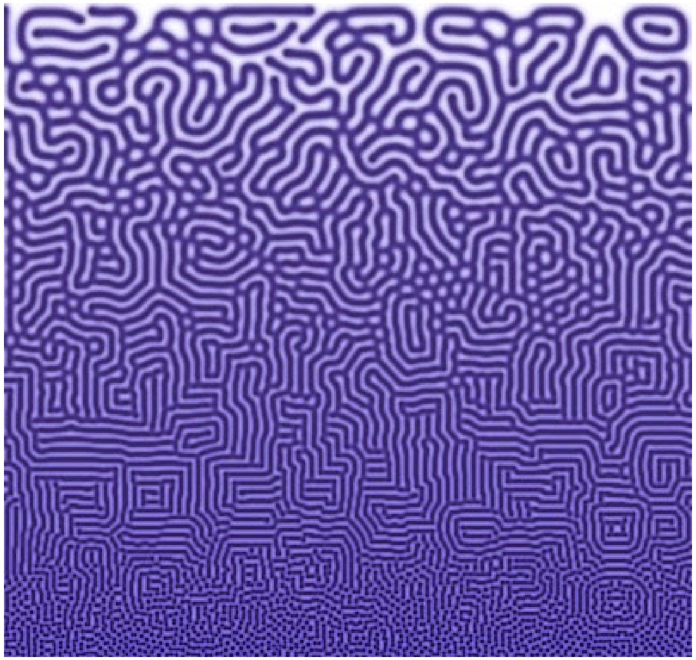
Computer modeling of physical phenomena



Lab IV – Gray-Scott reaction

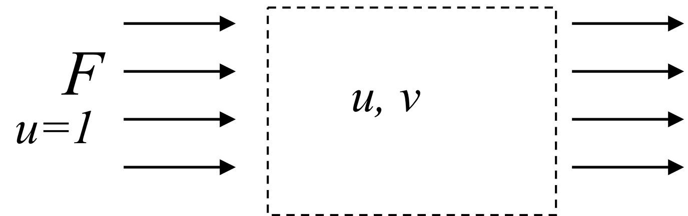
Gray-Scott system

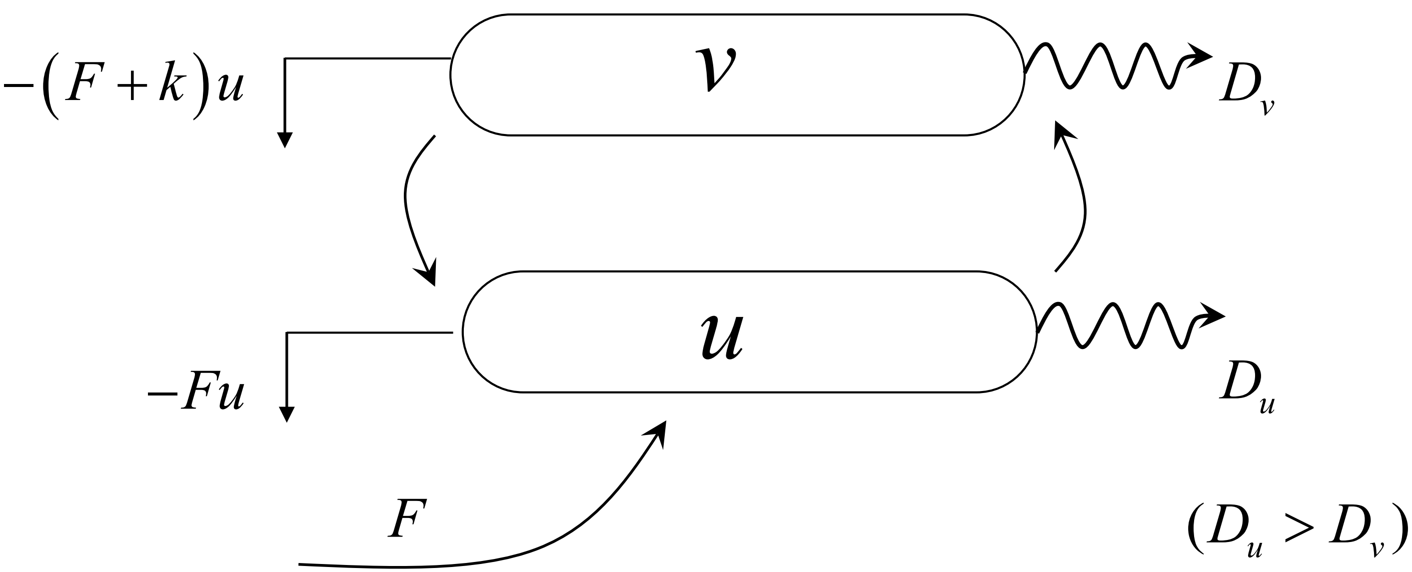
$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F\left(1-u\right)$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - \left(F+k\right)v$$

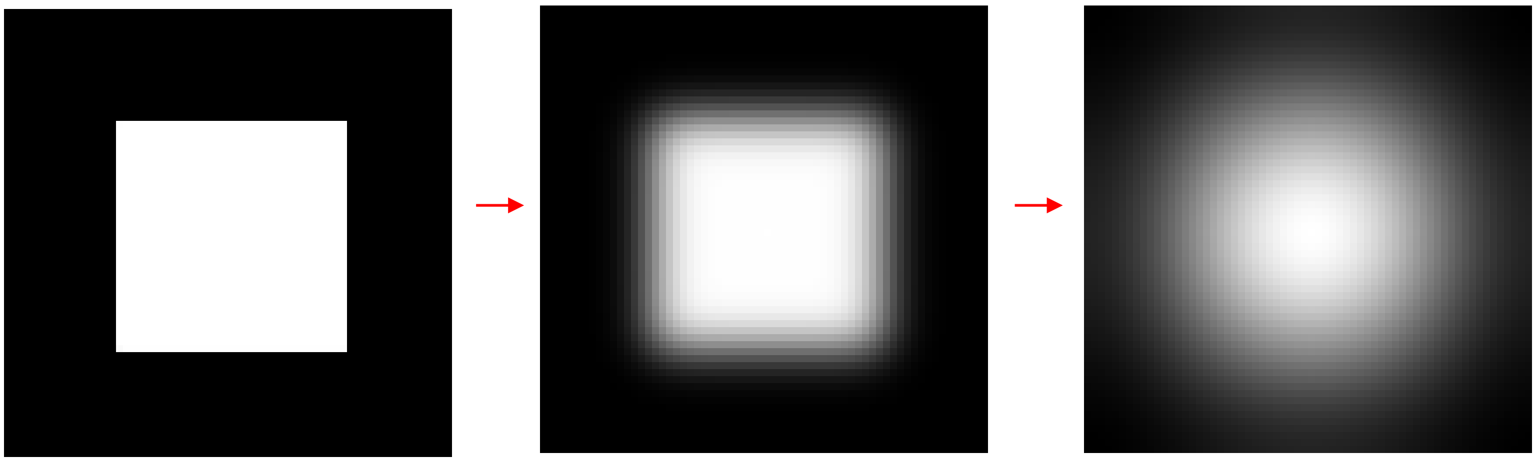
$$U + 2V \xrightarrow{1} 3V$$

$$V \xrightarrow{k} P$$

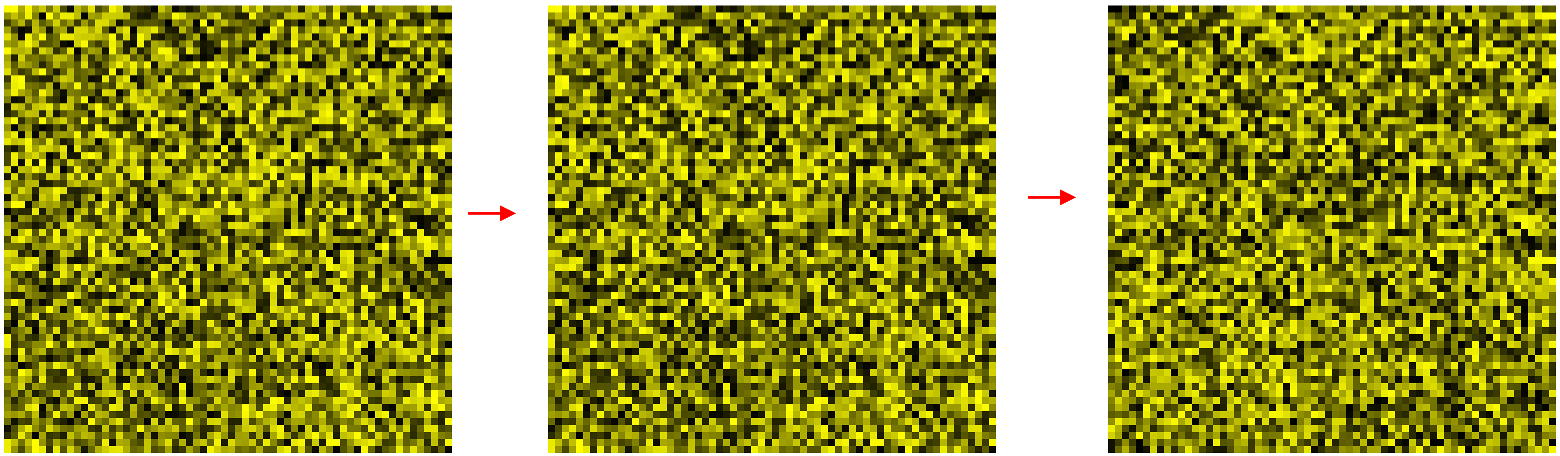




Diffusion only..,



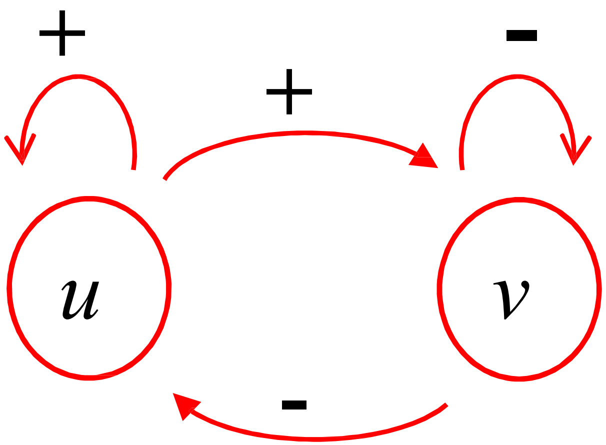
Reaction only...



Reaction + diffusion...

G-M system vs. G-S system

Instability conditions (Murray):

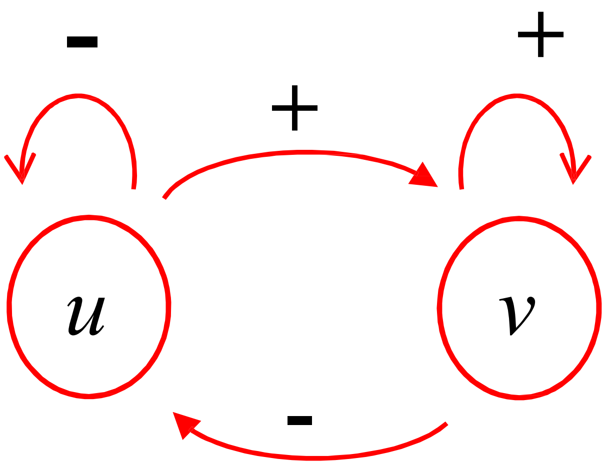


$(D_v > D_u)$

$$\frac{\partial u}{\partial t} = \nabla^2 u + a - u + \frac{u^2}{v}$$

$$\frac{\partial v}{\partial t} = d\nabla^2 v + \mu\left(u^2 - v\right)$$

Gierer and Meinhardt, 1972



$(D_u > D_v)$

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + F\left(1 - u\right)$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - \left(F + k\right)v$$

Gray and Scott, 1983

Problem no.1

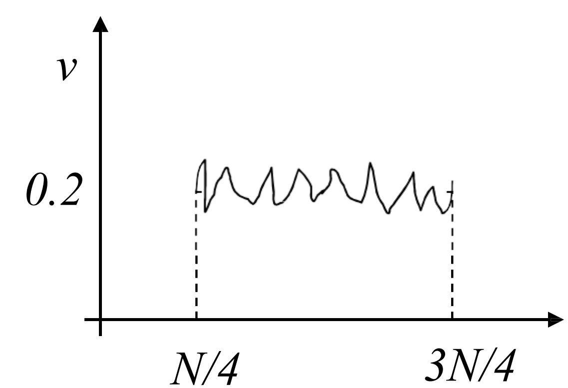
Implement 1d version of Gray-Scott system:

- divide the segment (0,2) into N=100 elementary intervals of length dx=0.02
- use periodic boundary conditions
- discretize the Laplace operator (second derivative after x)
- for time evolution, use the Euler algorithm (dt=1)
- exemplary parameters:

$$D_u=2\cdot 10^{-5},\ D_v=1\cdot 10^{-5},\ F=0.025,\ k = 0.055$$

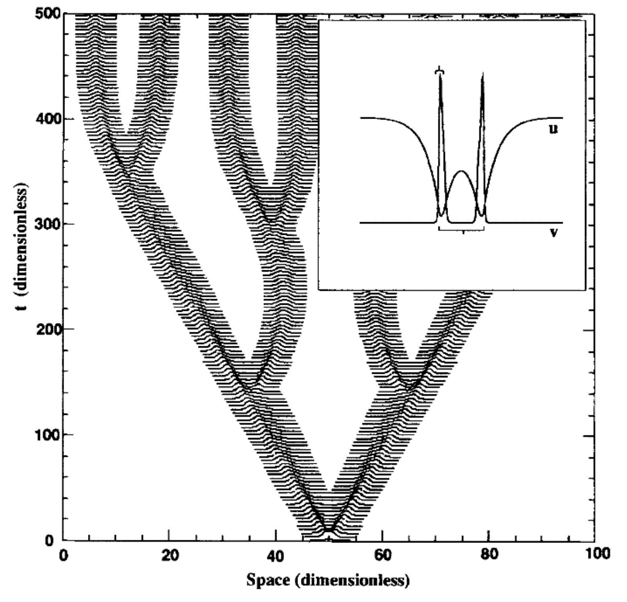
- as an initial condition use

```
u = ones(N)
v = zeros(N)
xs= np.arange(N)
for i in range(N/4,3*N/4):
    u[i] = random()*0.2+0.4
    v[i] = random()*0.2+0.2
```



What is the stationary state of a homogeneous system? How will the system evolve over time for the initial conditions given above? Will it reach a stationary state? What length scale will characterize the resulting structure? What will change for different F and k?

Spacetime diagram



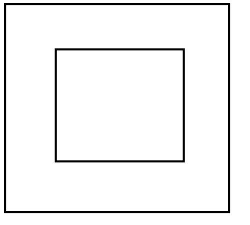
plot such a diagram, describing the evolution of the position of v(x) maxima

Problem no. 2

Implement a two-dimensional version of the Gray-Scott system:

- create a 100x100 grid and dx=dy=0.02
- again use periodic boundary conditions and Du/Dv=2
- as an initial condition take:

```
for i in range(N/4,3*N/4):
    for j in range(N/4,3*N/4):
        U[i][j] = random()*0.2+0.4
        V[i][j] = random()*0.2+0.2
```



How does the evolution look like for different values of F and k, e.g.

F = 0.025	F = 0.03	F= 0.01	F=0.04	F=0.06	F=0.037
k = 0.055	k = 0.062	k= 0.047	k=0.07	k=0.0615	k=0.06

(or other six if these look boring …)

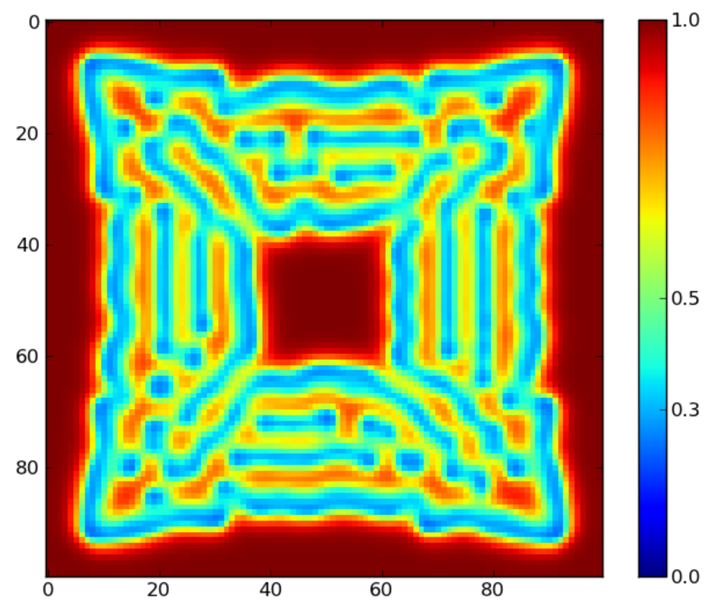
Extra task: make a systematic phase diagram of the system behavior for k=0.062 and different values of F

Hint

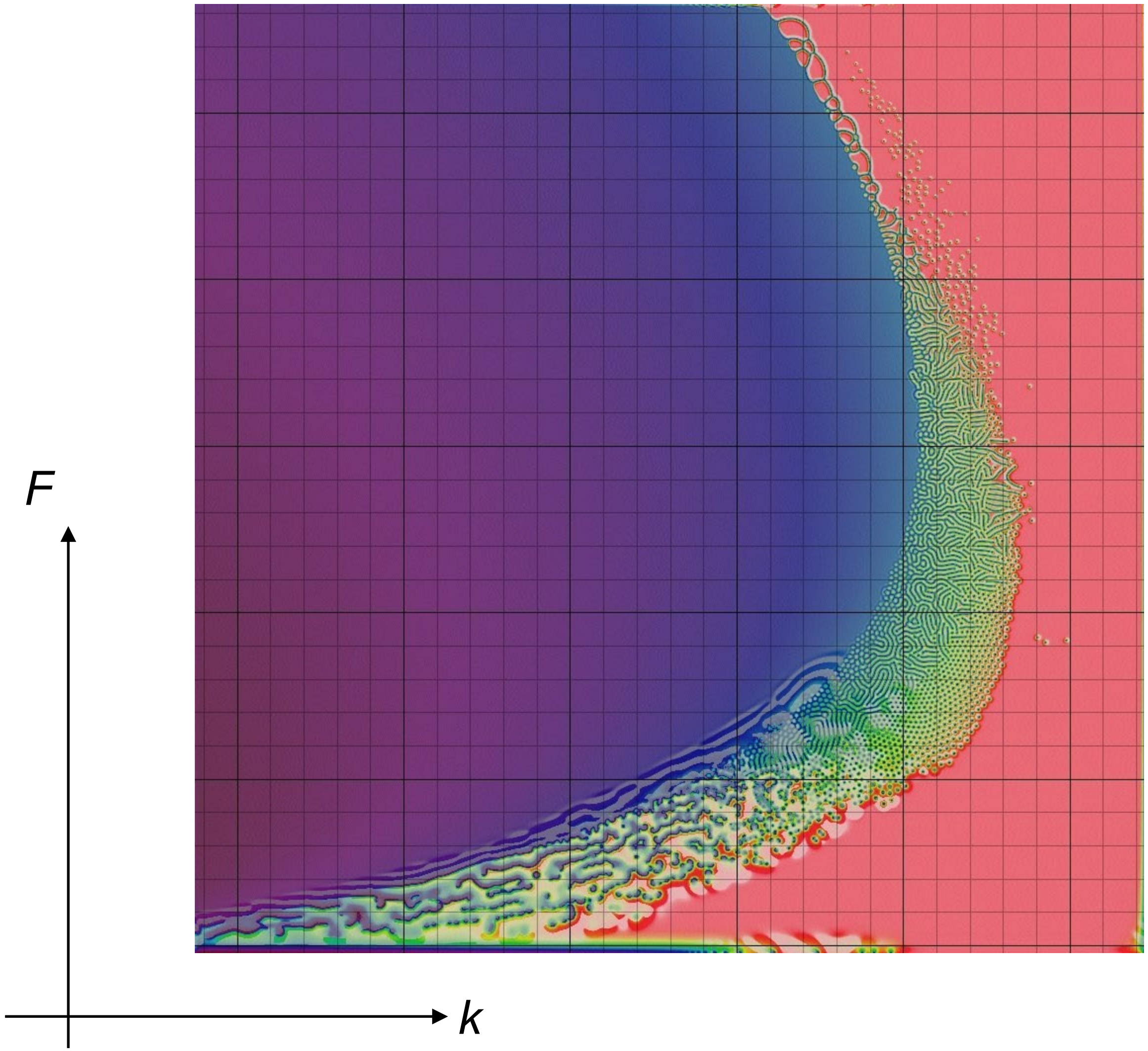
- Avoid loops over the matrix, use numpy.roll

Visualization:

```
import matplotlib
import matplotlib.pyplot as plt
fig=plt.figure()
ax=fig.add_subplot(111)
cax = ax.imshow(u, interpolation='nearest')
cax.set_clim(vmin=0, vmax=1)
cbar = fig.colorbar(cax, ticks=[0,0.3, 0.5,1], orientation='vertical')
plt.clf()
```



Xmorphia



http://mrob.com/pub/comp/xmorphia/

More about the system:

- http://mrob.com/pub/comp/xmorphia/
- http://groups.csail.mit.edu/mac/projects/amorphous/GrayScott/
- http://www.aliensaint.com/uo/java/rd/
- http://www.joakimlinde.se/java/ReactionDiffusion/
- http://complex.upf.es/~andreea/PACE/Self-replicating_spots.html
- J. E. Pearson., Complex patterns in a simple system, Science, 261:189-192, 1993.