Switch

▼ PBC

Double-click (or enter) to edit

```
# === MultiFate Reaction-Diffusion (Numba-accelerated, Model from figure) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox, Dropdown, ToggleButtons, jslink
from google.colab import output
output.enable_custom_widget_manager()
from IPython.display import display
from numba import njit, prange

def Initial_1():
    # ----- Grid -----
    N = 60

    # ----- Initial Conditions -----
    def square(N):
        """Uniform random high values for both species."""
        A0 = np.random.uniform(19.0, 20.0, (N, N))
        B0 = np.random.uniform(19.0, 20.0, (N, N))
        return A0, B0

    def random_300(N):
        """Place three sets (300 each) of special values for A and B at random coordinates."""
        pass

    A0, B0 = square(N)
    random_300(N)
    return A0, B0

njit(Initial_1)
```

```

nx, ny = N, N
A0 = np.zeros((nx, ny))
B0 = np.zeros((nx, ny))

num_total = 900
num_set = 300
total_points = nx * ny

# Species A
all_indices_A = np.random.choice(total_points, size=num_total, replace=False)
for k, val in enumerate([9.0, 0.5, 9.0]):
    part = all_indices_A[k * num_set:(k + 1) * num_set]
    coords = np.array(np.unravel_index(part, (nx, ny))).T
    A0[coords[:, 0], coords[:, 1]] = val

# Species B
all_indices_B = np.random.choice(total_points, size=num_total, replace=False)
for k, val in enumerate([9.0, 9.0, 0.5]):
    part = all_indices_B[k * num_set:(k + 1) * num_set]
    coords = np.array(np.unravel_index(part, (nx, ny))).T
    B0[coords[:, 0], coords[:, 1]] = val

return A0, B0

def radial_gradient_both(N, center=None,
                        A_inner=10.0, A_outer=1.0,
                        B_inner=10.0, B_outer=1.0):
    if center is None:
        center = (N // 2, N // 2)
    ii, jj = np.indices((N, N))
    r = np.sqrt((ii - center[0]) ** 2 + (jj - center[1]) ** 2)
    r = r / r.max()

    A = A_outer + (A_inner - A_outer) * np.exp(-4 * r)
    B = B_outer + (B_inner - B_outer) * np.exp(-4 * r)

    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))

    return A0, B0

def multi_gaussian(N, centers=[(30, 30), (15, 45), (45, 15)], A_inner=10, B_inner=10):
    A = np.zeros((N, N))
    B = np.zeros((N, N))
    rr, cc = np.indices((N, N))
    for cx, cy in centers:
        dist2 = (rr - cx) ** 2 + (cc - cy) ** 2
        A += A_inner * np.exp(-dist2 / (2 * 5.0 ** 2))
        B += B_inner * np.exp(-dist2 / (2 * 5.0 ** 2))

    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))

    return A0, B0

def sinusoidal_initial(N=60, noise_strength=0.1):
    """
    Sinusoidal checkerboard initial condition with small noise.
    Returns A0, B0 fields on an NxN grid.
    """
    x = np.linspace(0, 2*np.pi, N)
    y = np.linspace(0, 2*np.pi, N)
    X, Y = np.meshgrid(x, y)
    pattern = np.sin(X) * np.sin(Y)
    A = 19.0 + (pattern + 1) / 2
    B = 19.0 + (pattern + 1) / 2
    A0 = A + noise_strength * (np.random.rand(N, N) - 0.5)
    B0 = B + noise_strength * (np.random.rand(N, N) - 0.5)
    return A0, B0

# Dictionary to access IC functions
ic_options = {
    "Radial Gradient": radial_gradient_both,
    "Random 300": random_300,
    "Multi Gaussian Peaks": multi_gaussian,
    "Square": square,
}

```

```

        "Sinusoidal": sinusoidal_initial
    }

    # ----- Parameters -----
    Du, Dv = 0.0001, 0.0001      # diffusion coefficients (increase if patterns diffuse too slowly)
    alpha_u, alpha_v = 5.0, 5.0
    gamma_u, gamma_v = 1.0, 1.0
    dt = 0.2
    steps = 10000                # lower by default so interactive demo isn't too slow
    save_every = 1

    # ----- Numba kernels -----
    @njit(fastmath=True)
    def reaction_u(u_ij, v_ij, alpha_u, gamma_u):
        return alpha_u / (1.0 + v_ij * v_ij) - gamma_u * u_ij

    @njit(fastmath=True)
    def reaction_v(u_ij, v_ij, alpha_v, gamma_v):
        return alpha_v / (1.0 + u_ij * u_ij) - gamma_v * v_ij

    @njit(parallel=True, fastmath=True)
    def _step_periodic(A, B, Du, Dv, alpha_u, alpha_v, gamma_u, gamma_v, dt):
        nx, ny = A.shape
        Anew = np.empty_like(A)
        Bnew = np.empty_like(B)
        for i in prange(nx):
            im = (i - 1) % nx
            ip = (i + 1) % nx
            for j in range(ny):
                jm = (j - 1) % ny
                jp = (j + 1) % ny

                # 5-point Laplacian (no dx factor; Du/Dv absorb grid spacing)
                LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
                LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

                fA = reaction_u(A[i, j], B[i, j], alpha_u, gamma_u)
                fB = reaction_v(A[i, j], B[i, j], alpha_v, gamma_v)

                Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
                Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

        # enforce non-negativity
        for i in prange(nx):
            for j in range(ny):
                if Anew[i, j] < 0.0:
                    Anew[i, j] = 0.0
                if Bnew[i, j] < 0.0:
                    Bnew[i, j] = 0.0

        return Anew, Bnew

    # ----- Simulation Runner -----
    def run_sim(initial_condition):
        # Get initial condition by passing N to the selected IC function
        A0, B0 = ic_options[initial_condition](N)
        A_temp, B_temp = A0.copy(), B0.copy()
        # warmup
        A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha_u, alpha_v, gamma_u, gamma_v, dt)

        # Run simulation
        A_list = [A0.copy()]
        B_list = [B0.copy()]
        for s in range(1, steps + 1):
            A_temp, B_temp = _step_periodic(A_temp, B_temp, Du, Dv, alpha_u, alpha_v, gamma_u, gamma_v, dt)
            if s % save_every == 0:
                A_list.append(A_temp.copy())
                B_list.append(B_temp.copy())

        # Plotting function
        def plot_at_time(idx, species):
            plt.figure(figsize=(5, 5), dpi=150)
            if species == "A":
                data = A_list[idx]
                title = f"A Concentration (t={idx * save_every * dt:.2f})"
            else:
                data = B_list[idx]
                title = f"B Concentration (t={idx * save_every * dt:.2f})"
            return data, title

```

```

data = B_list[idx]
title = f"B Concentration (t={idx * save_every * dt:.2f})"
img = plt.imshow(data, cmap='inferno', origin='lower', interpolation='bilinear')
plt.colorbar(img)
plt.title(title)
plt.axis('off')
plt.show()

# Controls
species_toggle = ToggleButtons(options=["A", "B"], value="A", description="Species:", button_style="info")
play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100)
slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description="Frame")
jslink((play, 'value'), (slider, 'value'))

widgets = HBox([play, slider, species_toggle])
interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)
display(widgets, interact_ui)

# ----- Dropdown for IC -----
ic_dropdown = Dropdown(options=list(ic_options.keys()), value="Radial Gradient", description="Initial Condition:")
interact(run_sim, initial_condition=ic_dropdown)

Initial_1()

```

Initial Cond... Sinusoidal

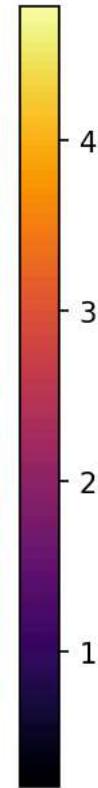
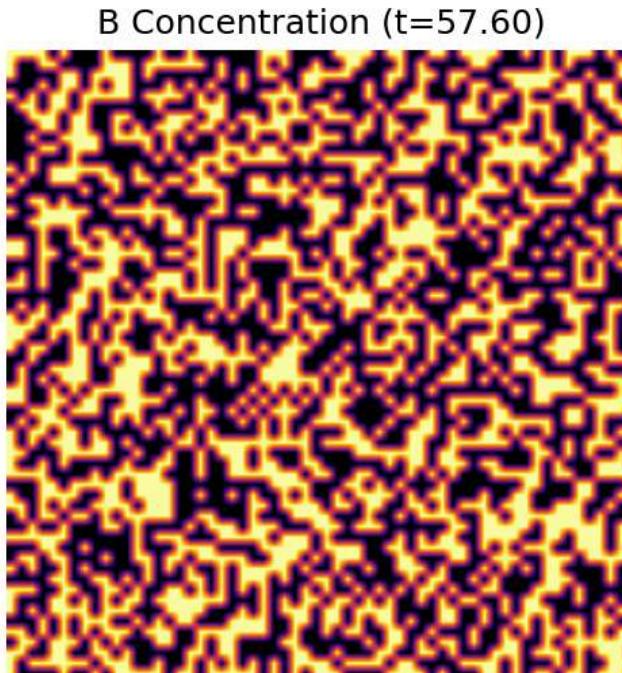
Frame

288

Species:

A

B



▶ ■ ⏪ Frame

288 Species:

A

B

Initial_1.<locals>.run_sim.<locals>.plot_at_time

NBC

<no docstring>

```

# === MultiFate Reaction-Diffusion (Numba-accelerated, Model from figure, Neumann BC) ===
import numpy as np
import matplotlib.pyplot as plt
from ipywidgets import interact, IntSlider, Play, HBox, Dropdown, ToggleButtons, jslink
from google.colab import output

```

```

output.enable_custom_widget_manager()
from IPython.display import display
from numba import njit, prange

def Initial_N1():
    # ----- Grid -----
    N = 60

    # ----- Initial Conditions -----
    def square(N):
        A0 = np.random.uniform(19.0, 20.0, (N, N))
        B0 = np.random.uniform(19.0, 20.0, (N, N))
        return A0, B0

    def random_300(N):
        nx, ny = N, N
        A0 = np.zeros((nx, ny))
        B0 = np.zeros((nx, ny))
        num_total = 900
        num_set = 300
        total_points = nx * ny

        all_indices_A = np.random.choice(total_points, size=num_total, replace=False)
        for k, val in enumerate([9.0, 0.5, 9.0]):
            part = all_indices_A[k * num_set:(k + 1) * num_set]
            coords = np.array(np.unravel_index(part, (nx, ny))).T
            A0[coords[:, 0], coords[:, 1]] = val

        all_indices_B = np.random.choice(total_points, size=num_total, replace=False)
        for k, val in enumerate([9.0, 9.0, 0.5]):
            part = all_indices_B[k * num_set:(k + 1) * num_set]
            coords = np.array(np.unravel_index(part, (nx, ny))).T
            B0[coords[:, 0], coords[:, 1]] = val

    return A0, B0

def radial_gradient_both(N, center=None,
                        A_inner=10.0, A_outer=1.0,
                        B_inner=10.0, B_outer=1.0):
    if center is None:
        center = (N // 2, N // 2)
    ii, jj = np.indices((N, N))
    r = np.sqrt((ii - center[0]) ** 2 + (jj - center[1]) ** 2)
    r = r / r.max()
    A = A_outer + (A_inner - A_outer) * np.exp(-4 * r)
    B = B_outer + (B_inner - B_outer) * np.exp(-4 * r)
    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))
    return A0, B0

def multi_gaussian(N, centers=[(30, 30), (15, 45), (45, 15)], A_inner=10, B_inner=10):
    A = np.zeros((N, N))
    B = np.zeros((N, N))
    rr, cc = np.indices((N, N))
    for cx, cy in centers:
        dist2 = (rr - cx) ** 2 + (cc - cy) ** 2
        A += A_inner * np.exp(-dist2 / (2 * 5.0 ** 2))
        B += B_inner * np.exp(-dist2 / (2 * 5.0 ** 2))
    A0 = A + np.random.uniform(0.0, 1.0, (N, N))
    B0 = B + np.random.uniform(0.0, 1.0, (N, N))
    return A0, B0

def sinusoidal_initial(N=60, noise_strength=0.1):
    x = np.linspace(0, 2*np.pi, N)
    y = np.linspace(0, 2*np.pi, N)
    X, Y = np.meshgrid(x, y)
    pattern = np.sin(X) * np.sin(Y)
    A = 19.0 + (pattern + 1) / 2
    B = 19.0 + (pattern + 1) / 2
    A0 = A + noise_strength * (np.random.rand(N, N) - 0.5)
    B0 = B + noise_strength * (np.random.rand(N, N) - 0.5)
    return A0, B0

ic_options = {
    "Radial Gradient": radial_gradient_both,
    "Random 300": random_300,
}

```

```

    "Multi Gaussian Peaks": multi_gaussian,
    "Square": square,
    "Sinusoidal": sinusoidal_initial
}

# ----- Parameters -----
Du, Dv = 0.0001, 0.0001
alpha_u, alpha_v = 5.0, 5.0
gamma_u, gamma_v = 1.0, 1.0
dt = 0.2
steps = 10000
save_every = 1

# ----- Numba kernels -----
@njit(fastmath=True)
def reaction_u(u_ij, v_ij, alpha_u, gamma_u):
    return alpha_u / (1.0 + v_ij * v_ij) - gamma_u * u_ij

@njit(fastmath=True)
def reaction_v(u_ij, v_ij, alpha_v, gamma_v):
    return alpha_v / (1.0 + u_ij * u_ij) - gamma_v * v_ij

@njit(parallel=True, fastmath=True)
def _step_neumann(A, B, Du, Dv, alpha_u, alpha_v, gamma_u, gamma_v, dt):
    nx, ny = A.shape
    Anew = np.empty_like(A)
    Bnew = np.empty_like(B)

    for i in prange(nx):
        im = max(i - 1, 0)      # Neumann BC
        ip = min(i + 1, nx - 1)
        for j in range(ny):
            jm = max(j - 1, 0)
            jp = min(j + 1, ny - 1)

            LapA = -4.0 * A[i, j] + A[im, j] + A[ip, j] + A[i, jm] + A[i, jp]
            LapB = -4.0 * B[i, j] + B[im, j] + B[ip, j] + B[i, jm] + B[i, jp]

            fA = reaction_u(A[i, j], B[i, j], alpha_u, gamma_u)
            fB = reaction_v(A[i, j], B[i, j], alpha_v, gamma_v)

            Anew[i, j] = A[i, j] + dt * (Du * LapA + fA)
            Bnew[i, j] = B[i, j] + dt * (Dv * LapB + fB)

    # enforce non-negativity
    for i in prange(nx):
        for j in range(ny):
            if Anew[i, j] < 0.0:
                Anew[i, j] = 0.0
            if Bnew[i, j] < 0.0:
                Bnew[i, j] = 0.0

    return Anew, Bnew

# ----- Simulation Runner -----
def run_sim(initial_condition):
    A0, B0 = ic_options[initial_condition](N)
    A_temp, B_temp = A0.copy(), B0.copy()

    # warmup
    A_temp, B_temp = _step_neumann(A_temp, B_temp, Du, Dv, alpha_u, alpha_v, gamma_u, gamma_v, dt)

    A_list = [A0.copy()]
    B_list = [B0.copy()]
    for s in range(1, steps + 1):
        A_temp, B_temp = _step_neumann(A_temp, B_temp, Du, Dv, alpha_u, alpha_v, gamma_u, gamma_v, dt)
        if s % save_every == 0:
            A_list.append(A_temp.copy())
            B_list.append(B_temp.copy())

    def plot_at_time(idx, species):
        plt.figure(figsize=(5, 5), dpi=150)
        data = A_list[idx] if species == "A" else B_list[idx]
        title = f"{species} Concentration (t={idx * save_every * dt:.2f})"
        img = plt.imshow(data, cmap='inferno', origin='lower', interpolation='bilinear')
        plt.colorbar(img)

```

```
plt.title(title)
plt.axis('off')
plt.show()

species_toggle = ToggleButtons(options=["A", "B"], value="A", description="Species:", button_style="info")
play = Play(value=0, min=0, max=len(A_list) - 1, step=1, interval=100)
slider = IntSlider(value=0, min=0, max=len(A_list) - 1, step=1, description="Frame")
jslink((play, 'value'), (slider, 'value'))

widgets = HBox([play, slider, species_toggle])
interact_ui = interact(plot_at_time, idx=slider, species=species_toggle)
display(widgets, interact_ui)

ic_dropdown = Dropdown(options=list(ic_options.keys()), value="Radial Gradient", description="Initial Condition:")
interact(run_sim, initial_condition=ic_dropdown)

Initial N1()
```

Initial Cond [Radial Gradient]