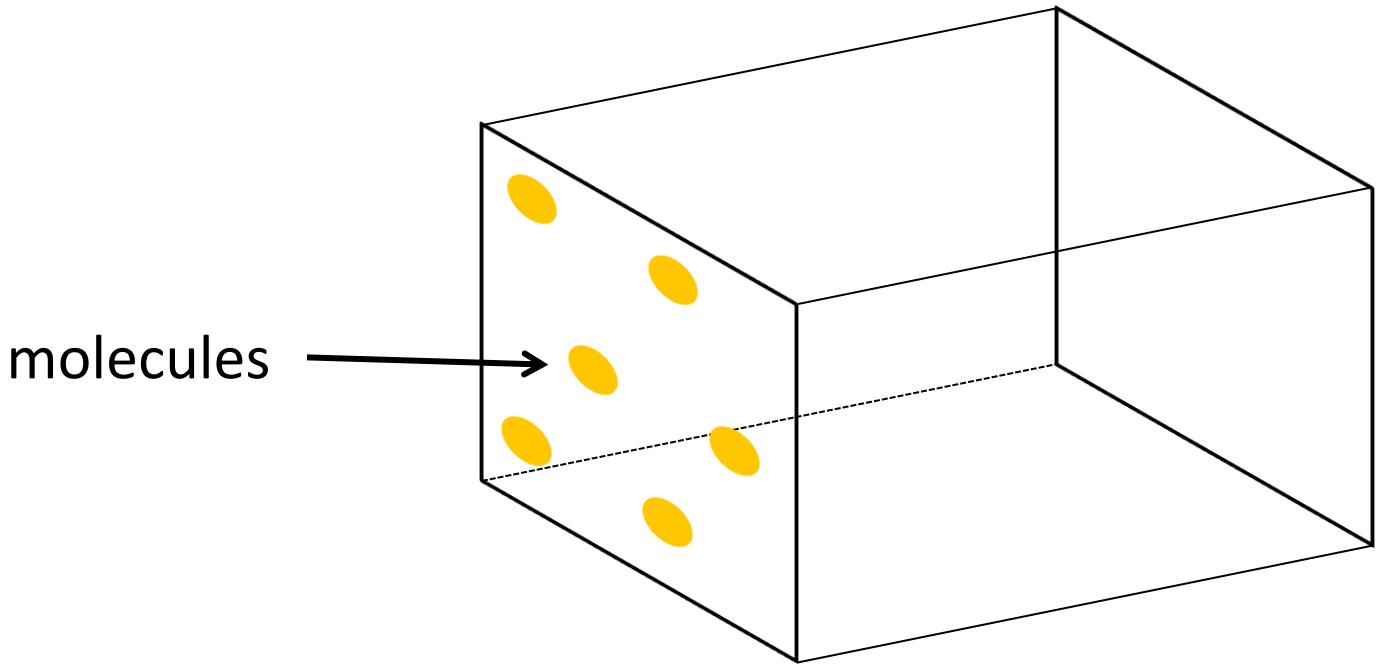
PFE 9

Palubicki

Diffusion

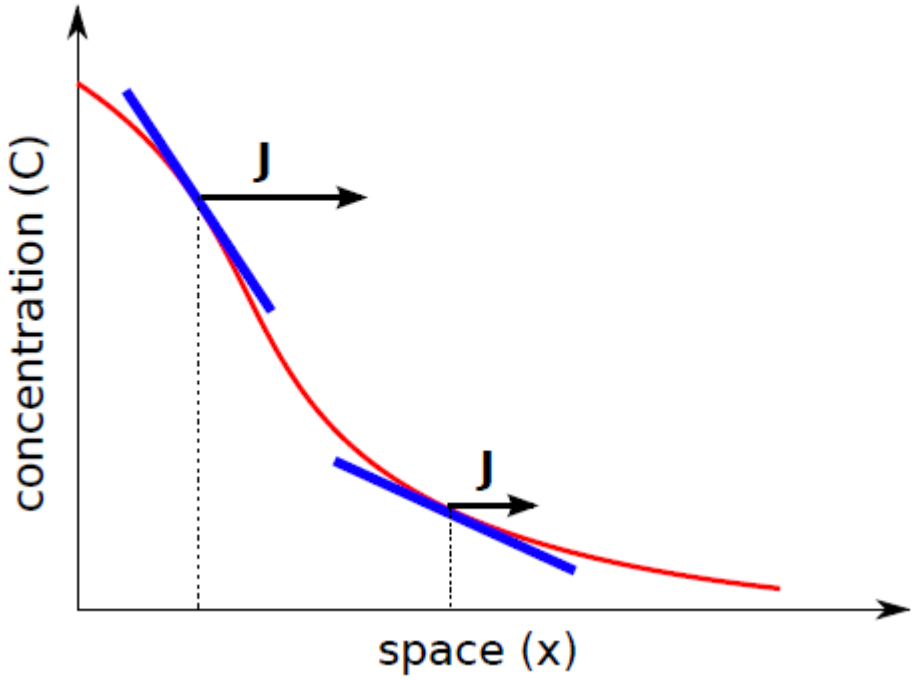


Ficks First Law

$$\dot{V} = \frac{(c_1 - c_2) \cdot A \cdot D}{x}$$

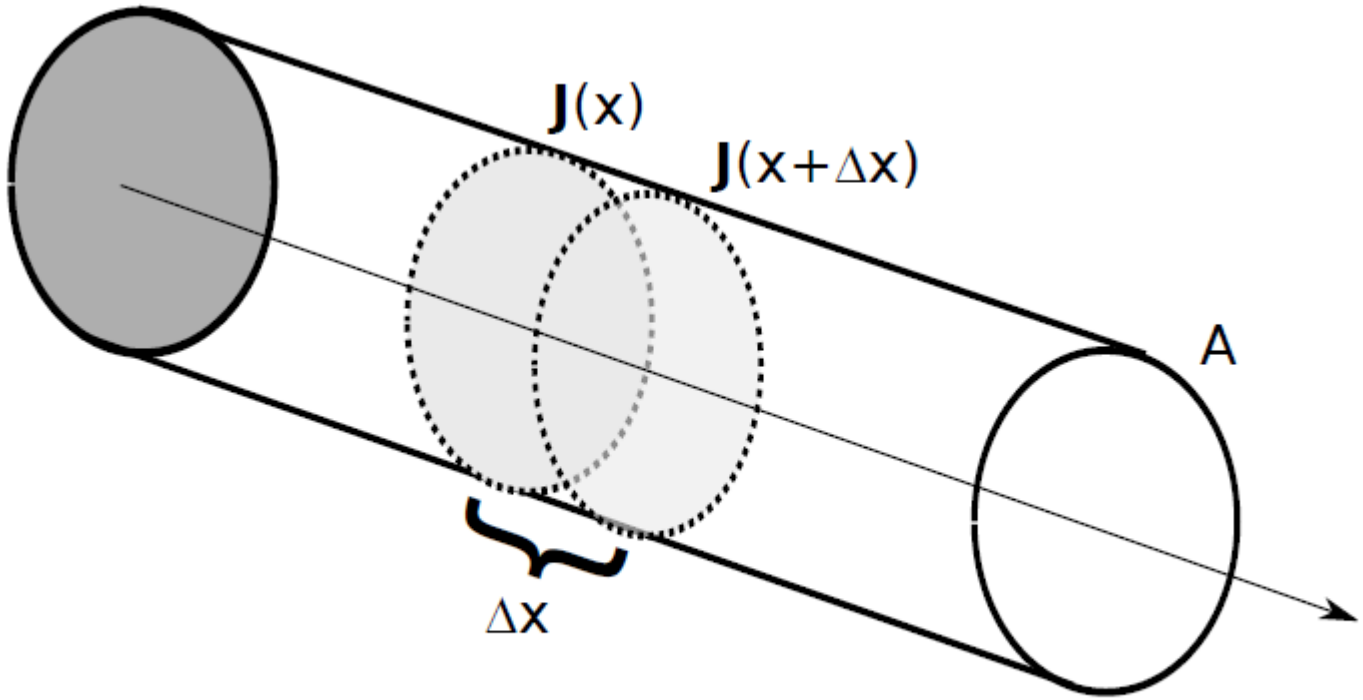
$$J = -D\nabla c$$

Flux Gradient



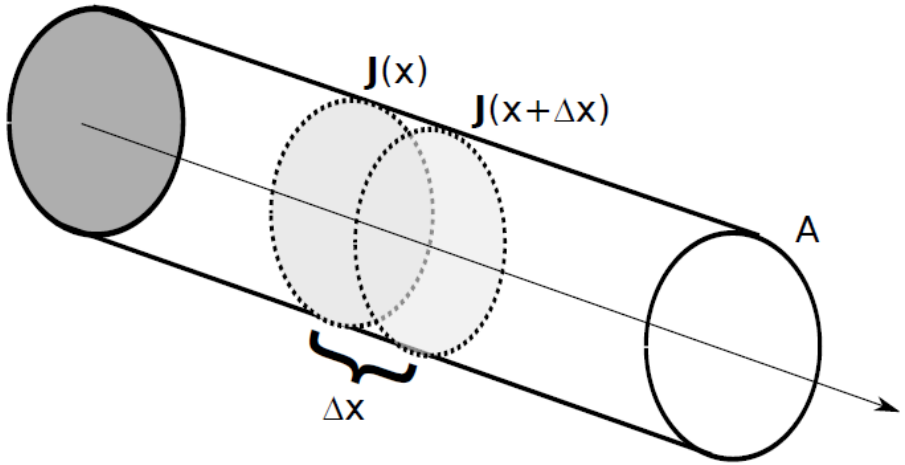
Continuity equation

- How does the number of particles change at a given position?
- For a cylinder at a position x to $x + \Delta x$:



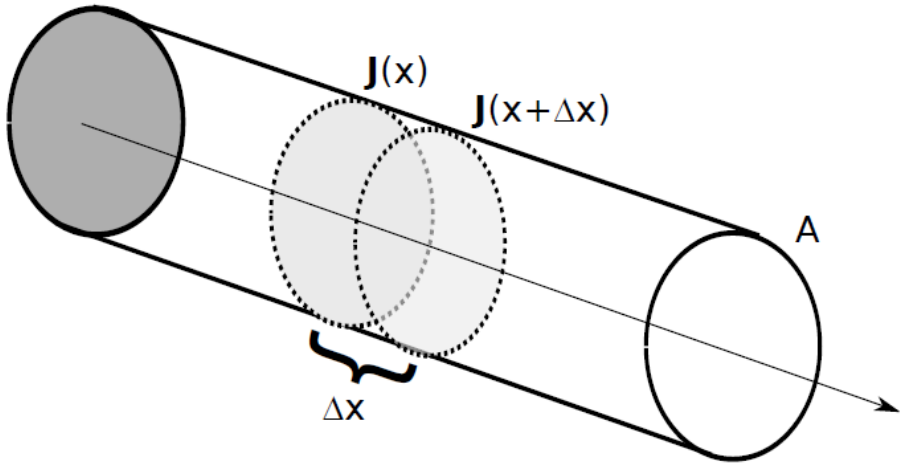
Continuity equation

- Number of particles:
  - $N = cA\Delta x$
  - Where A is the area of the cross-section
  - c, concentration of particles
  - Δx, length of the cylinder



Continuity equation

- Number of particles:
  - $N = cA\Delta x$
  - Where A is the area of the cross-section
  - c, concentration of particles
  - Δx, length of the cylinder
- Then the rate of change of the number of particles over time t is given by the fluxes at positions x and $x + \Delta x$:
- $\frac{\partial(cA\Delta x)}{\partial t} = AJ(x) - AJ(x + \Delta x) \pm \sigma A\Delta x$



Continuity equation

- $\frac{\partial(cA\Delta x)}{\partial t} = AJ(x) - AJ(x + \Delta x) \pm \sigma A\Delta x$

Continuity equation

- $\frac{\partial(cA\Delta x)}{\partial t} = AJ(x) - AJ(x+\Delta x) \pm \sigma A\Delta x$

- $\frac{\partial c(x,t)}{\partial t} = \frac{J(x)-J(x+\Delta x)}{\Delta x} \pm \sigma$

Continuity equation

- $\frac{\partial(cA\Delta x)}{\partial t} = AJ(x) - AJ(x+\Delta x) \pm \sigma A\Delta x$
- $\frac{\partial c(x,t)}{\partial t} = \frac{J(x)-J(x+\Delta x)}{\Delta x} \pm \sigma$
- When Δx is becoming close to zero:
- $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} \pm \sigma$

Continuity equation

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- When Δx is becoming close to zero:
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Continuity equation

- $\frac{\partial(cA\Delta x)}{\partial t} = AJ(x) - AJ(x+\Delta x) \pm \sigma A\Delta x$
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- When Δx is becoming close to zero:
- $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} \pm \sigma = \frac{\partial\left(D\frac{\partial c}{\partial x}\right)}{\partial x} \pm \sigma = D\frac{\partial^2 c}{\partial x^2} \pm \sigma$

Ficks 2nd Law of Diffusion

Laplace Operator

- The Laplace operator is a **second-order differential operator** in the **n-dimensional Euclidean space**, defined as the **divergence** $(\nabla \cdot)$ of the **gradient** (∇f)

- $\Delta f(x, y) = \nabla \cdot \nabla f$

Gradient ∇f

- The gradient of a scalar-valued differentiable function f of several variables, is a vector-valued function ∇ f : $R^n \rightarrow R^n$ whose value at a point is a tangent vector to f.

$$\nabla f = \frac{\partial f}{\partial x}\mathbf{i} + \frac{\partial f}{\partial y}\mathbf{j}$$

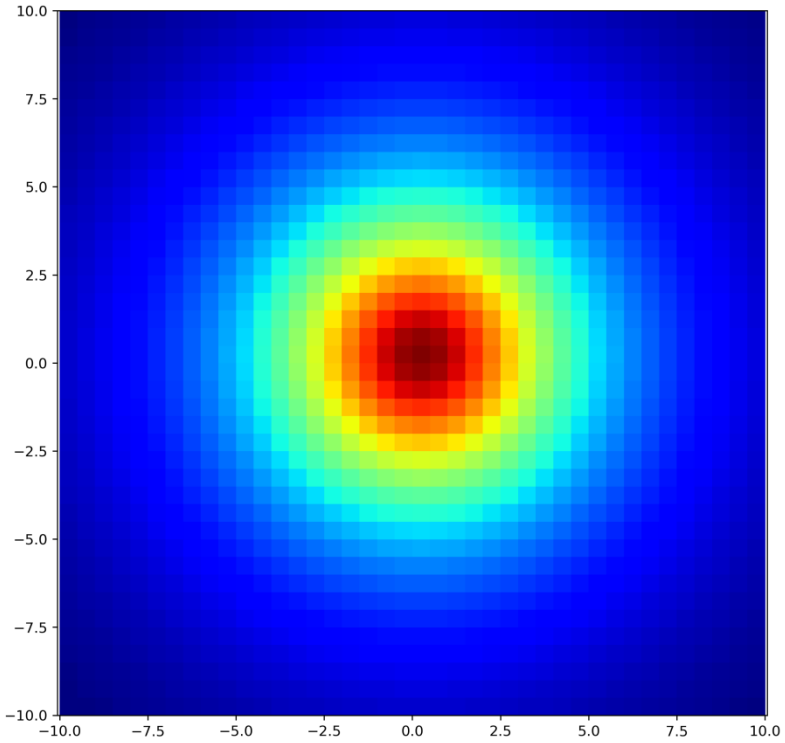
where **i**, **j** are the standard unit vectors in the directions of the *x*, *y* coordinates

Example

```
x = y = np.linspace(-10., 10., 41)
xv, yv = np.meshgrid(x, y, indexing=’ij’)
fv = h0/(1 + (xv**2+yv**2)/(R**2)) # Some function
```

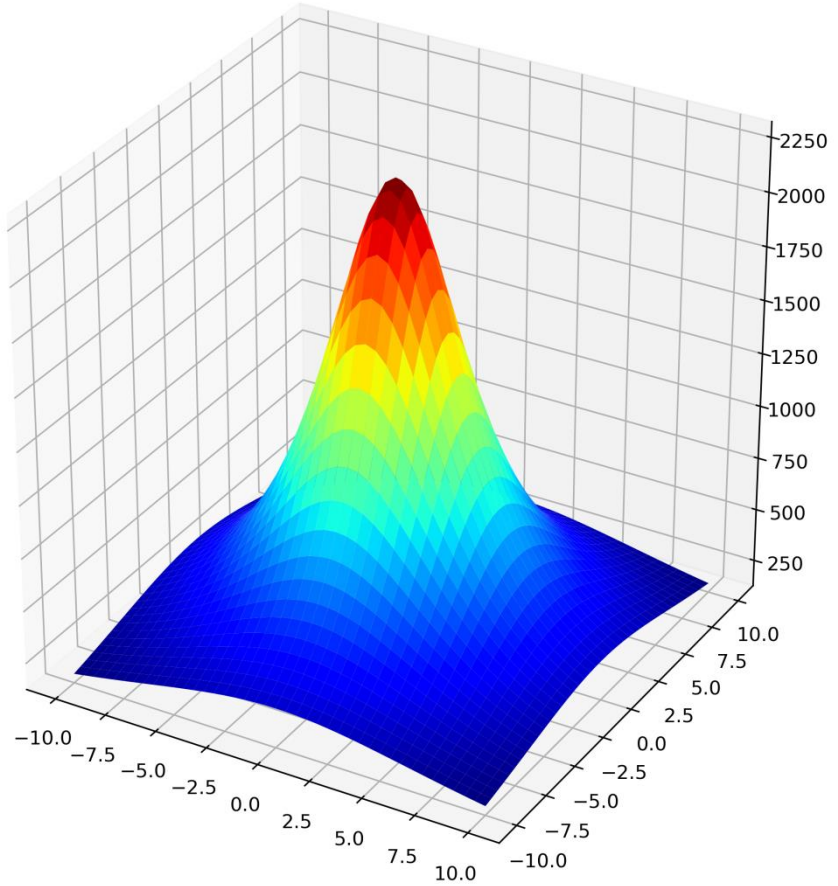
Example

```
plt.pcolormesh(x,y,fv, cmap = 'jet')
```



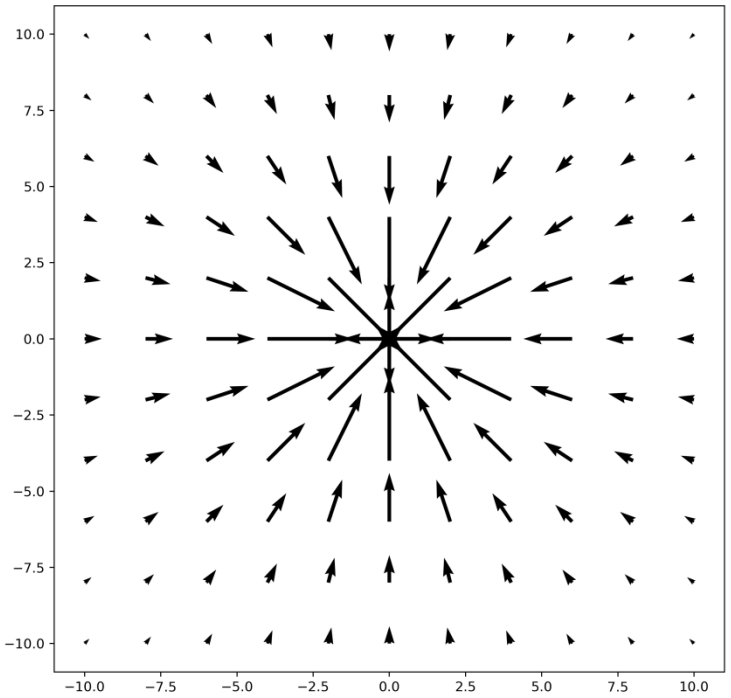
Example

```
ax.plot_surface(xv, yv, fv, cmap='jet')
```



Gradient Computation ∇f

```
dhdx, dhdy = np.gradient(fv) # dh/dx, dh/dy
```



quiver

Gradient Computation ∇f

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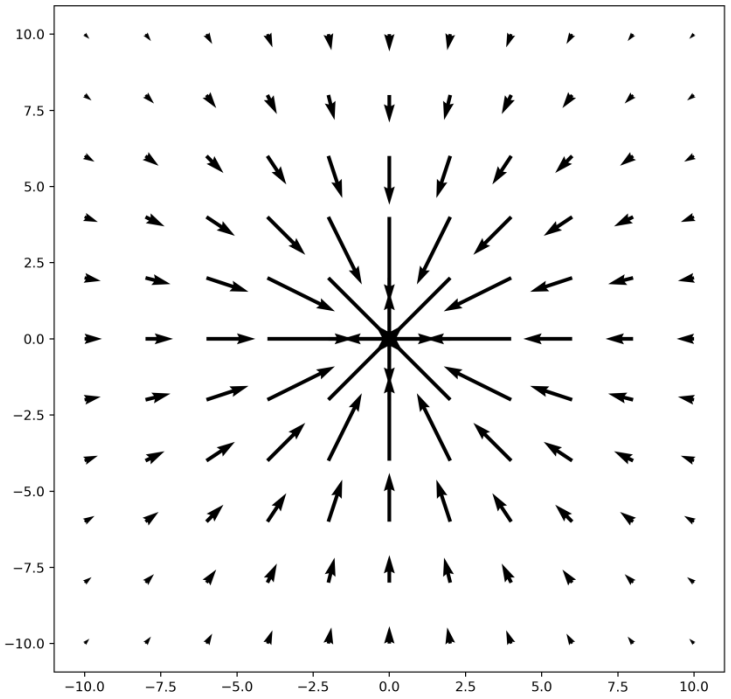
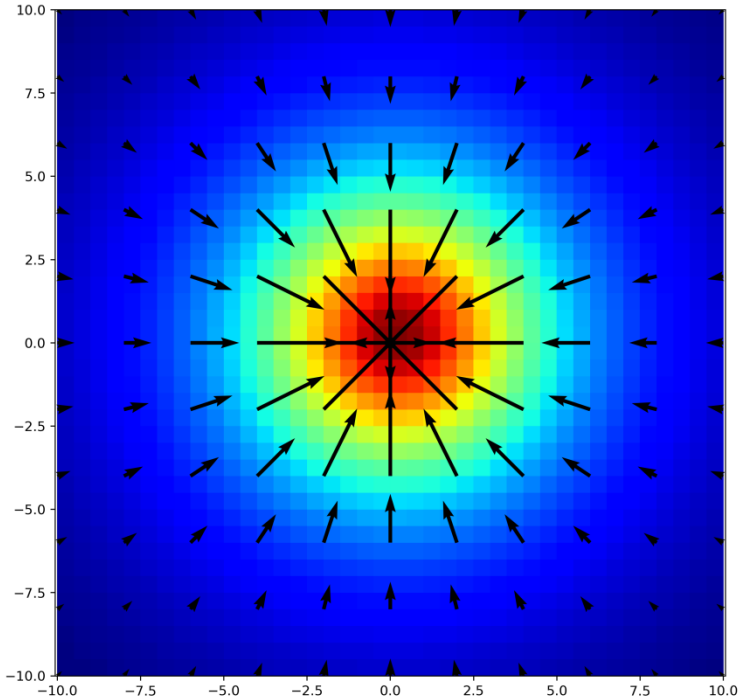


quiver



pcolormesh + quiver

Gradient Computation ∇f

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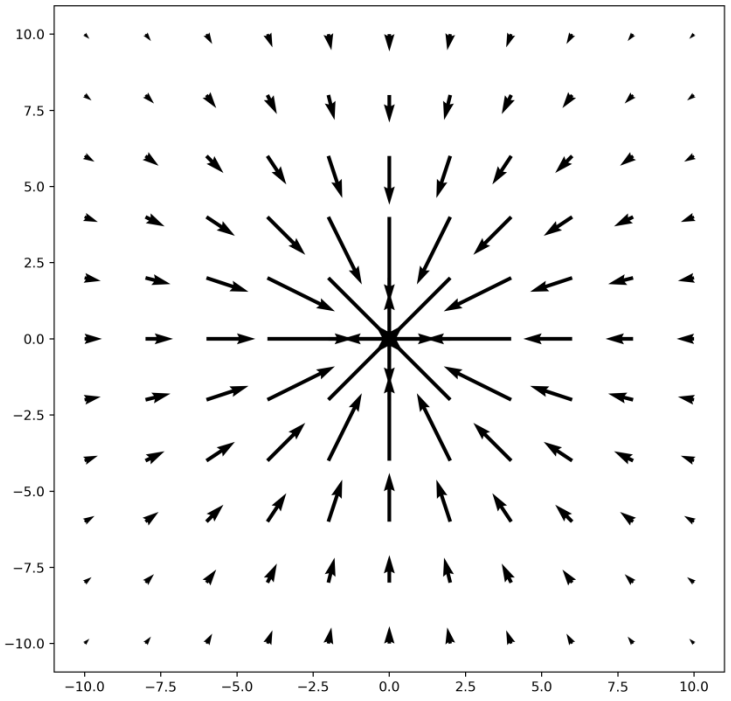
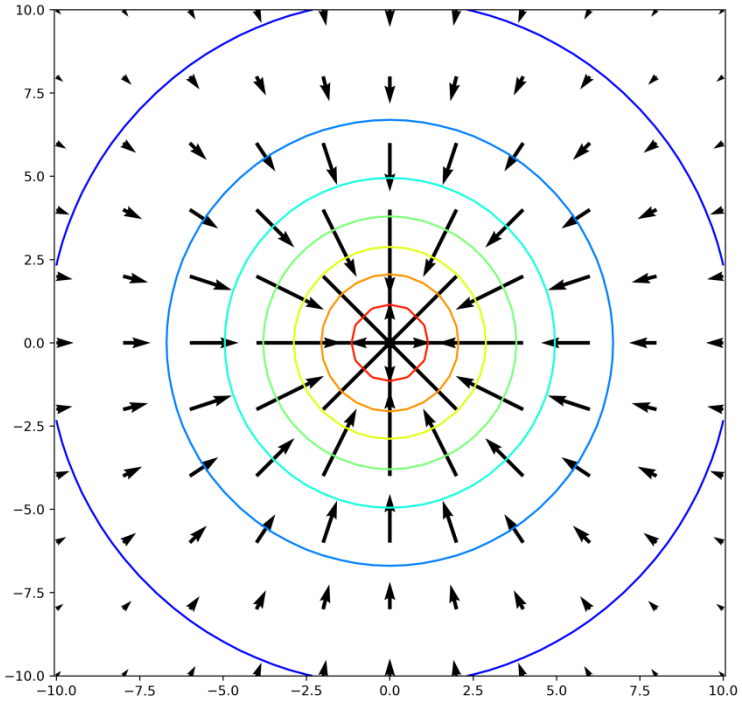
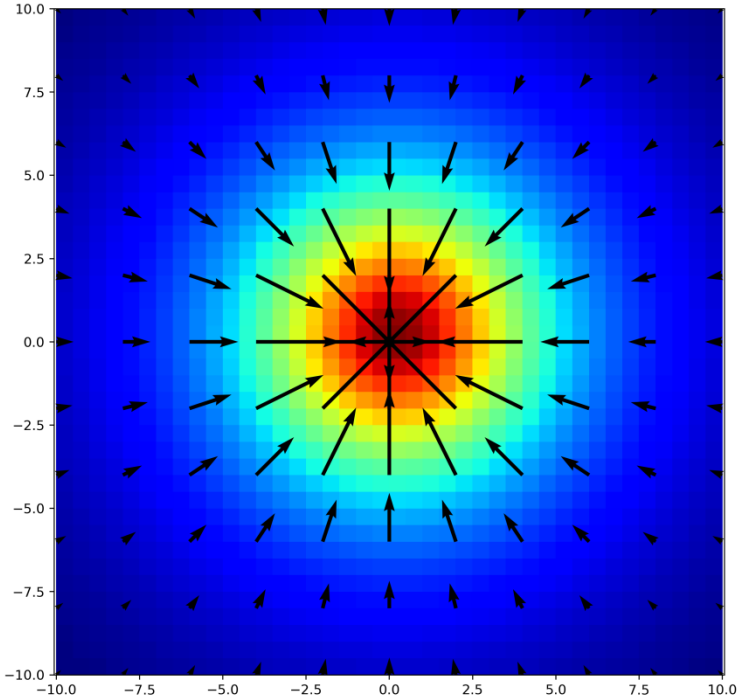


quiver



contour + quiver

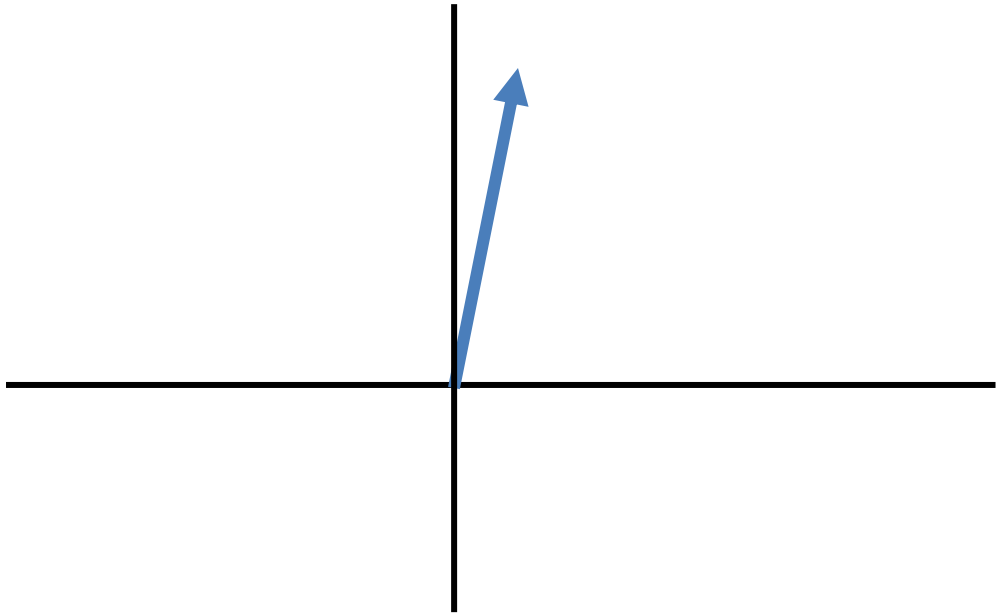


pcolormesh + quiver

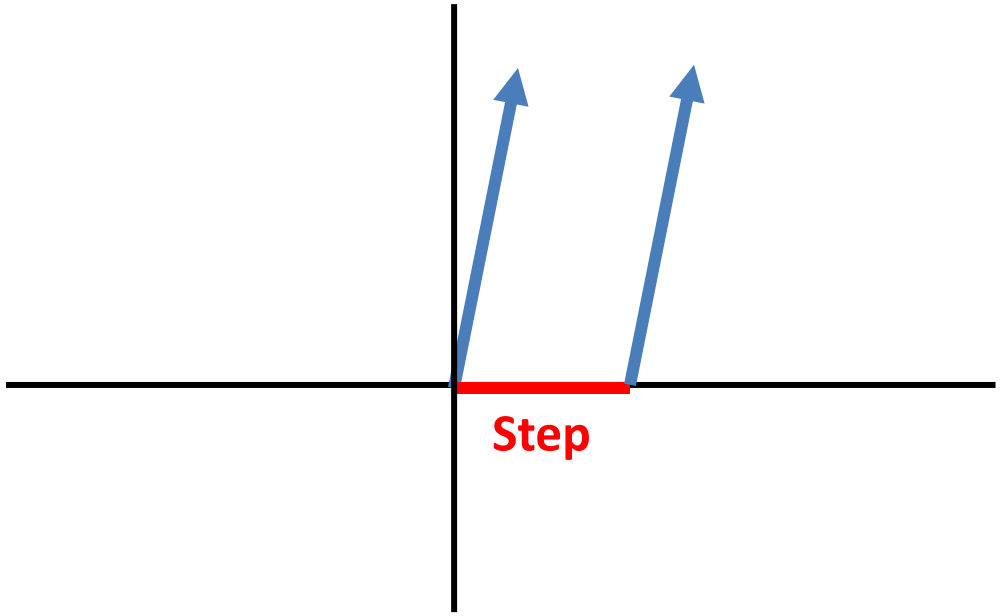
2D Divergence $\nabla \cdot$

$$\nabla \cdot (\mathbf{V}(x,y)) = \frac{\partial \, \mathbf{V}_x(x,y)}{\partial x} + \frac{\partial \, \mathbf{V}_y(x,y)}{\partial y}$$

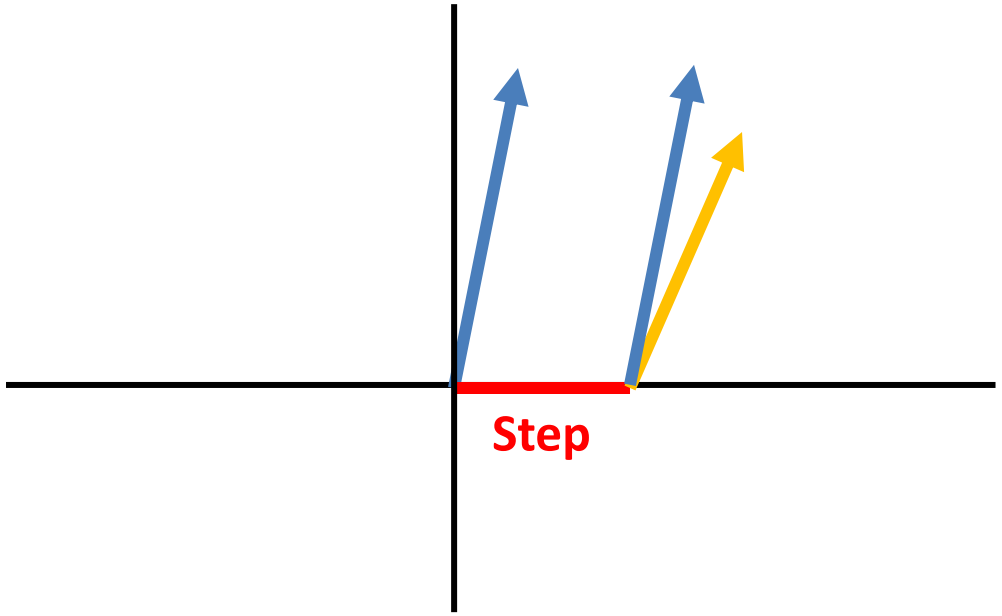
Geometric Interpretation of Divergence



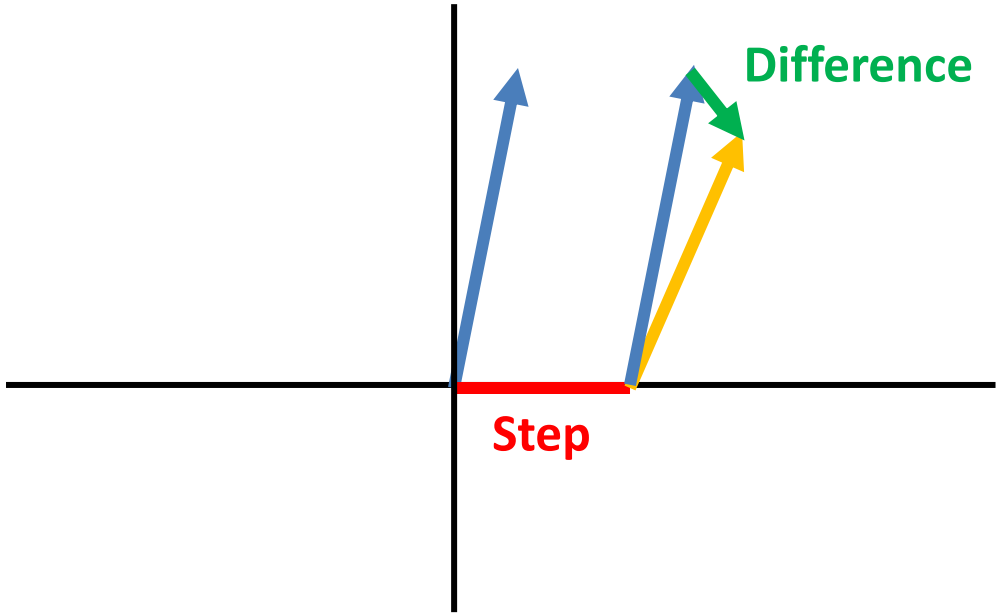
Geometric Interpretation of Divergence



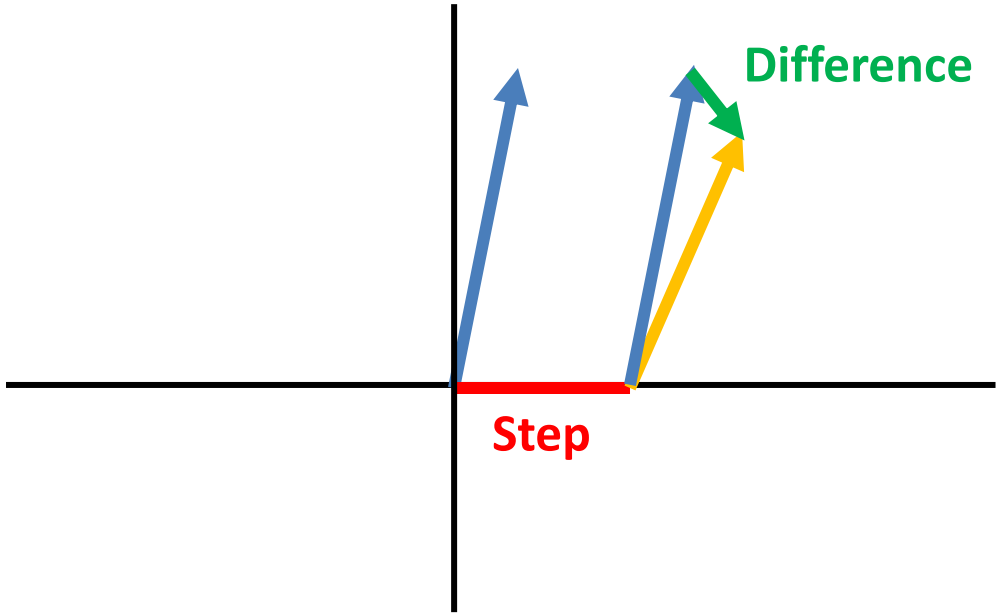
Geometric Interpretation of Divergence



Geometric Interpretation of Divergence

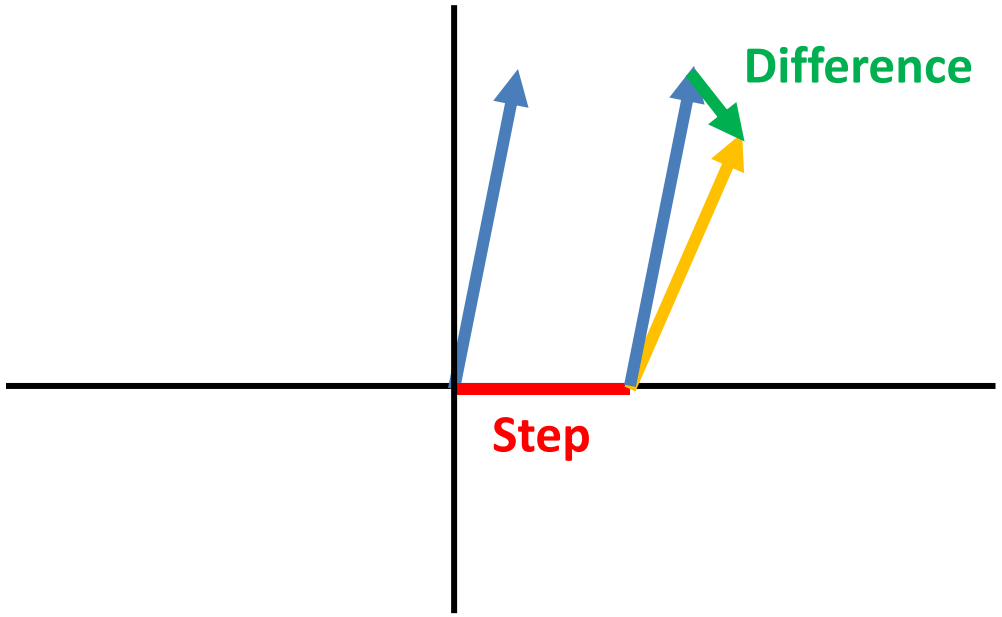


Geometric Interpretation of Divergence



$$\textbf{Step} \cdot \textbf{Difference}$$

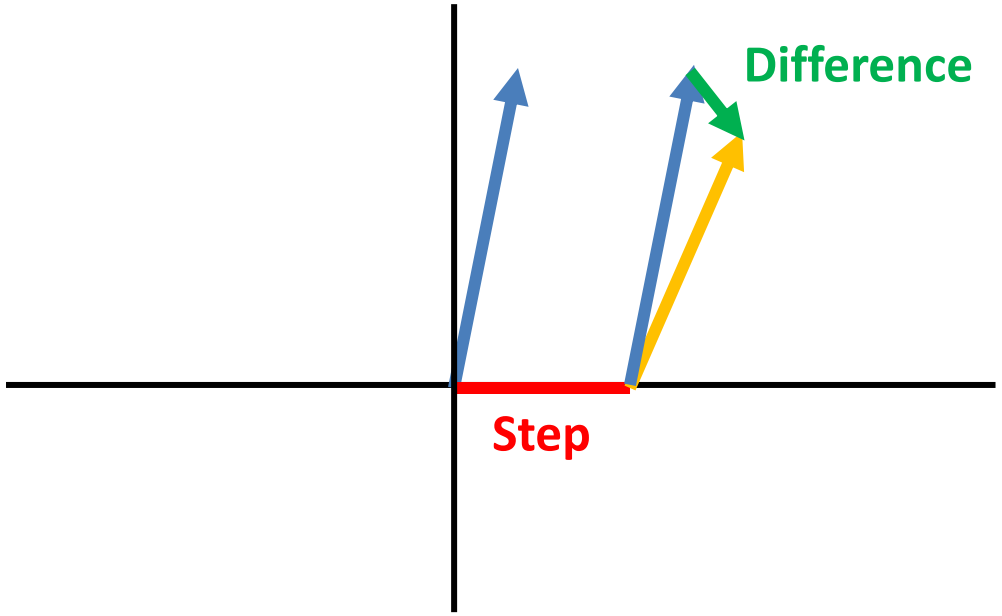
Geometric Interpretation of Divergence



Example: $(1, 0) \cdot (0.2, -0.2) = 1 \cdot 0.2 + 0 \cdot (-0.2) = 0.2$

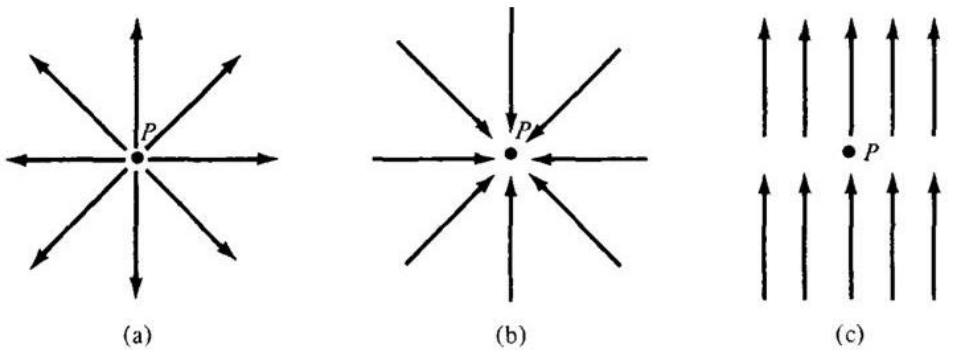
Step $\cdot$ **Difference**

Geometric Interpretation of Divergence



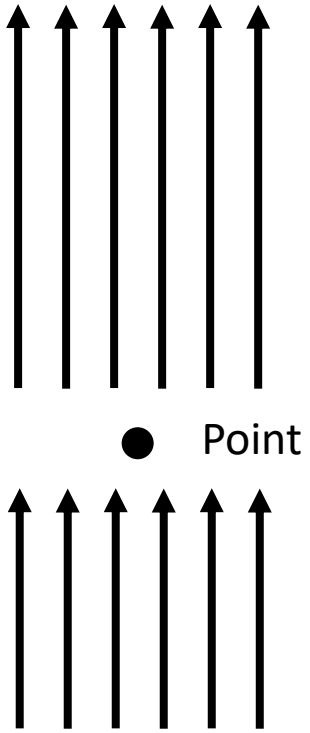
$$\frac{\partial \mathbf{V}_x(x,y)}{\partial x} + \frac{\partial \mathbf{V}_y(x,y)}{\partial y} \xrightarrow{\text{Averaged}} \textbf{Step} \cdot \textbf{Difference}$$

Divergence $\nabla \cdot$



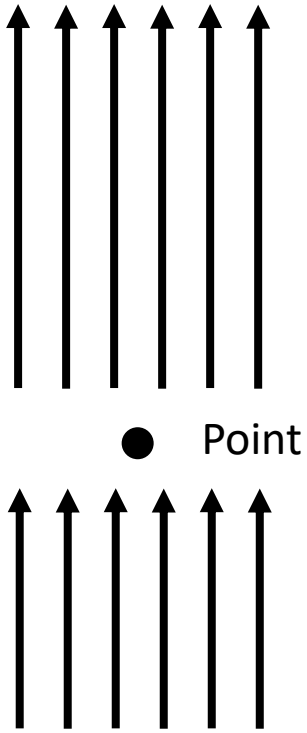
(a) Positive divergence, (b) negative divergence, (c) zero divergence.

Example Case



Example Case

Positive Divergence



Ficks 2nd Law

- $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x}$

Ficks 2nd Law

- $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} = \frac{\partial\left(D\frac{\partial c}{\partial x}\right)}{\partial x}$

Ficks 2nd Law

- $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} = \frac{\partial\left(D\frac{\partial c}{\partial x}\right)}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$

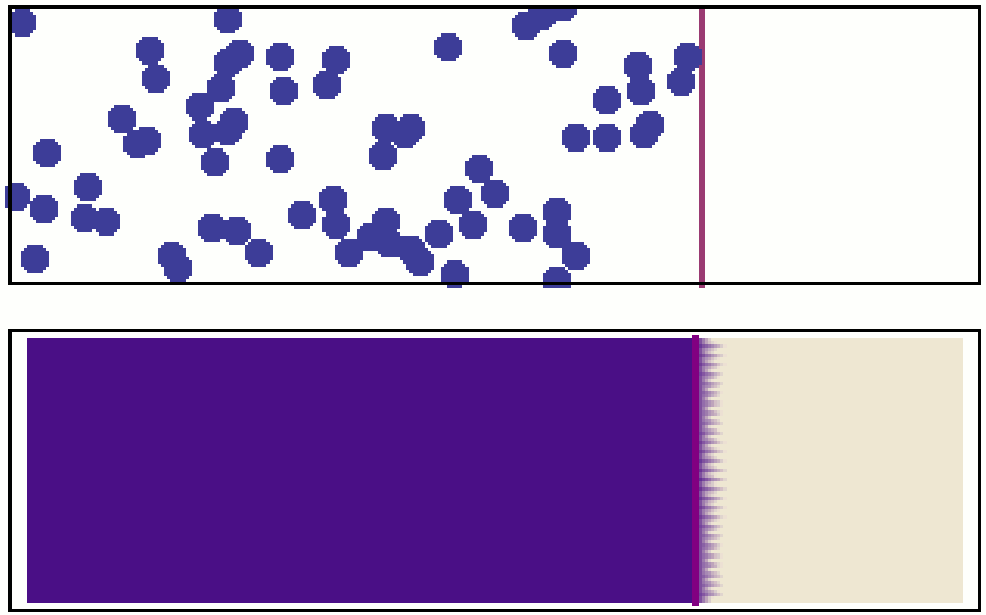
Ficks 2nd Law > 1D

- $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} = \frac{\partial\left(D\frac{\partial c}{\partial x}\right)}{\partial x} = D\frac{\partial^2 c}{\partial x^2} = D(\nabla \cdot \nabla c)$

Ficks 2nd Law > 1D

- $\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} = \frac{\partial\left(D\frac{\partial c}{\partial x}\right)}{\partial x} = D\frac{\partial^2 c}{\partial x^2} = D(\nabla \cdot \nabla c) = D\Delta c$

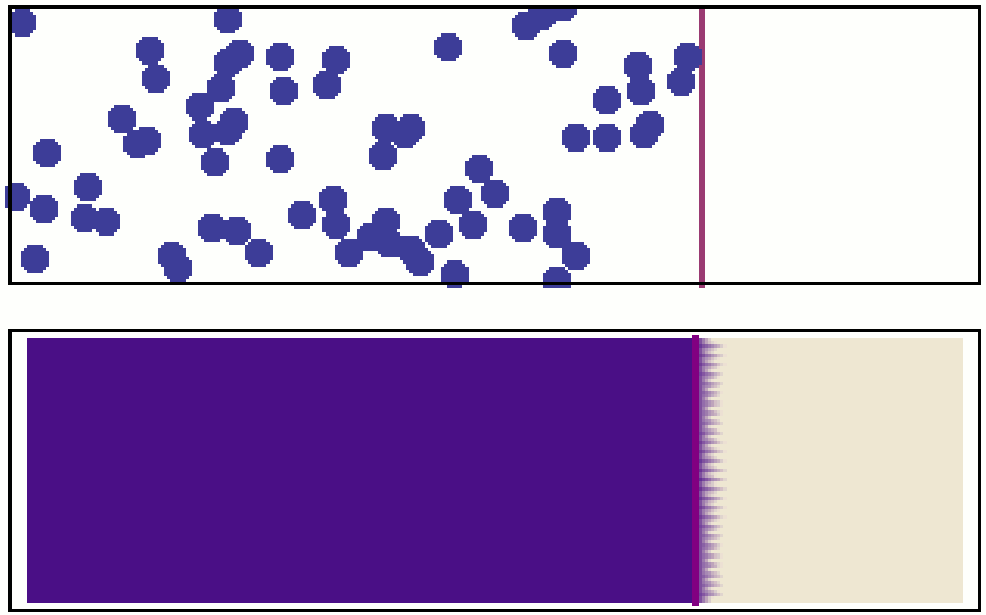
Ficks 2nd Law: $\frac{\partial c(x,t)}{\partial t} = D\Delta c$



Discrete model

Continuous model

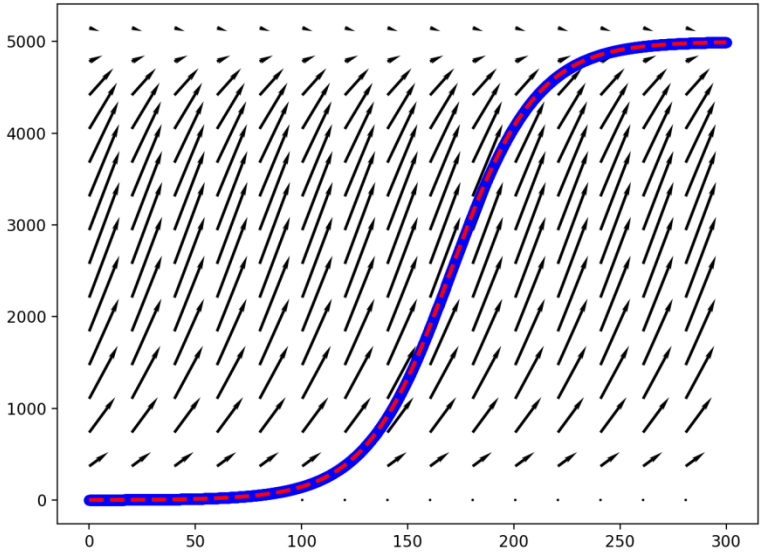
$c(x,t)$ depends on both space and time



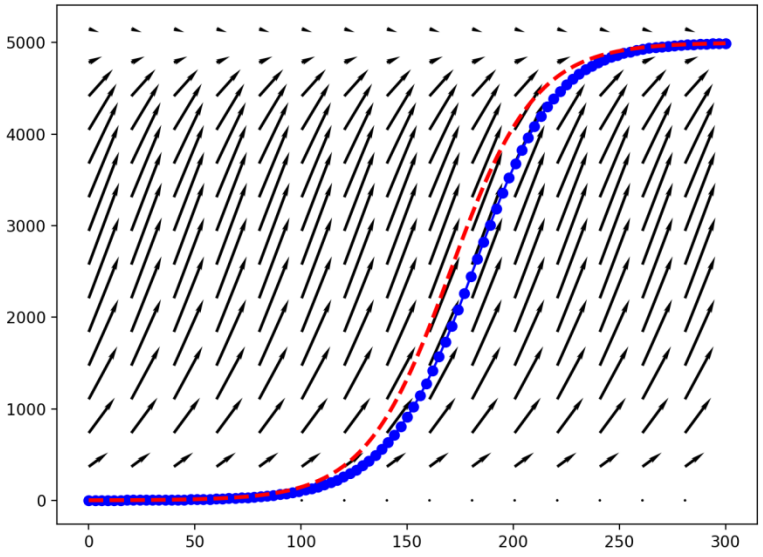
Discrete model

Continuous model

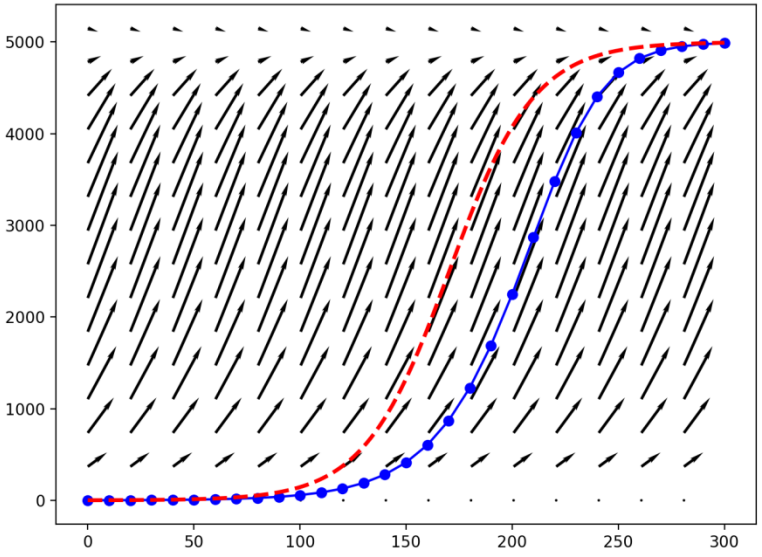
Discretization of Time



dt = 0.1



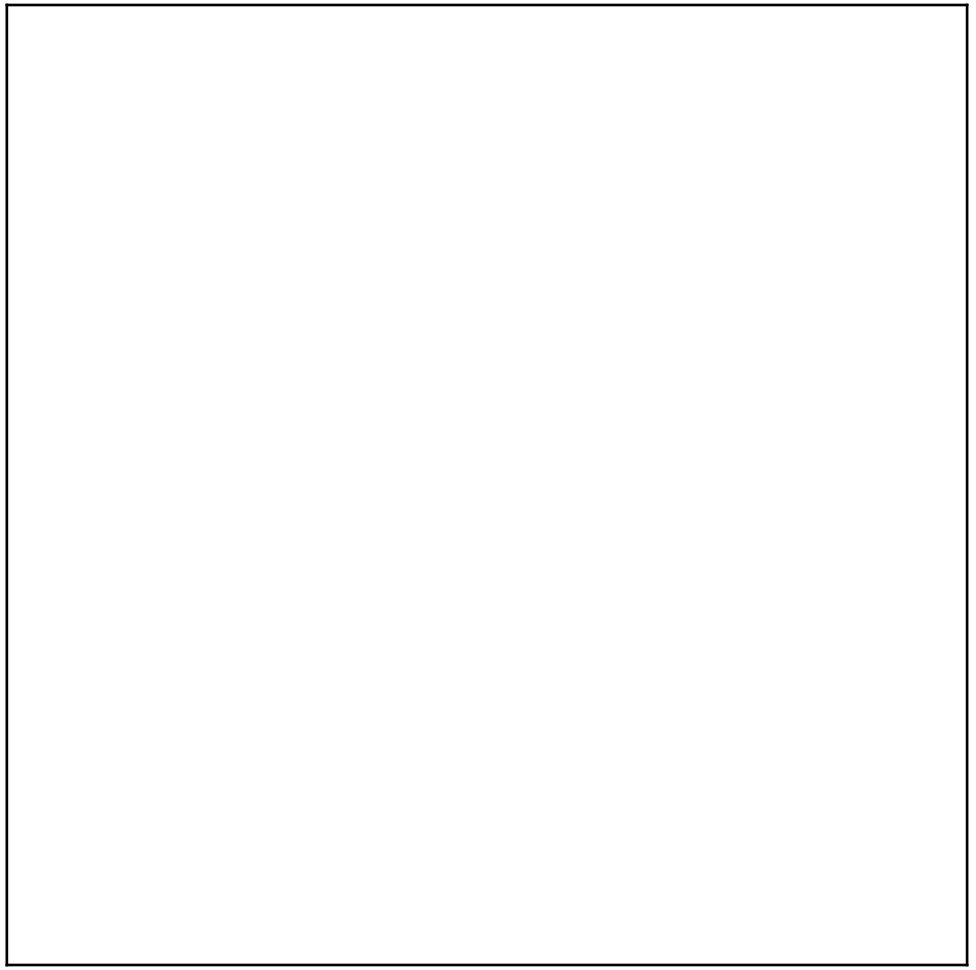
dt = 3



dt = 10

Follow the vector field: `x[n+1] = x[n] + dt*f(x[n], t[n])`

Discretization of 2D Space



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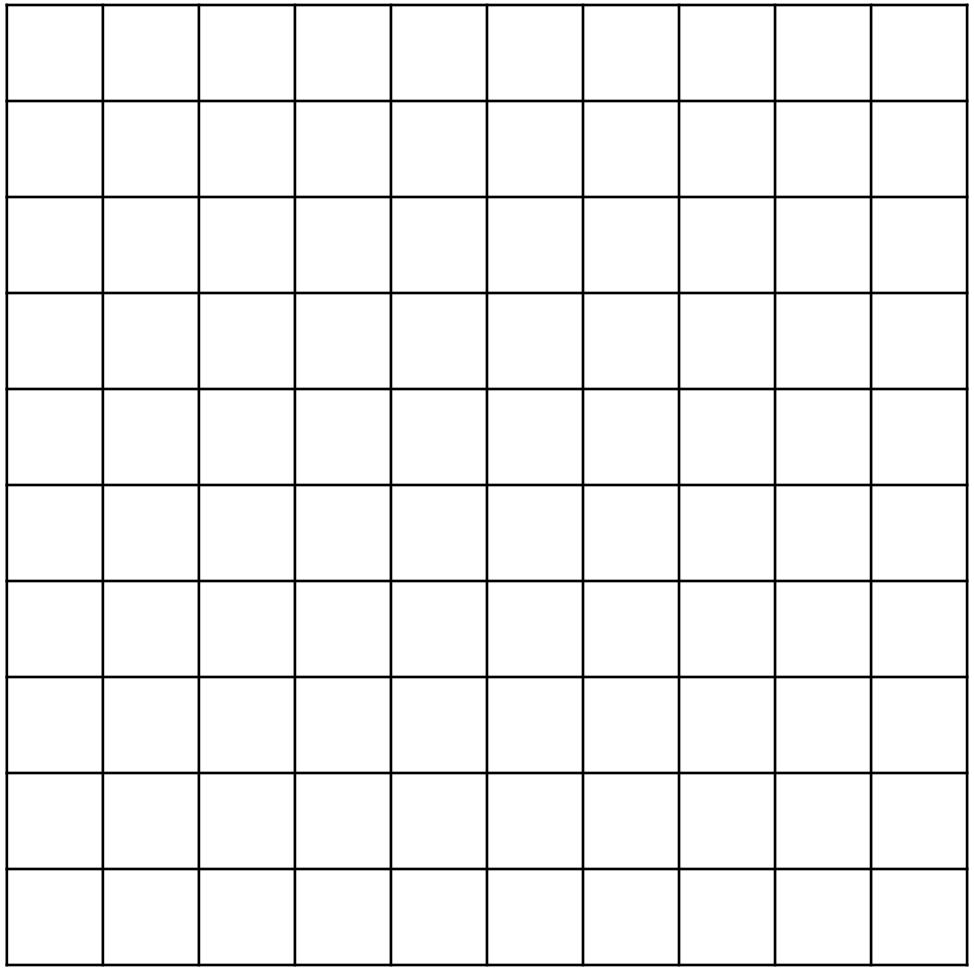

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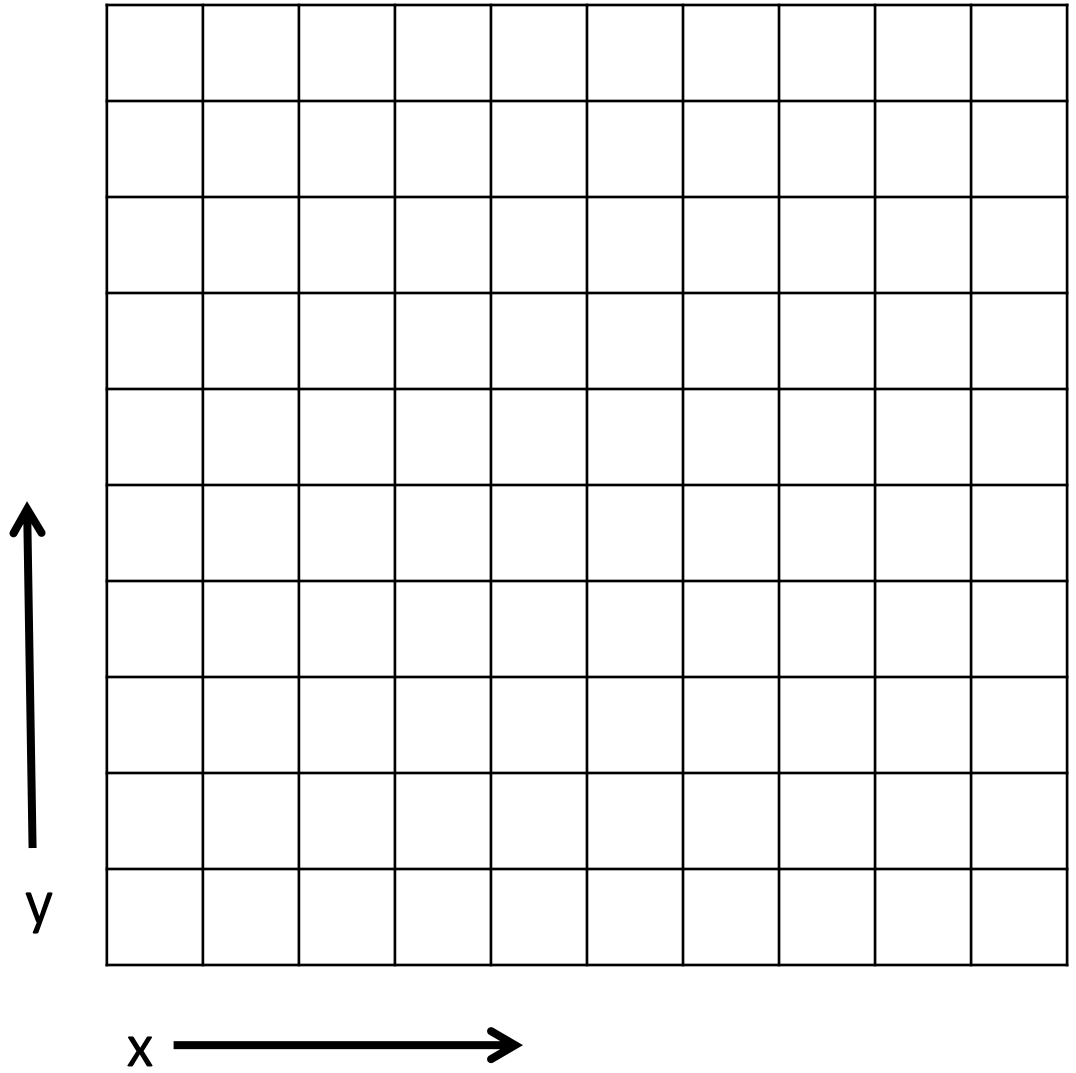
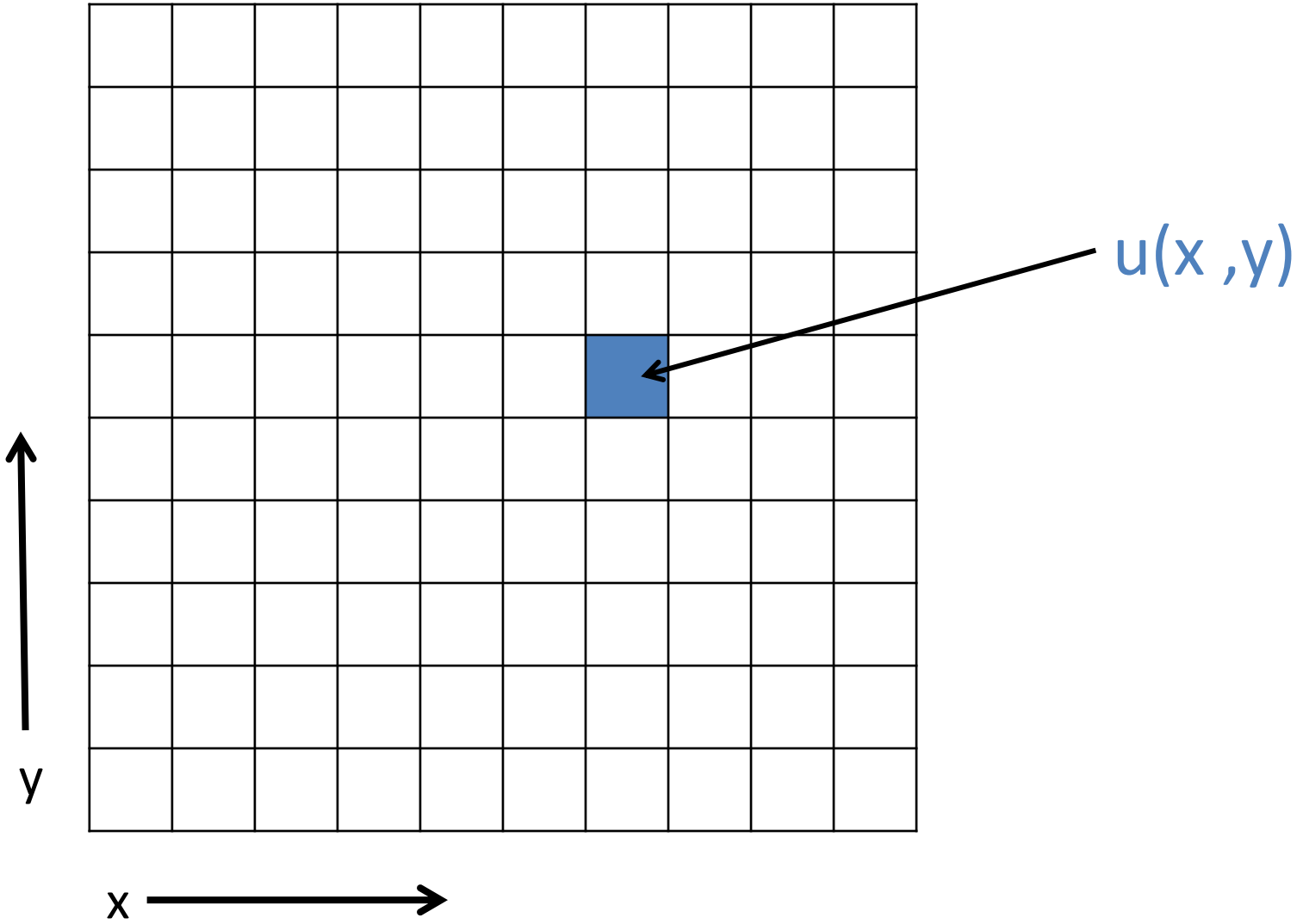


Discretization of 2D Space



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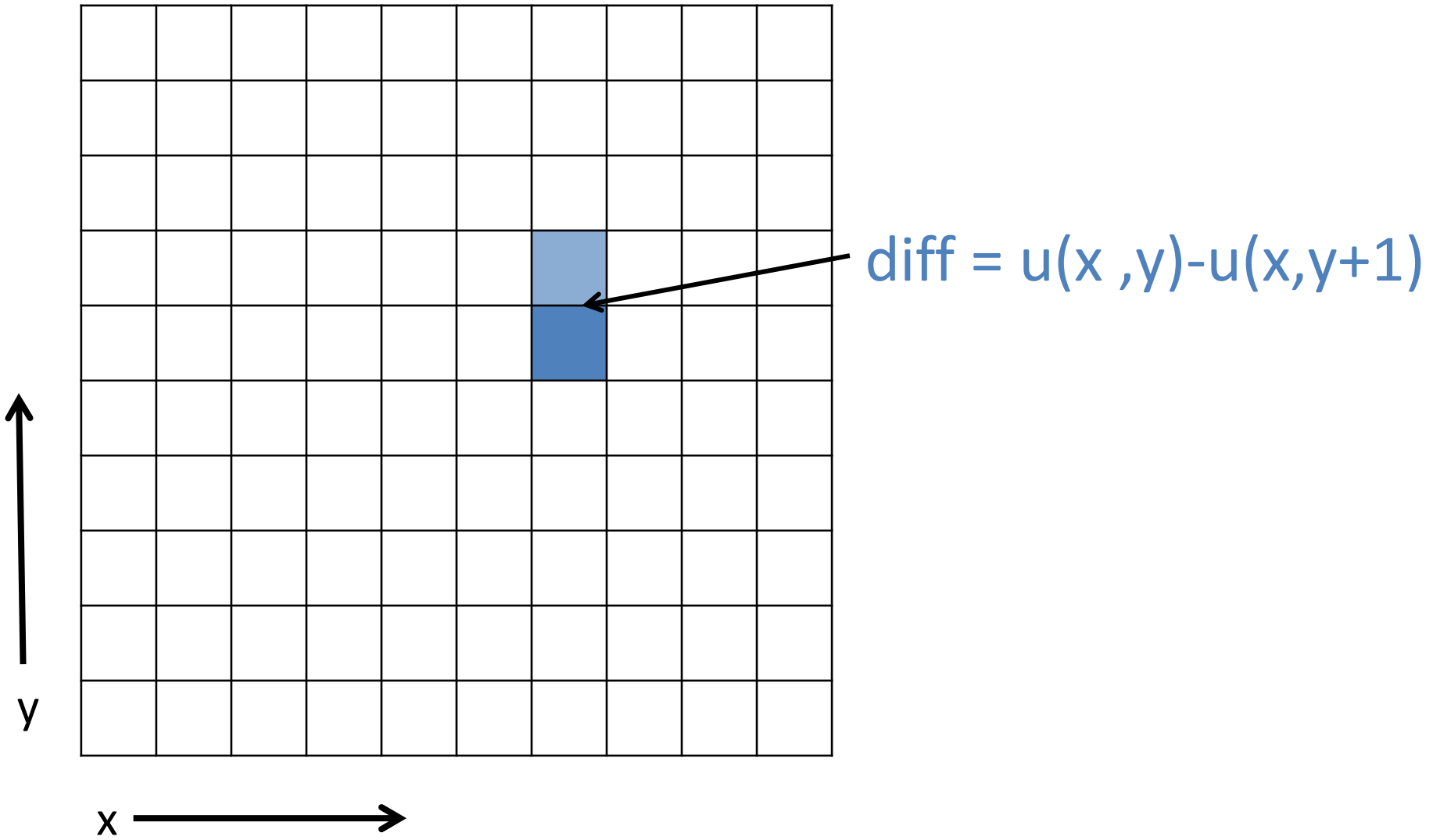

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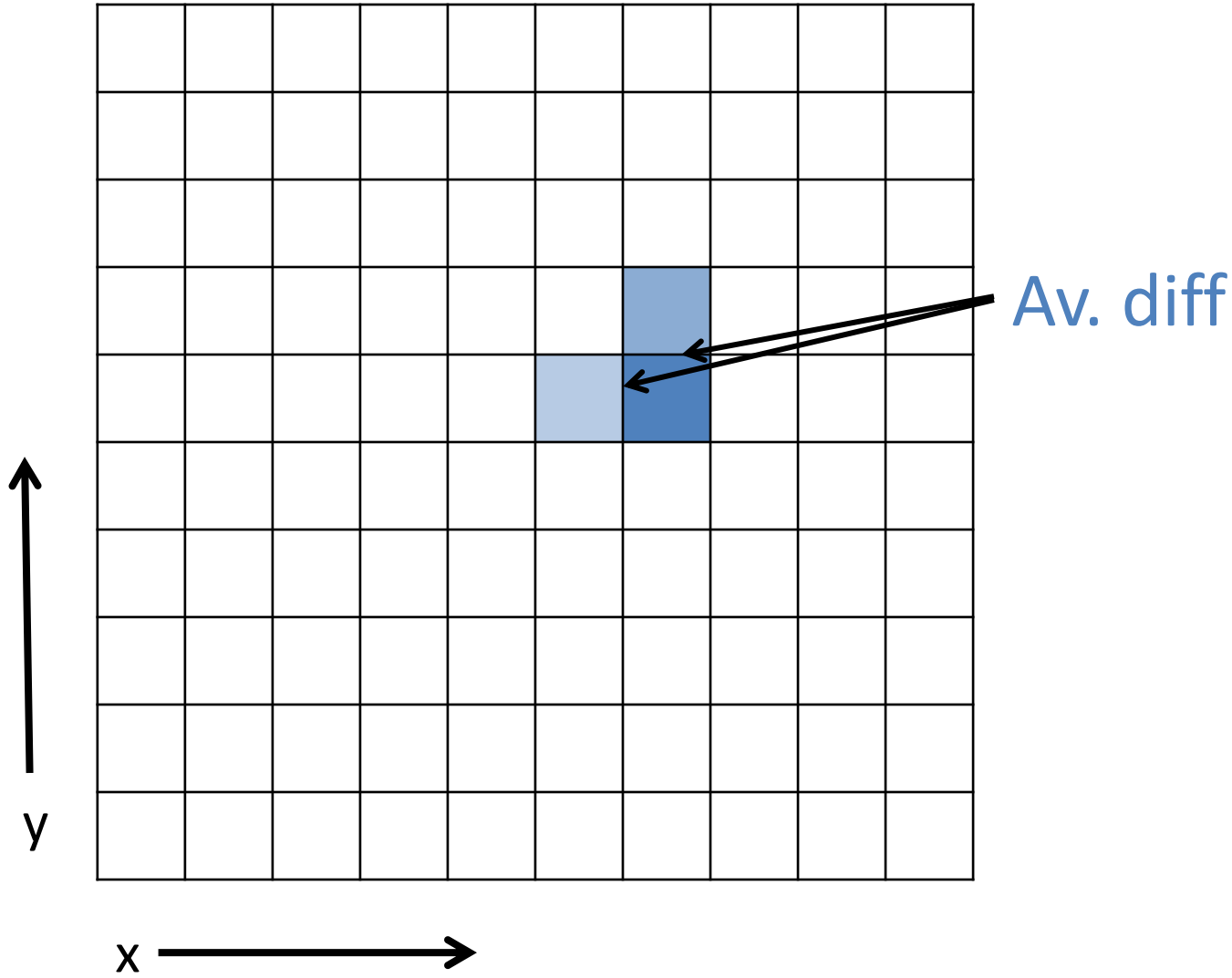
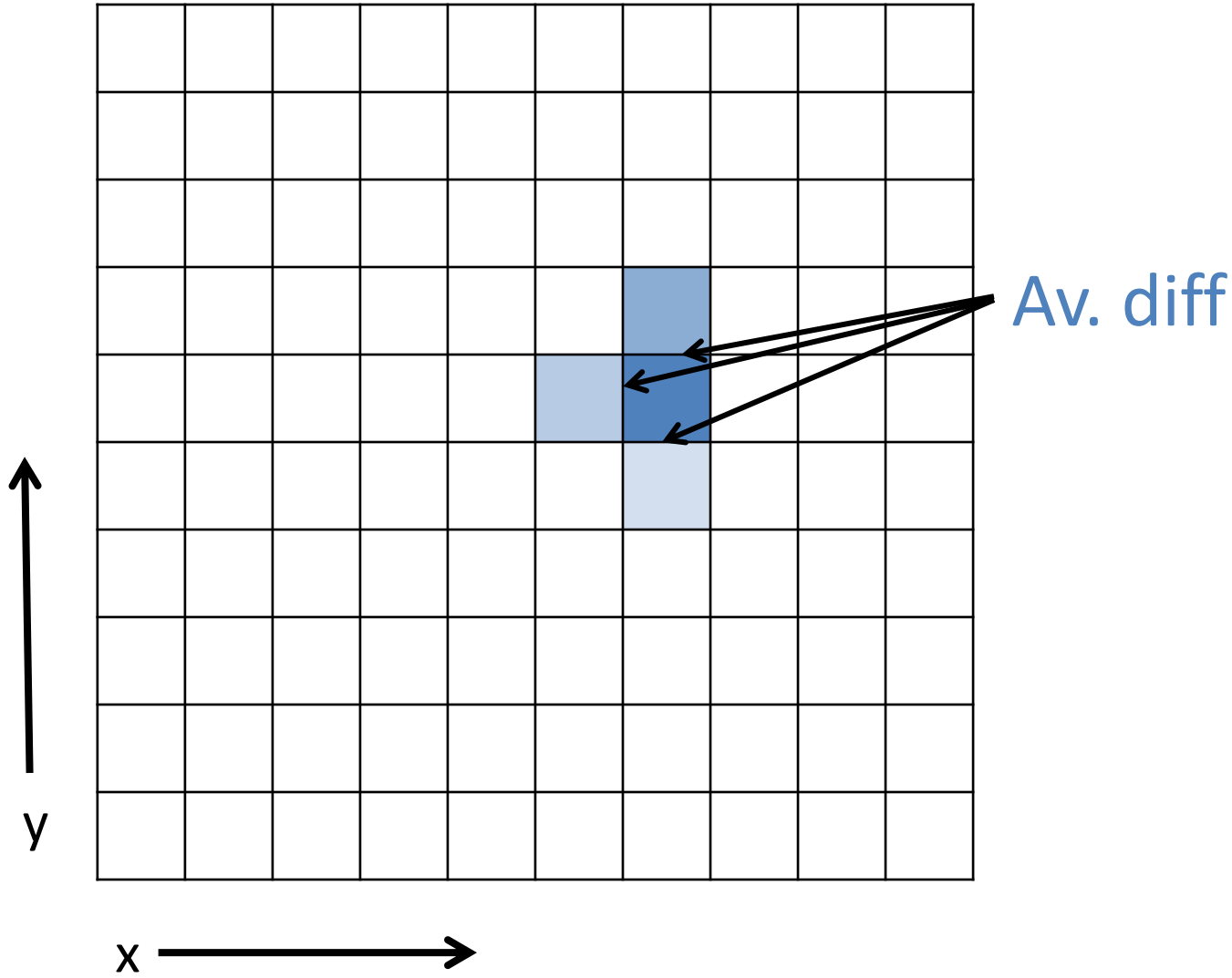


Discretization of 2D Space



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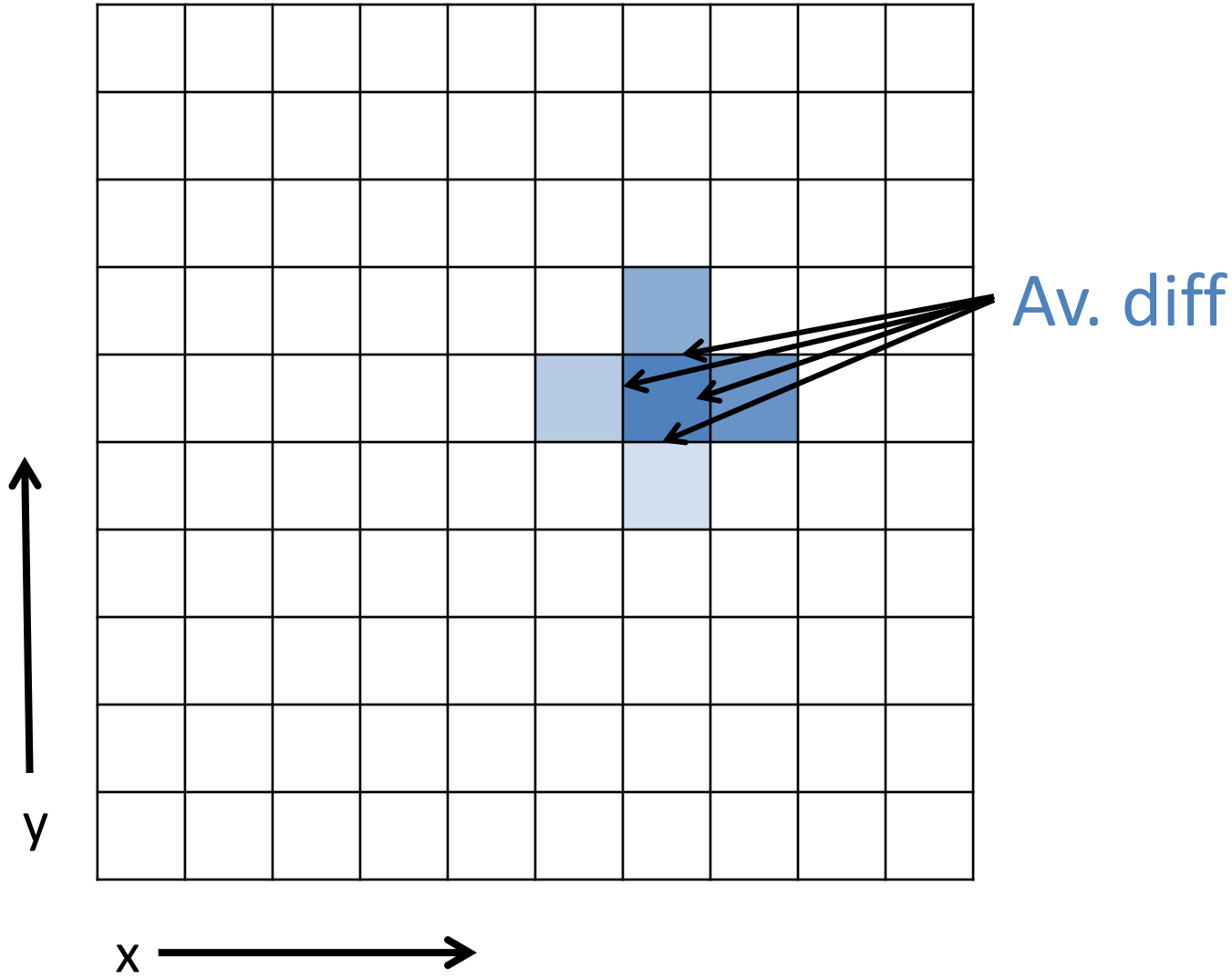

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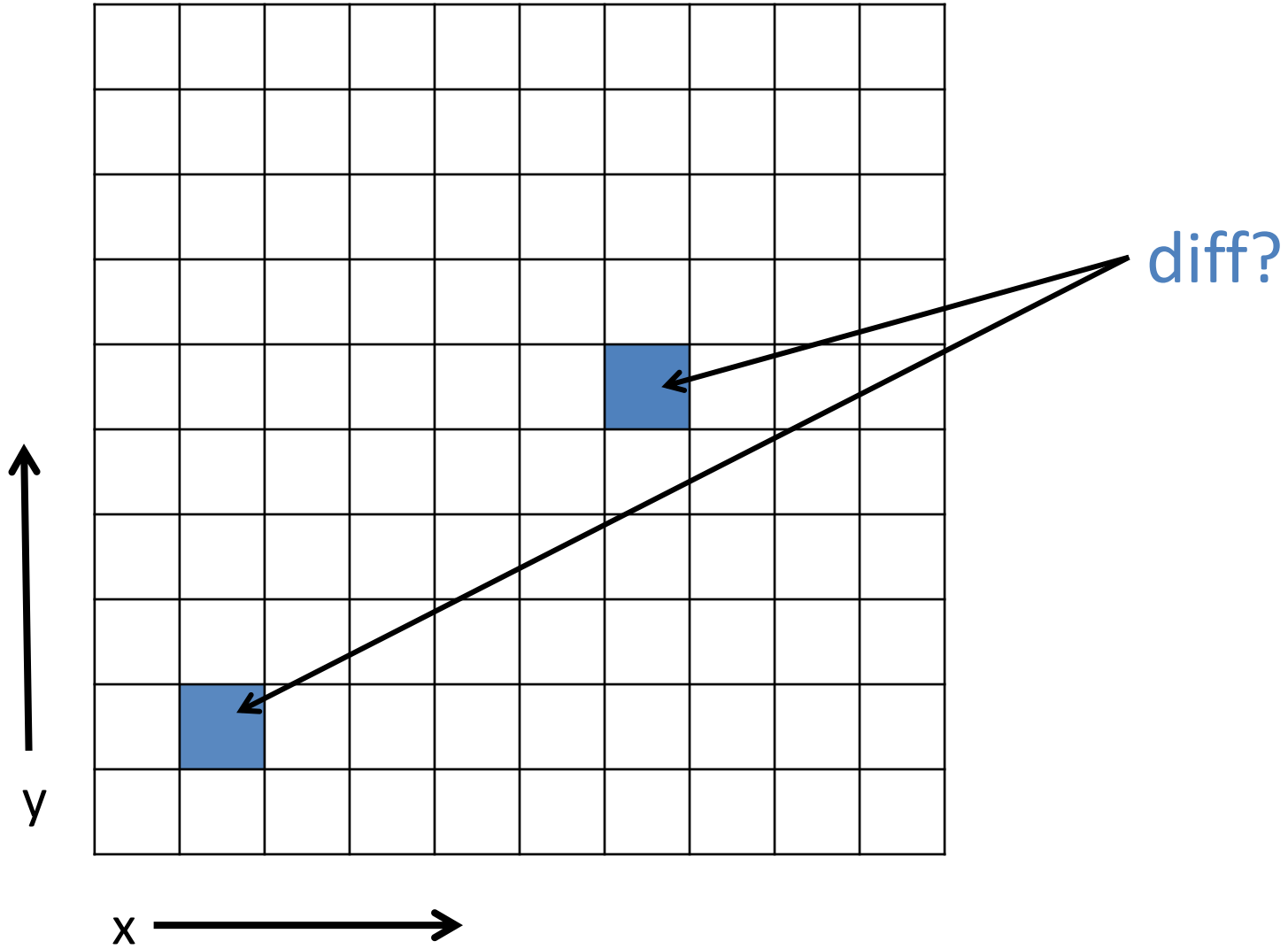

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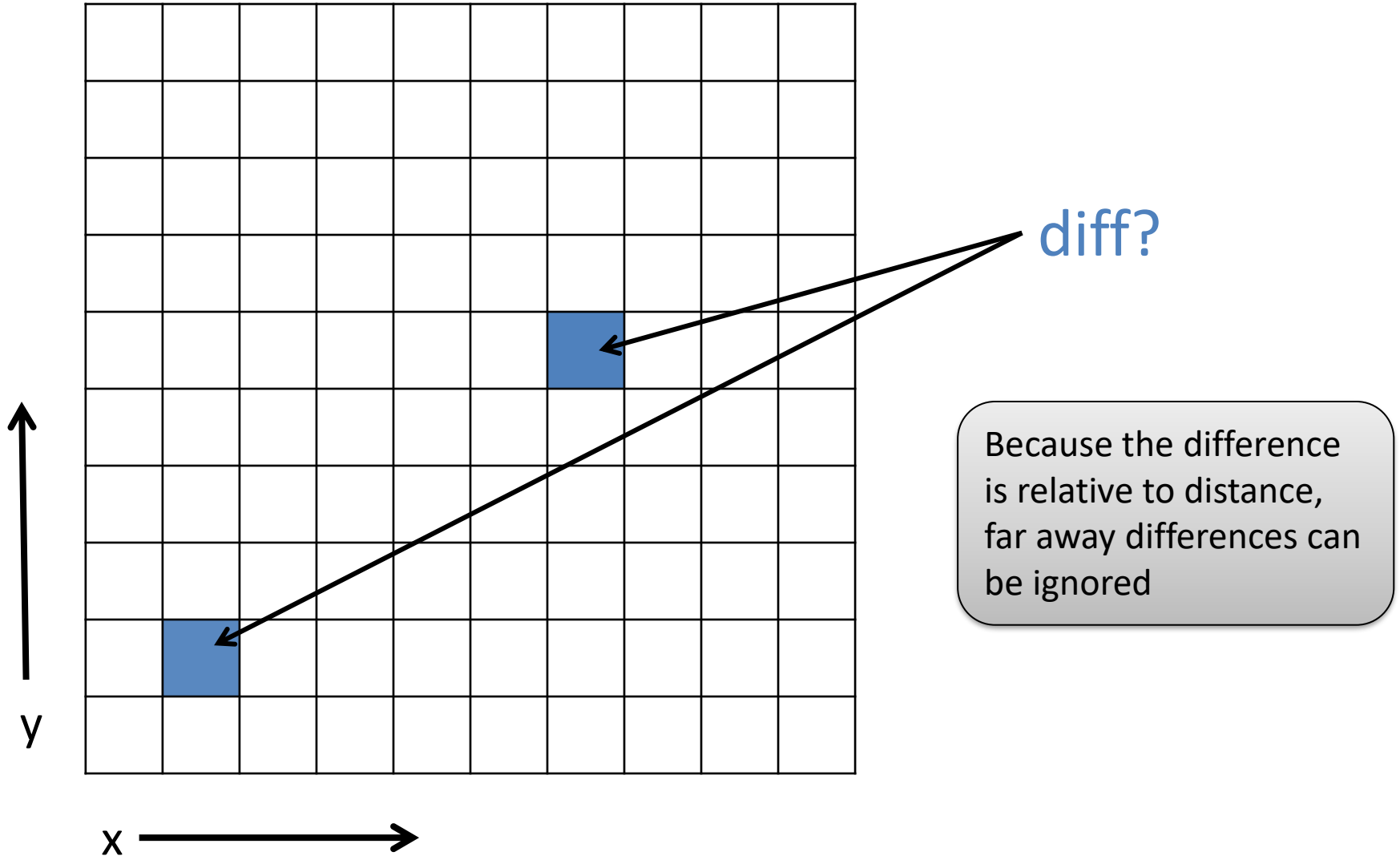


Because the difference is relative to distance, far away differences can be ignored

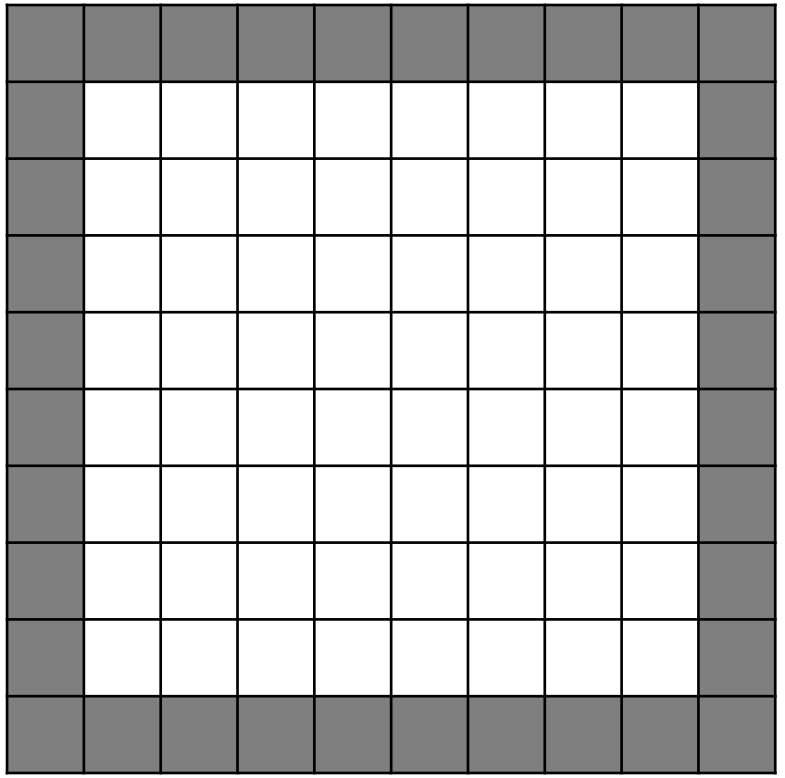
Discrete Laplace Operator

$$\Delta u(x,y) \simeq \frac{u(x+h,y)+u(x-h,y)+u(x,y+h)+u(x,y-h)-4u(x,y)}{dx^2}$$

Discrete Space represented by Array

- Define array of size of discrete grid + 2 (for padding)

```
U = np.random.rand(size, size)
```

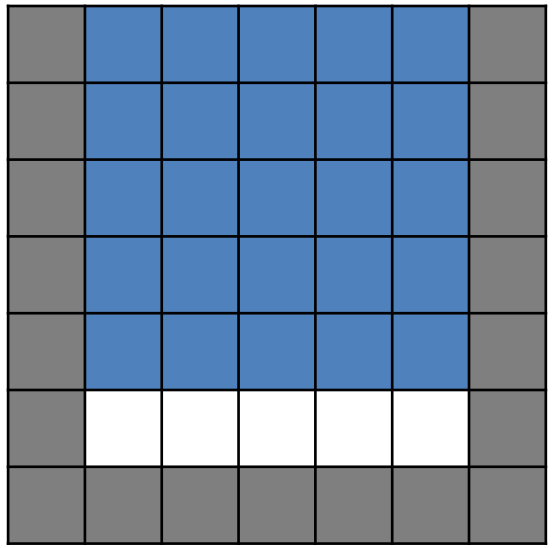


Discrete Laplacian in Python

```
# dx length of grid cell side

def laplacian(Z):
    Ztop = Z[0:-2, 1:-1]
    Zleft = Z[1:-1, 0:-2]
    Zbottom = Z[2:, 1:-1]
    Zright = Z[1:-1, 2:]
    Zcenter = Z[1:-1, 1:-1]
    return (Ztop + Zleft + Zbottom + Zright -4 * Zcenter) / dx**2
```

Discrete Laplacian in Python



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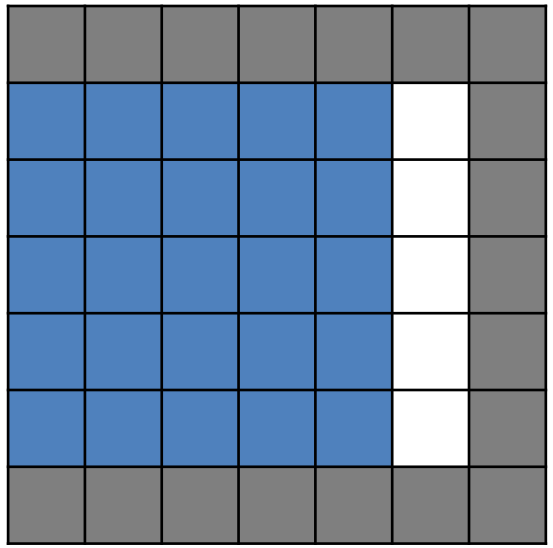

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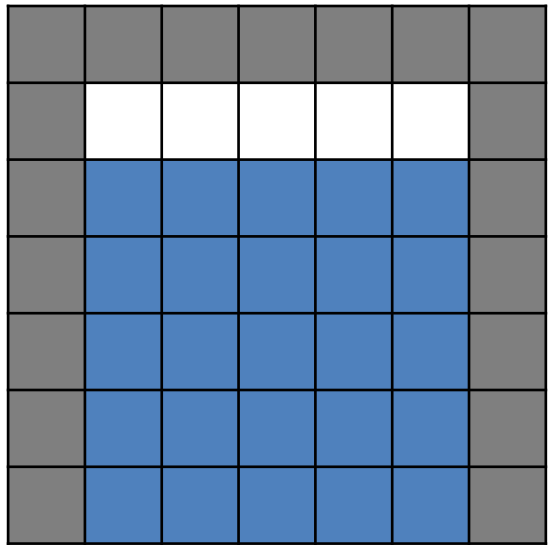
Discrete Laplacian in Python



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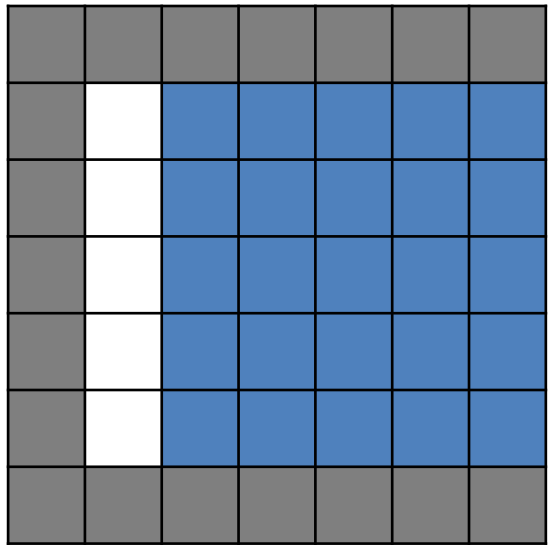
    Zleft = Z[1:-1, 0:-2]
    Zbottom = Z[2:, 1:-1]
    Zright = Z[1:-1, 2:]
    Zcenter = Z[1:-1, 1:-1]
    return (Ztop + Zleft + Zbottom + Zright -4 * Zcenter) / dx**2
```

Discrete Laplacian in Python



```
# dx length of grid cell side

def laplacian(Z):
    Ztop = Z[0:-2, 1:-1]
    Zleft = Z[1:-1, 0:-2]
    Zbottom = Z[2:, 1:-1]
    Zright = Z[1:-1, 2:]
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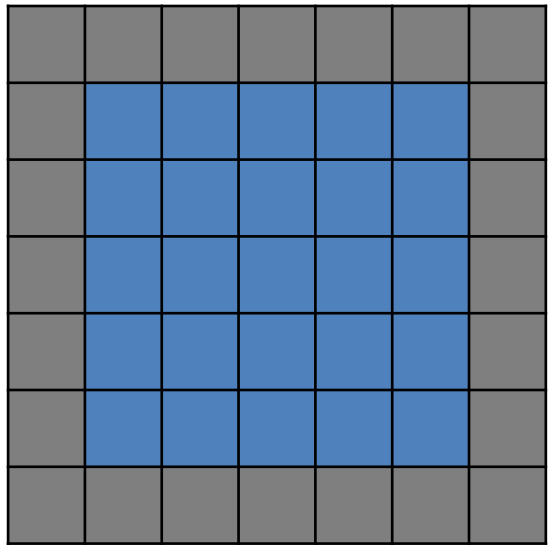
Discrete Laplacian in Python



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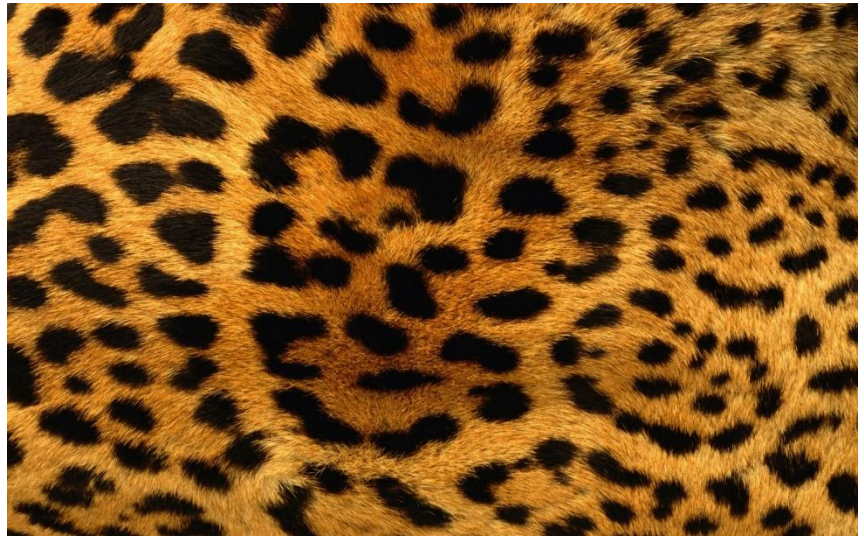
```

Modeling of pigmentation patterns with DE

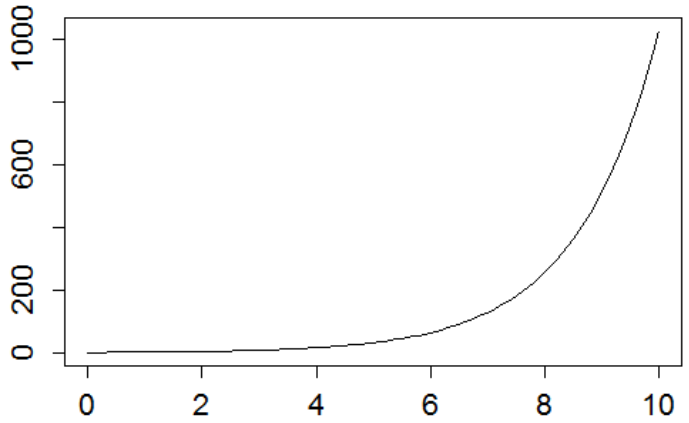


Reaction-Diffusion Equations

$$\frac{\partial c}{\partial t} = \underbrace{\mathrm{D}\frac{\partial^2 c}{\partial x^2}}_{\text{Diffusion}} + \underbrace{f(c)}_{\text{Reaction}}$$

Reaction in 0D Space

- E.g. Population growth model
- $\frac{dc}{dt} = Kc$
- $\mathrm{c}(t) = C_0 e^{Kt}, C_0 = c(0)$



Activator-Inhibitor model

- $\frac{\partial u}{\partial t} = u^3 - v - k + D_u \frac{\partial^2 u}{\partial x^2}$

- $\frac{\partial v}{\partial t} = a(u - v + D_v \frac{\partial^2 v}{\partial x^2})$

Activator-Inhibitor model

- $\frac{\partial u}{\partial t} = u^3 - v - k + D_u \frac{\partial^2 u}{\partial x^2}$

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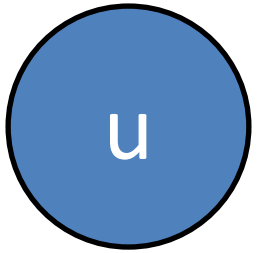

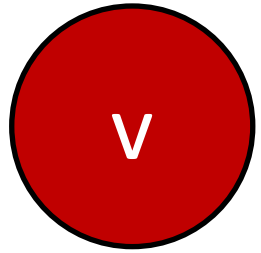

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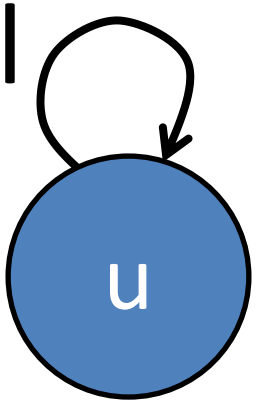

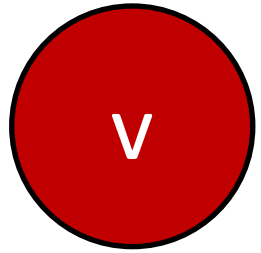

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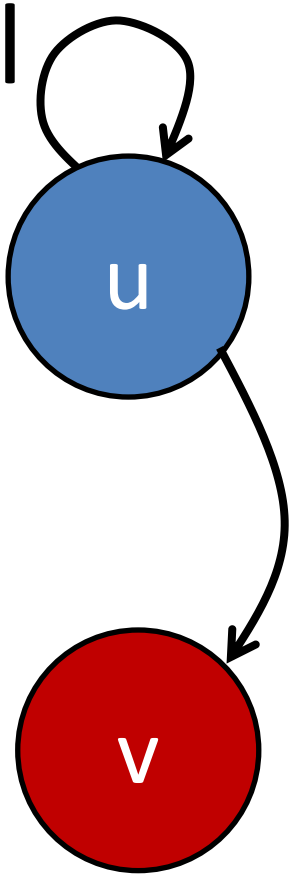

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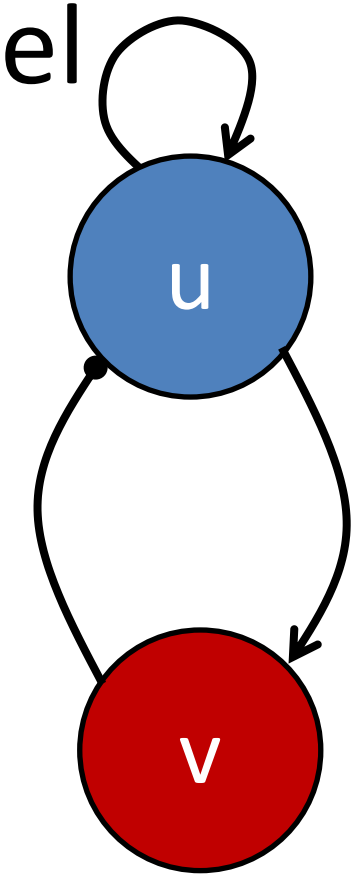

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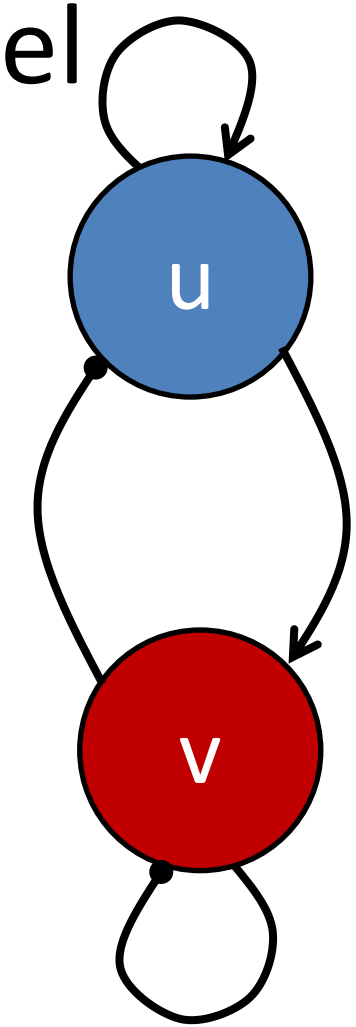

Activator-Inhibitor model

- $\frac{\partial u}{\partial t} = u^3 - v - k + D_u \frac{\partial^2 u}{\partial x^2}$

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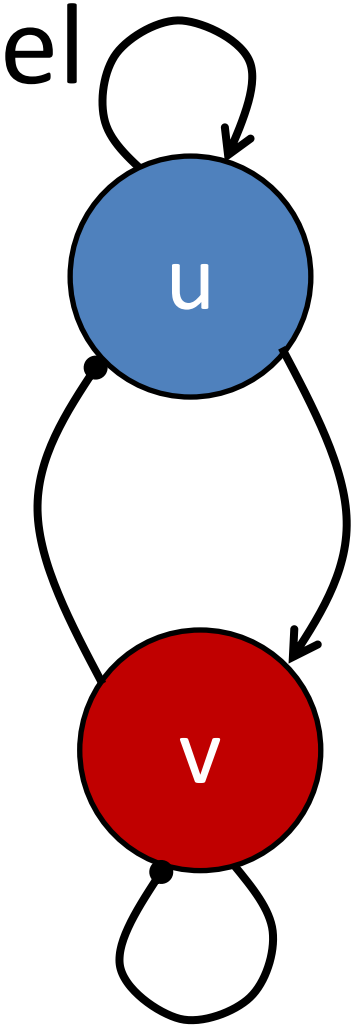


Constant Synthesis /Degradation

Python Implementation

```
deltaU = laplacian(U)
deltaV = laplacian(V)

Uc = U[1:-1, 1:-1]
Vc = V[1:-1, 1:-1]

U[1:-1, 1:-1], V[1:-1, 1:-1] = \
    Uc + dt * (Du * deltaU + Uc - Uc**3 - Vc + k),\
    Vc + dt * (Dv * deltaV + Uc - Vc) * a
```

Python Implementation

Loop over number of simulation steps

```
deltaU = laplacian(U)
deltaV = laplacian(V)

Uc = U[1:-1, 1:-1]
Vc = V[1:-1, 1:-1]

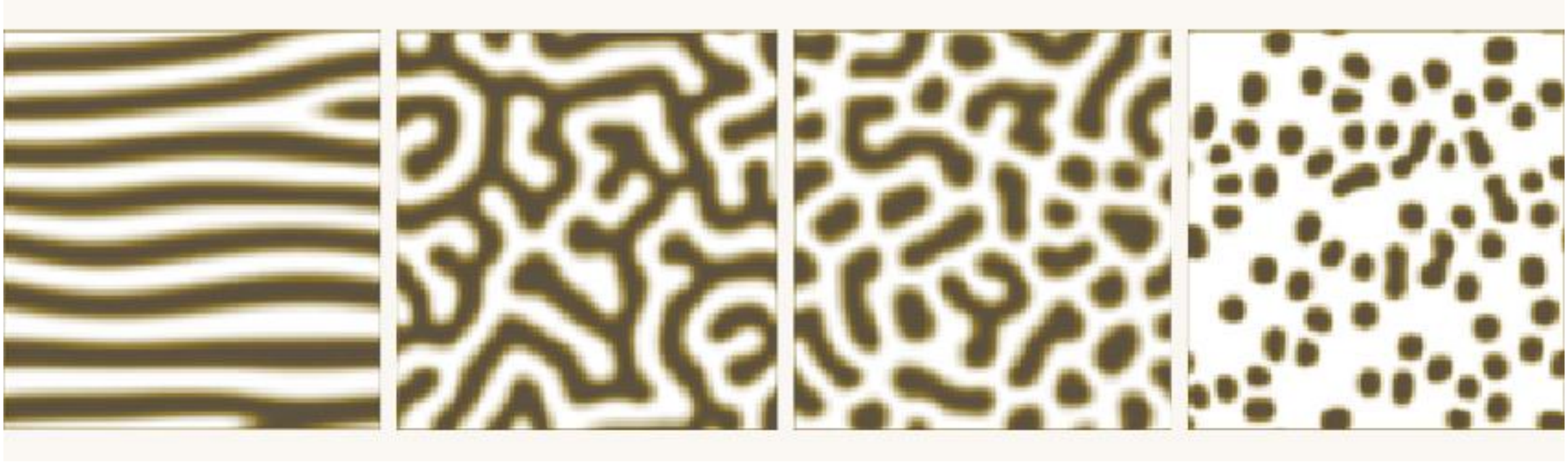
U[1:-1, 1:-1], V[1:-1, 1:-1] = \
    Uc + dt * (Du * deltaU + Uc - Uc**3 - Vc + k),\
    Vc + dt * (Dv * deltaV + Uc - Vc) * a
```

Fill Padding Values

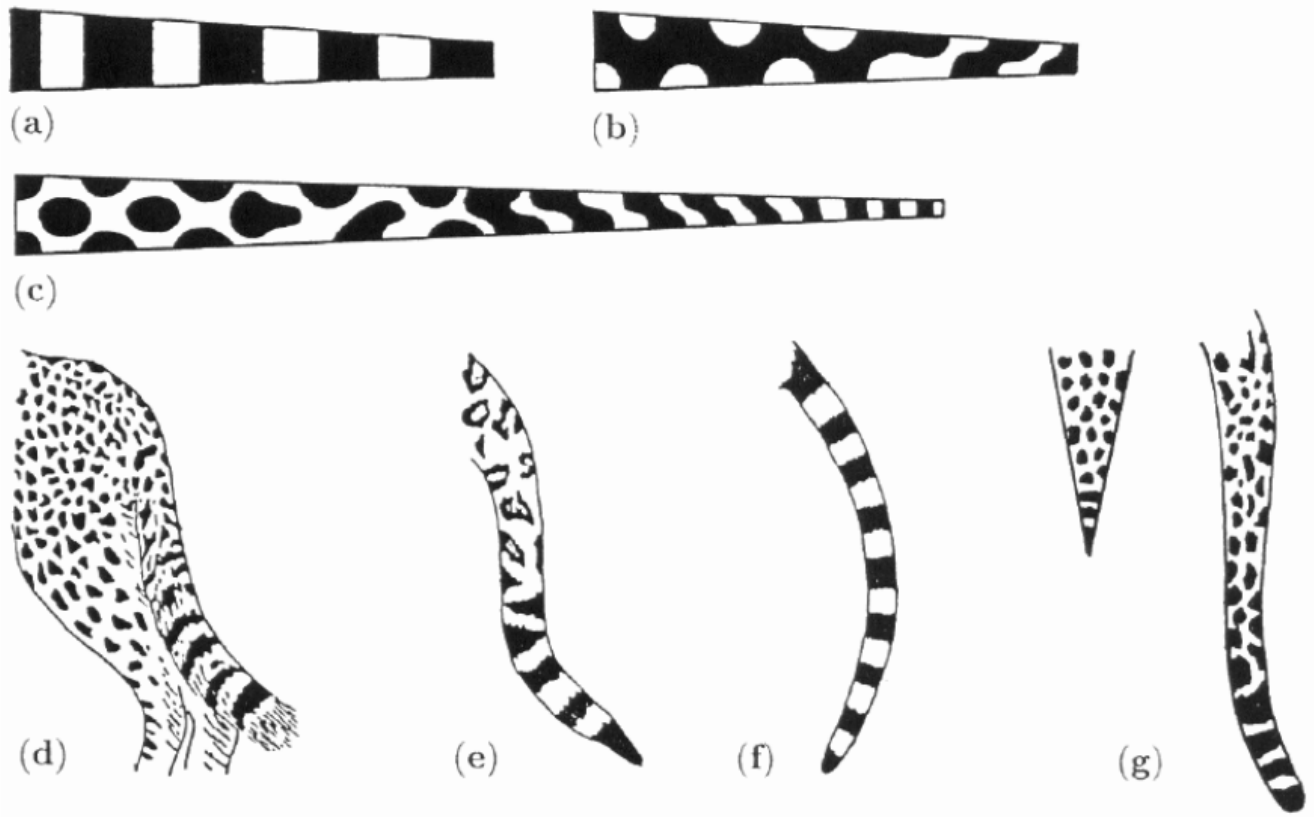
Loop over number of simulation steps

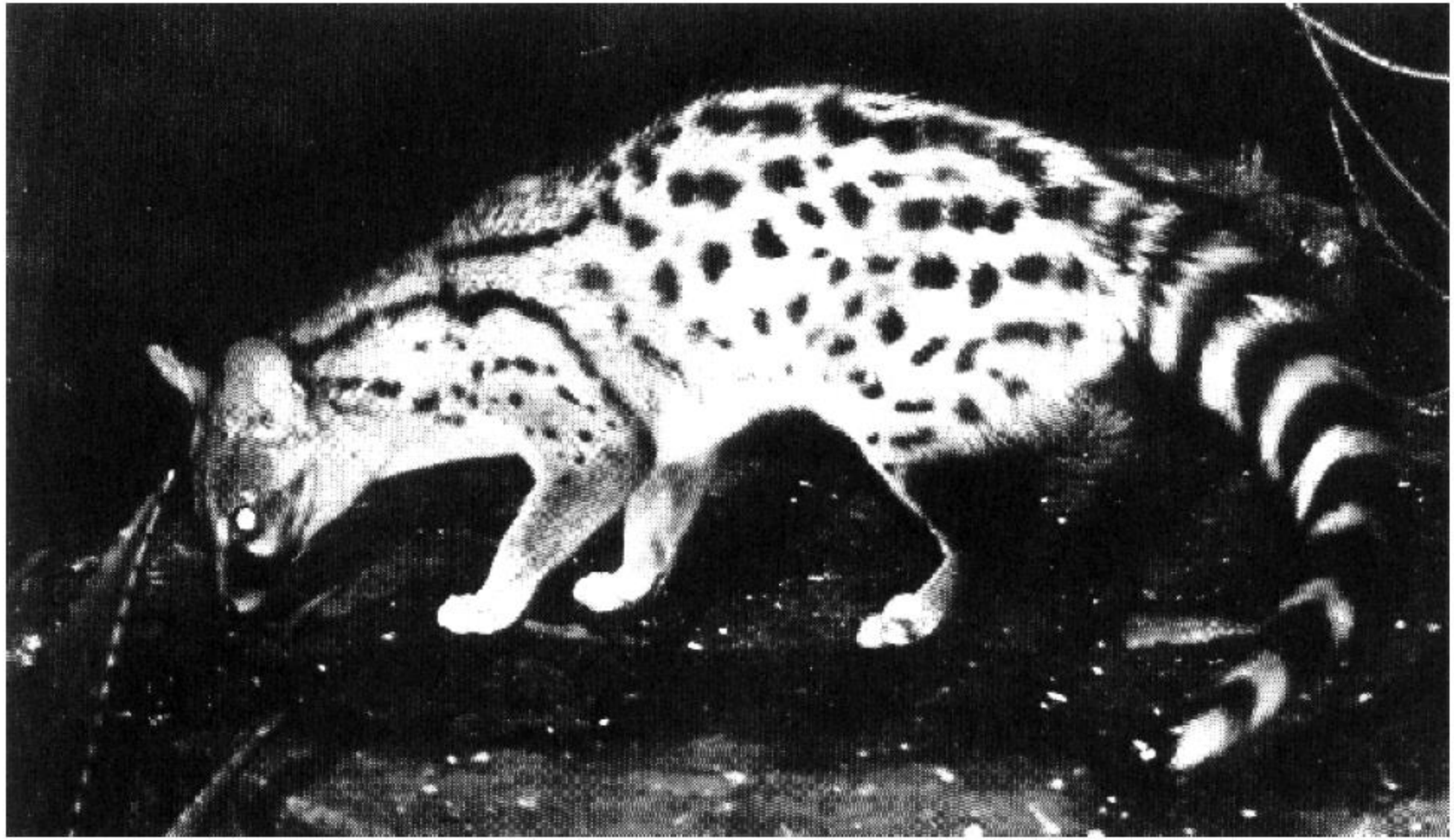
```
for Z in (U, V):
        Z[0, :] = Z[1, :]
        Z[-1, :] = Z[-2, :]
        Z[:, 0] = Z[:, 1]
        Z[:, -1] = Z[:, -2]
```

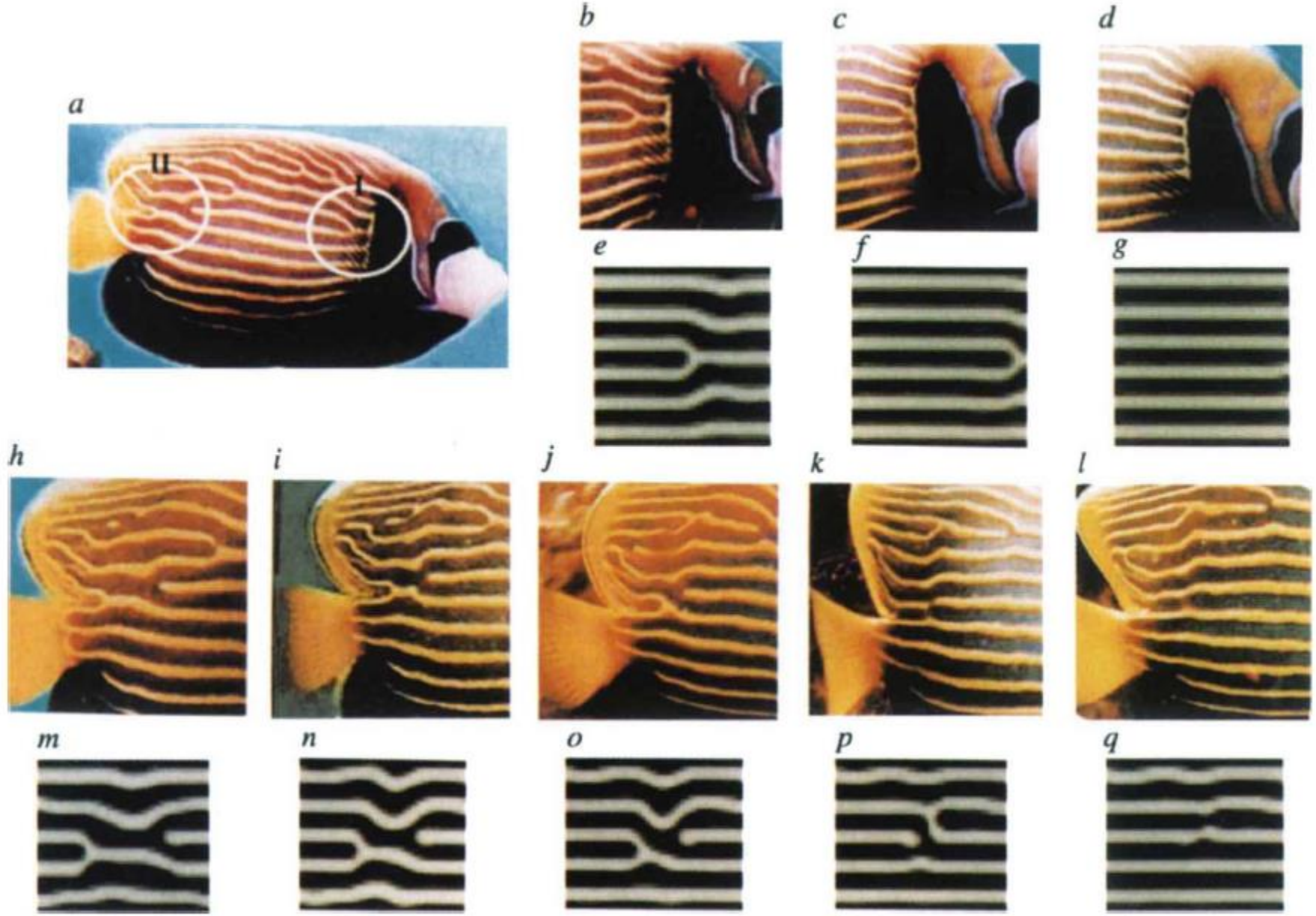
Parameter Space Exploration



Animal tails







Kondo S. et al, Nature 1995

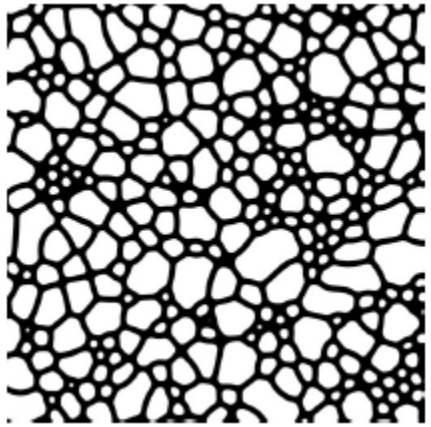
Reaction Diffusion in 3D

Gray-Scott model

- $\frac{\partial u}{\partial t} = -uv^2 + f(1-u) + D_u \frac{\partial^2 u}{\partial x^2}$

- $\frac{\partial v}{\partial t} = uv^2 - (k+f)v + D_v \frac{\partial^2 v}{\partial x^2}$






Exercise

- Implement the activator inhibitor model in python. Use a uniform grid size of 100, dx = 0.02, dt = 0.001, T = 15, a = 6, Dv = 5e-3. Visualize using matplotlib all a selection of patterns of stripes and spots. Visualize in an image plot a few consecutive time steps for a selected pattern. Parameters to change are k and Du, try ranges from -0.5 to 0.15 for k and 3e-5 to 1.4e-4 for Du. Report the settings for parameter values that give you spot, stripe, gap and noise patterns.