



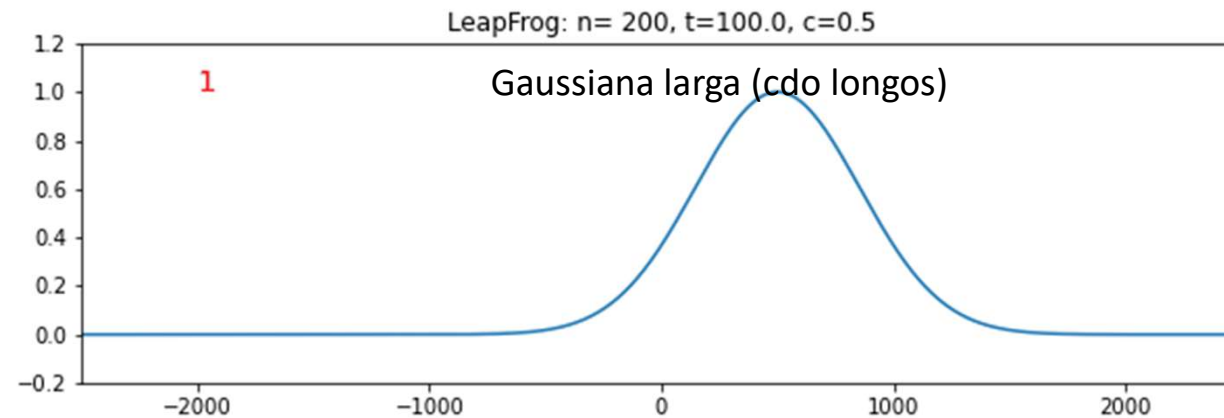
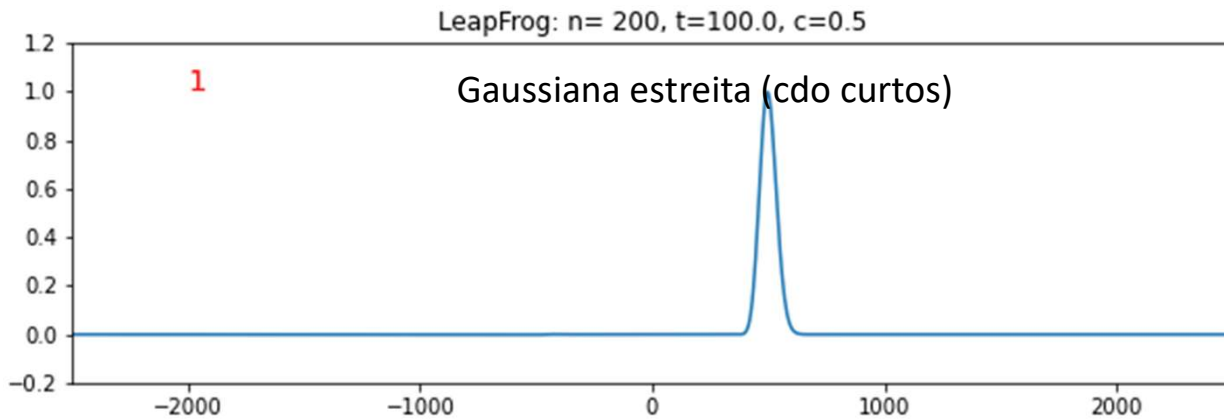
Ciências
ULisboa

Modelação Numérica 2022

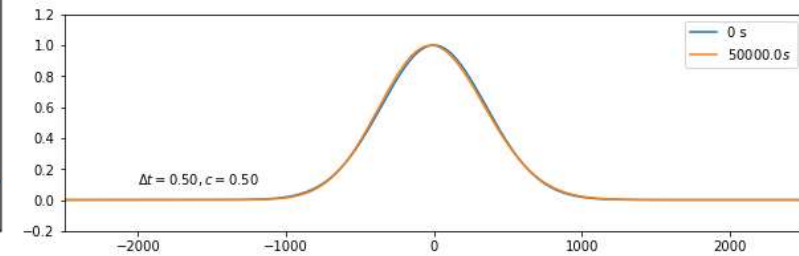
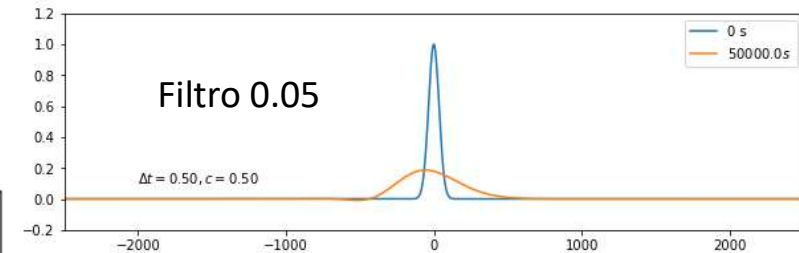
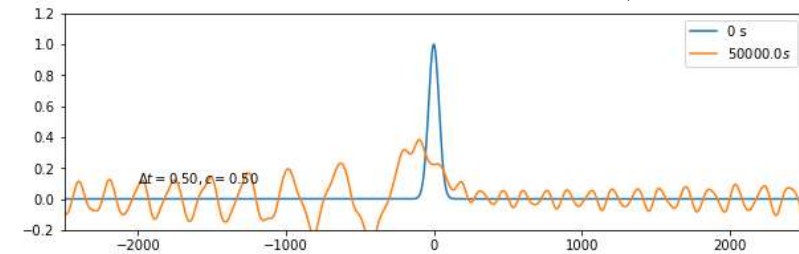
Aula 9

Equação de advecção-difusão.

Advecção linear LeapFrog



Após 50 voltas



Equação de **adveção**-difusão (linear, 2D)

$$\frac{\partial T}{\partial t} = -u \frac{\partial T}{\partial x} - v \frac{\partial T}{\partial y} + K_D \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

$$u, v = \text{const}$$

$$K_D = \text{const}$$

É uma simplificação (2D, linear) da equação (transferência de calor num fluido sem fontes de calor):

$$\frac{\partial \theta}{\partial t} = -(\vec{v} \cdot \nabla) \theta + \kappa_D \nabla^2 \theta$$

Casos particulares: $\vec{v} = 0$ (equação da difusão/condução); $\kappa_D = 0$ (equação da adveção)

Usando diferenças centradas

$$\frac{\partial T}{\partial t} = -u \frac{\partial T}{\partial x} - v \frac{\partial T}{\partial y} + K_D \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n-1}}{2\Delta t} = -u \frac{T_{i+1,j}^n - T_{i-1,j}^n}{2\Delta x} - v \frac{T_{i,j+1}^n - T_{i,j-1}^n}{2\Delta x} + K_D \left(\frac{T_{i-1,j}^n + T_{i+1,j}^n - 2T_{i,j}^n}{\Delta x^2} + \frac{T_{i,j-1}^n + T_{i,j+1}^n - 2T_{i,j}^n}{\Delta y^2} \right)$$

Não funciona. É **instável**.

Usando diferenças centradas (Leapfrog **explícito** com difusão em $n - 1$)

$$T_{i,j}^{n+1} = T_{i,j}^{n-1} +$$
$$+ 2\Delta t \left(-u \frac{T_{i+1,j}^n - T_{i-1,j}^n}{2\Delta x} - u \frac{T_{i,j+1}^n - T_{i,j-1}^n}{2\Delta x} \right.$$
$$\left. + K_D \left(\frac{T_{i-1,j}^{n-1} + T_{i+1,j}^{n-1} - 2T_{i,j}^{n-1}}{\Delta x^2} + \frac{T_{i,j-1}^{n-1} + T_{i,j+1}^{n-1} - 2T_{i,j}^{n-1}}{\Delta y^2} \right) \right)$$

É **condicionalmente estável**.

FTCS (**explícito** com difusão em n)

$$T_{i,j}^{n+1} = T_{i,j} +$$
$$+\Delta t \left(-u \frac{T_{i+1,j}^n - T_{i-1,j}^n}{2\Delta x} - u \frac{T_{i,j+1}^n - T_{i,j-1}^n}{2\Delta x} \right.$$
$$\left. + K_D \left(\frac{T_{i-1,j}^n + T_{i+1,j}^n - 2T_{i,j}^n}{\Delta x^2} + \frac{T_{i,j-1}^n + T_{i,j+1}^n - 2T_{i,j}^n}{\Delta y^2} \right) \right)$$

É **condicionalmente estável**.

Usando diferenças centradas (**implícito** com difusão em $n + 1$)

$$T_{i,j}^{n+1} - 2\Delta t K_D \left(\frac{T_{i-1,j}^{n+1} + T_{i+1,j}^{n+1} - 2T_{i,j}^{n+1}}{\Delta x^2} + \frac{T_{i,j-1}^{n+1} + T_{i,j+1}^{n+1} - 2T_{i,j}^{n+1}}{\Delta y^2} \right) \\ = T_{i,j}^{n-1} + 2\Delta t \left(-u \frac{-T_{i+1,j}^n T_{i-1,j}^n}{2\Delta x} - v \frac{T_{i,j+1}^n - T_{i,j-1}^n}{2\Delta y} \right)$$

É **absolutamente estável**, mas requiere a solução de um sistema de (muitas) equações simultâneas.

Adveção-difusão

```
import numpy as np
import matplotlib.pyplot as plt
def advdif(imethod,asel,u,kD,nt,dt,passo):
    methods=['FTCS','LF']
    method=methods[imethod]
    timefil=[asel,1-2*asel,asel]
    nx=500;dx=1;Lx=nx/2*dx
    c0=u*dt/dx
    c1=u*dt/(2*dx)
    c2=kD*dt/dx**2
    c2LF=kD*2*dt/dx**2
    x=np.arange(-Lx,Lx,dx)
    ...
```



```

...
if u>0:
    nvolta=int(2*Lx/u/dt)
    nt=nvolta*2+1
    passo=nvolta
Wx=10;x0=0
TI=np.exp(-(x-x0)/Wx)**2)
T=np.copy(TI);TP=np.copy(T);TM=np.copy(T)
plt.plot(x,T,label='0')
meanT=np.mean(T)
plt.plot([-Lx,Lx],[meanT,meanT],color='gray',linestyle='dashed',alpha=0.5,label='Mean')
if method=='LF':
    plt.title(r'$%5s,u=%3.1f,k_D=%3.2f,\sigma=%3.2f,\sigma_k=%3.2f$' % (method,u,kD,c0,c2LF))
else:
    plt.title(r'$%5s,u=%3.1f,k_D=%3.2f,\sigma=%3.2f,\sigma_k=%3.2f$' % (method,u,kD,c1,c2))
it0=1
if method=='LF':
    it0=2
    for ix in range(nx):
        ixm=ix-1;ixp=ix+1
        if ixm<0:
            ixm=nx-1
        elif ixp>nx-1:
            ixp=0
        T[ix]=0.5*(TM[ixm]+TM[ixp])-u*dt/dx*(TM[ixp]-TM[ixm])\
            +kD*dt*((TM[ixm]+TM[ixp]-2*TM[ix])/dx**2)

```

```

for it in range(it0,nt):
    for ix in range(nx):
        ixm=ix-1;ixp=ix+1
        if ixm<0: #fronteira cíclica
            ixm=nx-1
        elif ixp>nx-1:
            ixp=0
        if method=='FTCS':
            TP[ix]=T[ix]-u*dt/(2*dx)*(T[ixp]-T[ixm])\
                +kD*dt*((T[ixm]+T[ixp]-2*T[ix])/dx**2)
        elif method=='LF':
            TP[ix]=TM[ix]-u*dt/dx*(T[ixp]-T[ixm])\
                +kD*2*dt*((TM[ixm]+TM[ixp]-2*TM[ix])/dx**2)

    if method=='LF':
        T=timefil[0]*TM+timefil[1]*T+timefil[2]*TP #filtro temporal
    TM=np.copy(T);T=np.copy(TP) #update temporal
    if it%passo==0:
        plt.plot(x,T,label=str(it))
plt.legend()
return c0,c1,c2

```

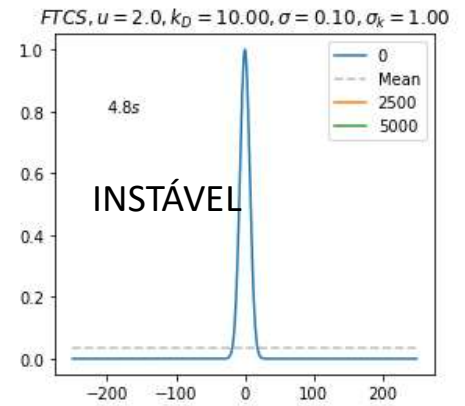
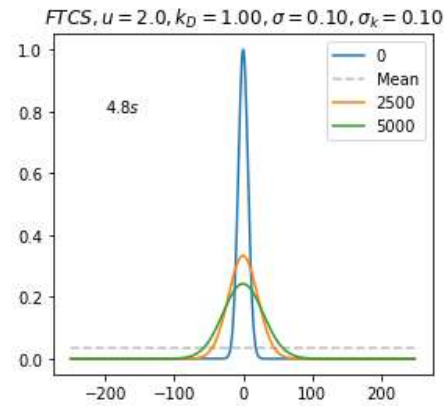
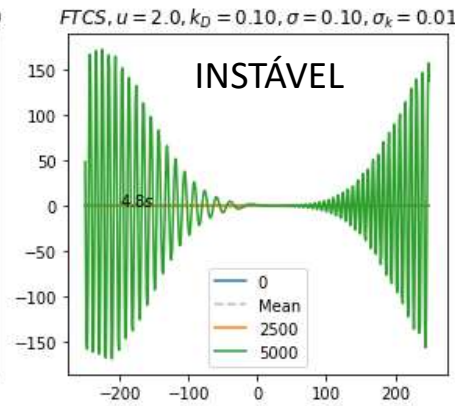
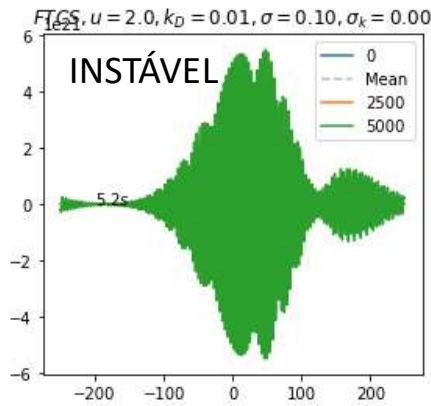
Teste de sensibilidade

```
asel=0.05; #asel=0.  
nt=5001;passo=2500;dt=0.1  
for u in[0,2]:  
    for imethod in[0,1]:  
        kP=0  
        plt.figure(figsize= (20,4))  
        for kD in[0.01,0.1,1,10]:  
            kP=kP+1  
            plt.subplot(1,4,kP)  
            c0,c1,c2=advdif(imethod,asel,u,kD,nt,dt,passo)
```

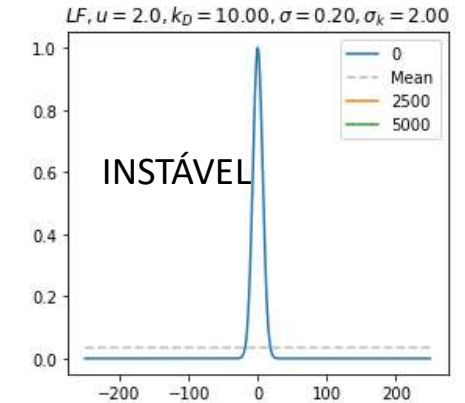
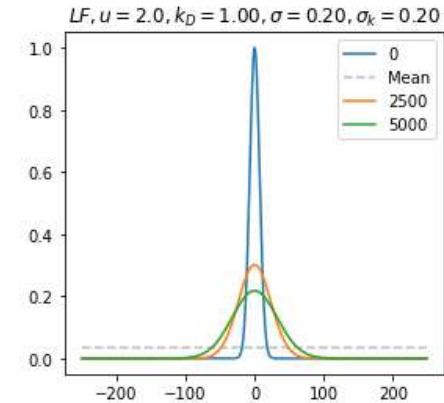
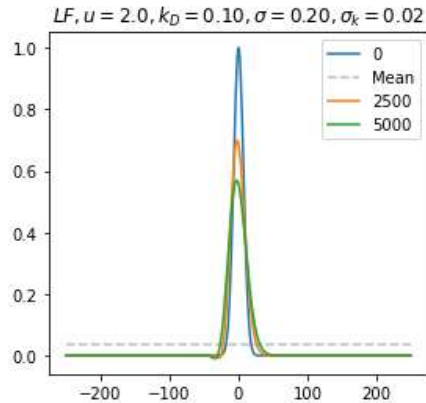
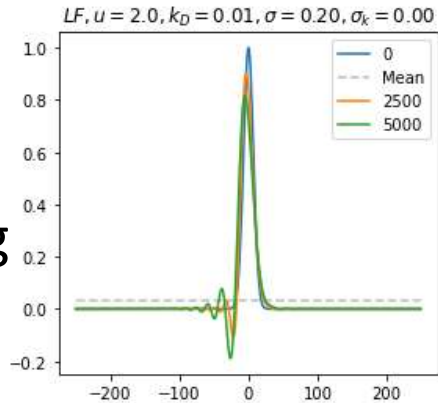
$$u = 2, \Delta x = 1, \Delta t = 0.1$$

 $k_D \rightarrow$

FTCS



Leapfrog
s/filtro

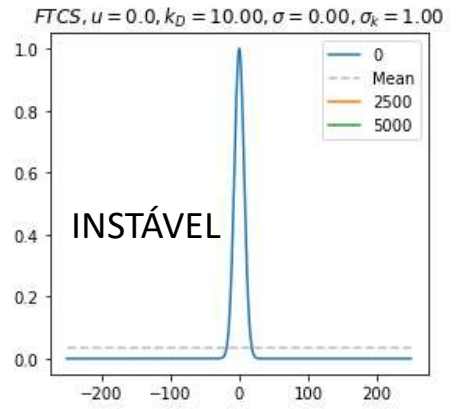
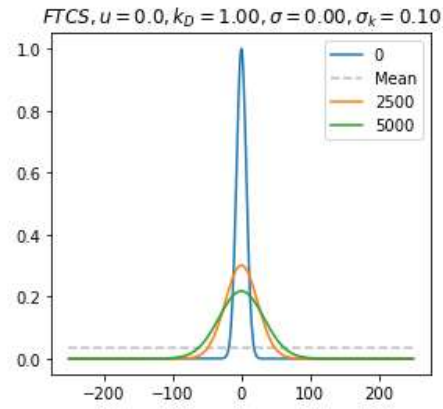
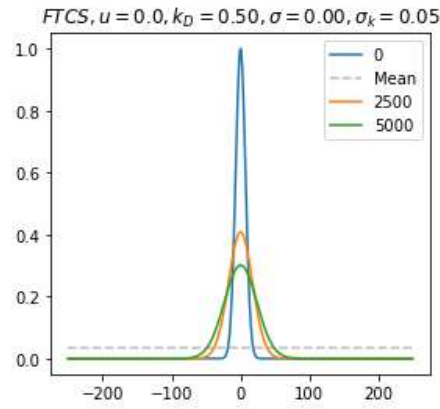
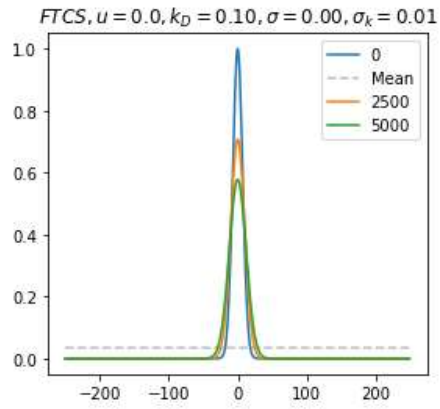


Alguns difusão **estabiliza** o FCTS e reduz a dispersão no leapfrog. **Muita difusão: instável**

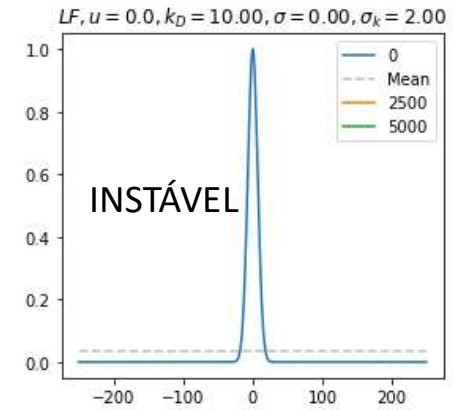
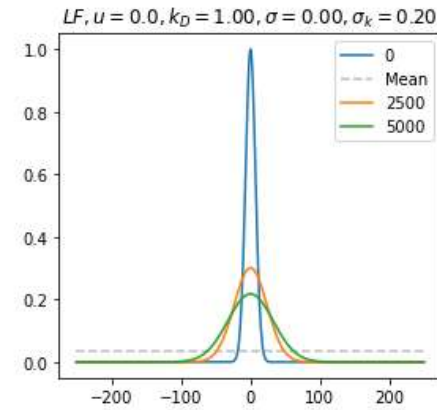
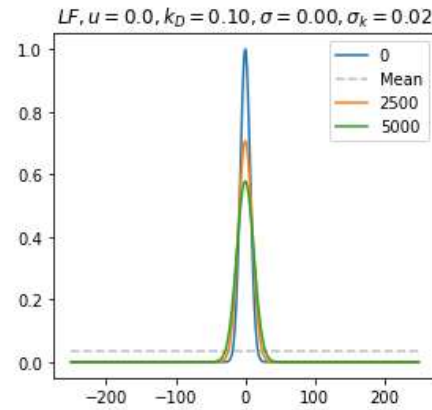
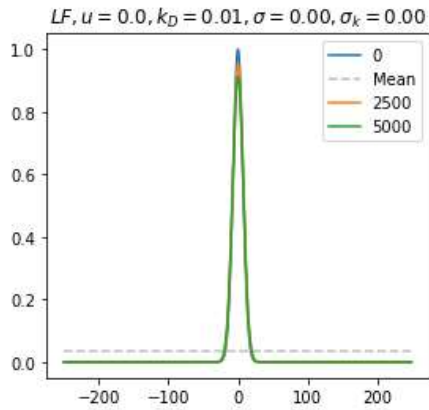
$u = 0$

$k_D \rightarrow$

FTCS



Leapfrog
s/ filtro



Estabilidade da solução da equação de advecção difusão

Leapfrog:

$$T_{i,j}^{n+1} = T_{i,j}^{n-1} - \frac{u\Delta t}{\Delta x} (T_{i+1,j}^n - T_{i-1,j}^n) + \frac{K_D 2\Delta t}{\Delta x^2} (T_{i-1,j}^{n-1} + T_{i+1,j}^{n-1} - 2T_{i,j}^{n-1})$$

FCTS:

$$T_{i,j}^{n+1} = T_{i,j}^n - \frac{u\Delta t}{2\Delta x} (T_{i+1,j}^n - T_{i-1,j}^n) + \frac{K_D \Delta t}{\Delta x^2} (T_{i-1,j}^n + T_{i+1,j}^n - 2T_{i,j}^n)$$

A estabilidade depende dos dois números adimensionais

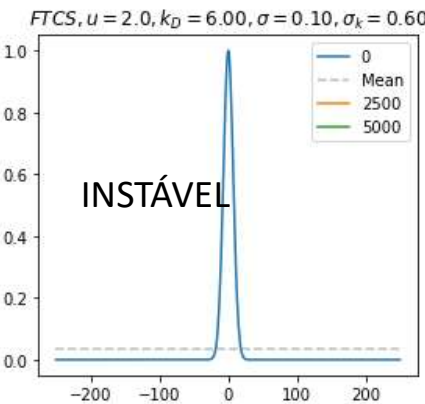
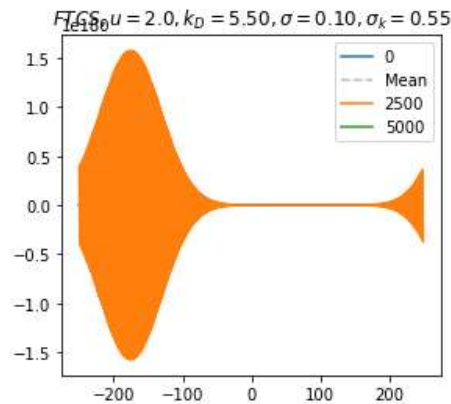
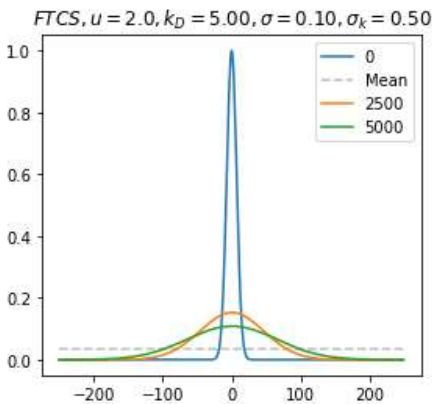
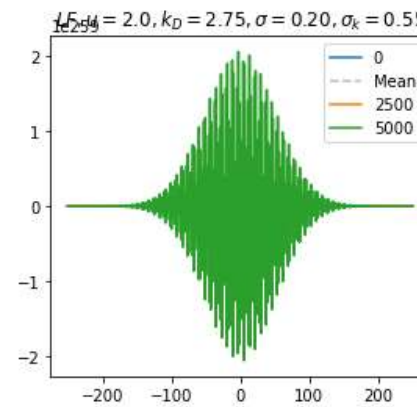
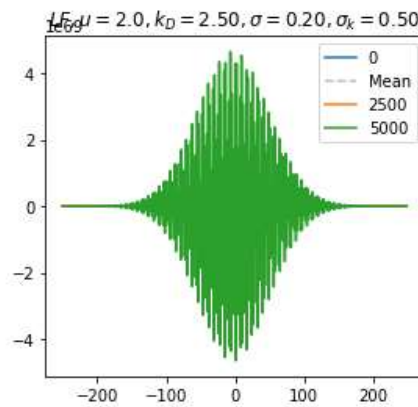
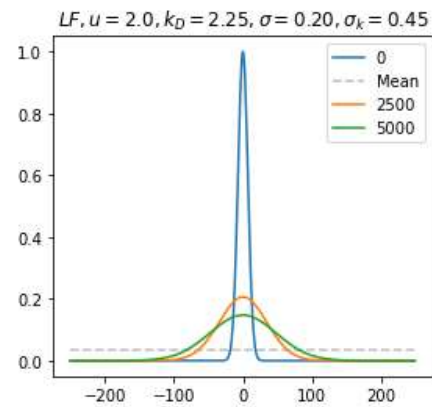
$$\sigma = \frac{u\Delta t}{\Delta x} \leq 1 \text{ (Número de Courant)}, \sigma_k = \frac{K_D 2\Delta t}{\Delta x^2} \leq \frac{1}{2} \text{ (Leapfrog)}$$

$$\sigma = \frac{u\Delta t}{2\Delta x} \leq 1, \sigma_k = \frac{K_D \Delta t}{\Delta x^2} \leq \frac{1}{2} \text{ (FTCS)}$$

Teste de sensibilidade a k_D : condição $\sigma_k \leq 0.5$

Leapfrog

$$\sigma_k = \frac{K_D 2\Delta t}{\Delta x^2}$$

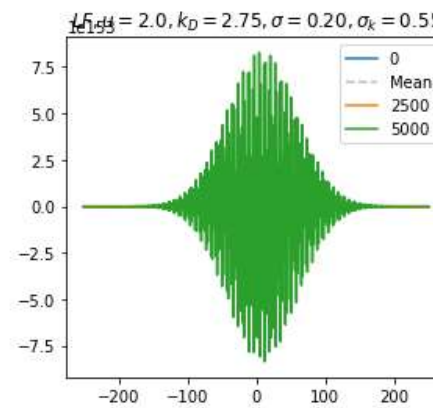
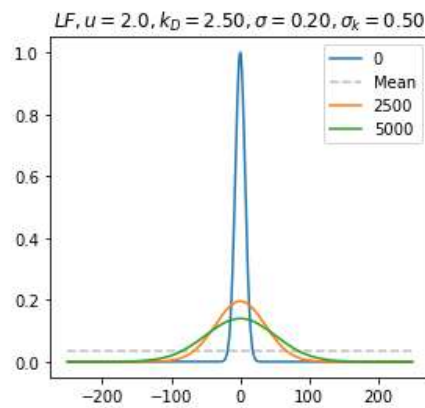
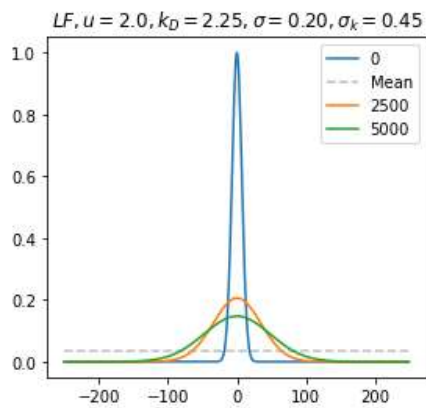


FTCS

$$\sigma_k = \frac{K_D \Delta t}{\Delta x^2}$$

Teste de sensibilidade a k_D (leapfrog)

$$\sigma_k = \frac{K_D 2\Delta t}{\Delta x^2}$$



Não melhora muito...

Leapfrog com
filtro temporal
Robert-Aselin
(0.05)

Advecção difusão em 2D (leapfrog)

$$T_{i,j}^{n+1} = T_{i,j}^{n-1} +$$

```

x=np.arange(-Lx,Lx,dx)
y=np.arange(-Ly,Ly,dy)
xis=np.zeros((nx,ny))
yps=np.zeros((nx,ny))
for iy in range(ny):
    xis[:,iy]=x
for ix in range(nx):
    yps[ix,:]=y

```

$$+2\Delta t \left(-u \frac{T_{i+1,j}^n - T_{i-1,j}^n}{2\Delta x} - v \frac{T_{i,j+1}^n - T_{i,j-1}^n}{2\Delta x} \right) + K_D \left(\frac{T_{i-1,j}^{n-1} + T_{i+1,j}^{n-1} - 2T_{i,j}^{n-1}}{\Delta x^2} + \frac{T_{i,j-1}^{n-1} + T_{i,j+1}^{n-1} - 2T_{i,j}^{n-1}}{\Delta y^2} \right)$$

...

```

TP[ix,iy]=TM[ix,iy]-u*dt/dx*(T[ixp,iy]-T[ixm,iy])-v*dt/dy*(T[ix,iyp]-T[ix,iym])\
+kD*2*dt*((TM[ixm,iy]+TM[ixp,iy]-2*TM[ix,iy])/dx**2+(TM[ix,iym]+TM[ix,iyp]-2*TM[ix,iy])/dy**2)

```

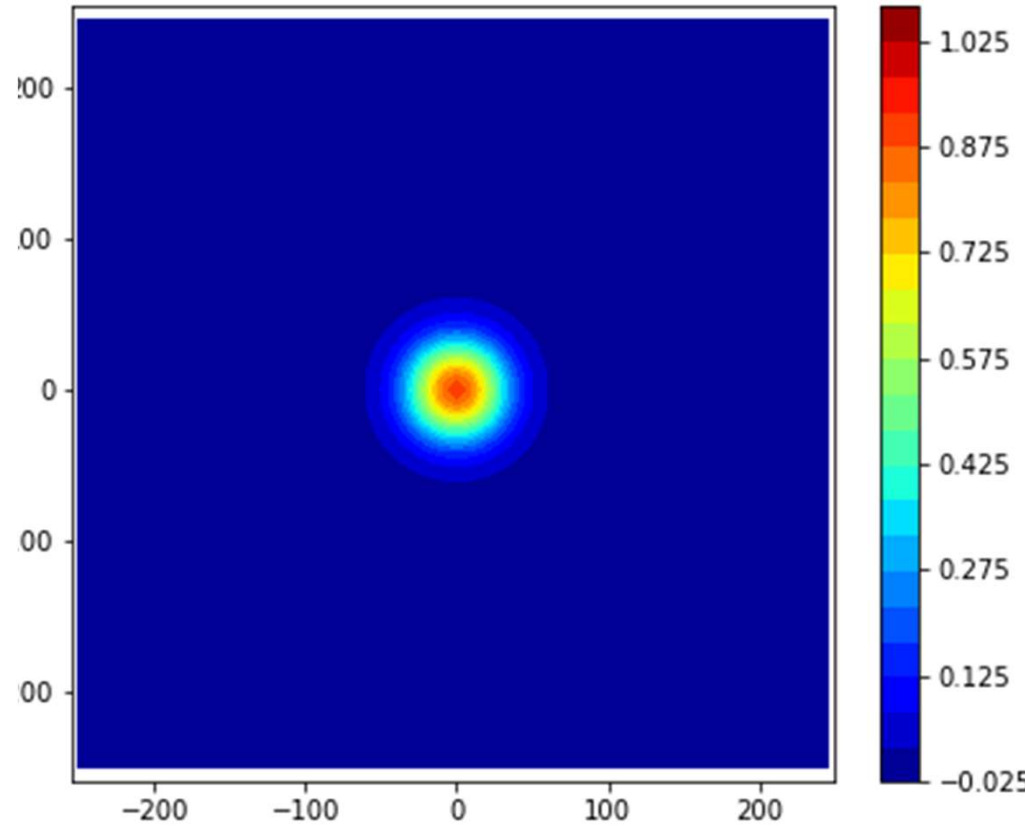
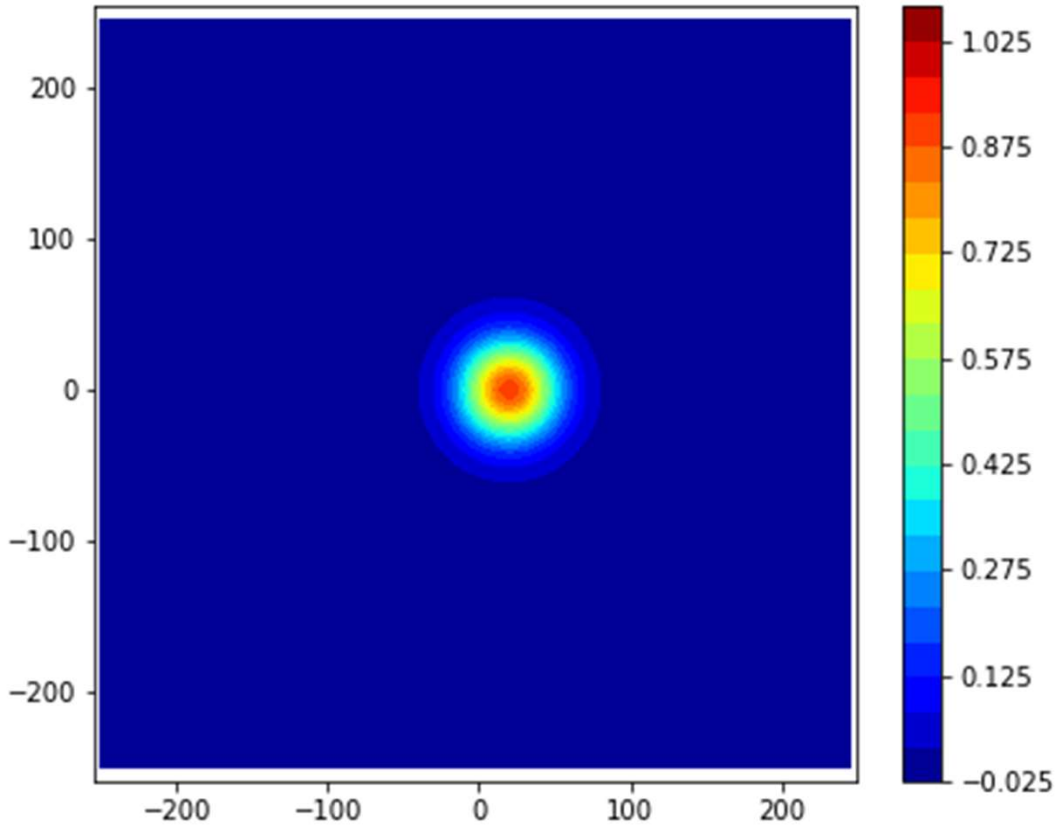
...

Caso 2D Leapfrog

$$u = 0$$

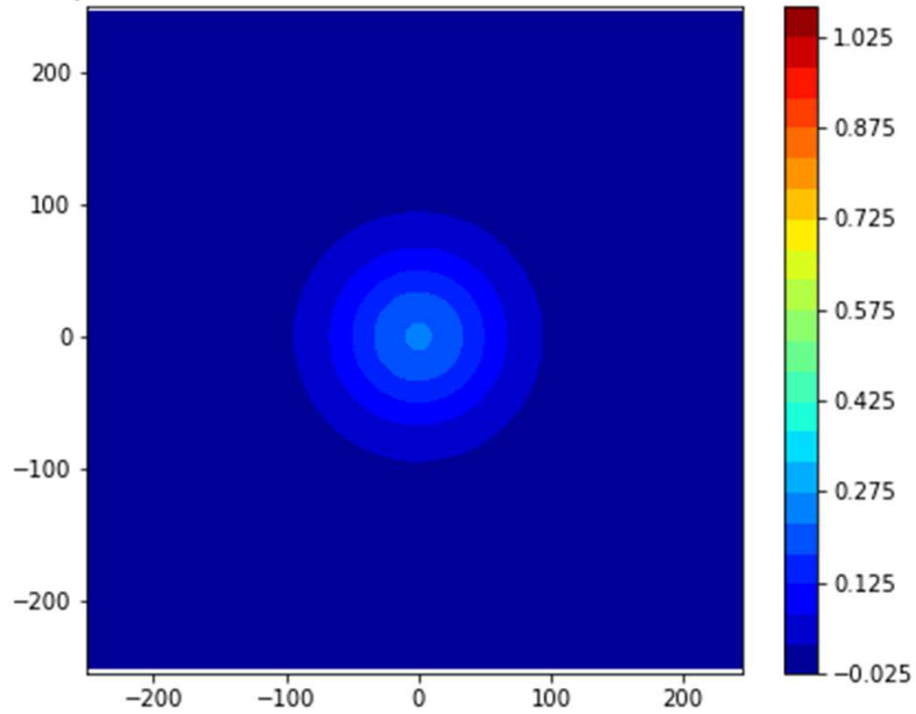
dvDif. by. LF: $u = 2.0, v = 0.0, k_D = 5.0, \sigma = 0.57, filtro = 0.05, t = 10s$

f. by. LF: $u = 0.0, v = 0.0, k_D = 5.0, \sigma = 0.00, filtro = 0.05, t = 10s$

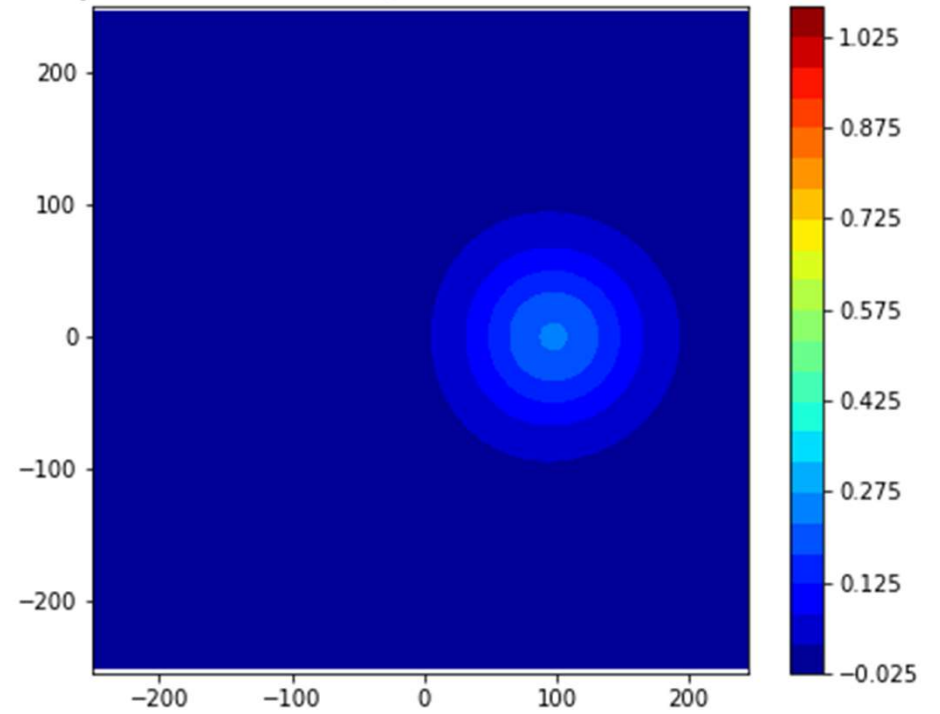


$$u = 0$$

|vDif. by. LF: $u = 0.0, v = 0.0, k_D = 5.0, \sigma = 0.00, \text{filtro} = 0.05, t = 299s$



|vDif. by. LF: $u = 2.0, v = 0.0, k_D = 5.0, \sigma = 0.57, \text{filtro} = 0.05, t = 299s$



É possível estabelecer um método **absolutamente estável**

Vamos recordar o **teorema do ponto médio**

$$\int_a^b f(x) dx = f(\bar{x})(b - a)$$

$$\frac{\partial T}{\partial t} = -u \frac{\partial T}{\partial x} + K_D \frac{\partial^2 T}{\partial x^2}$$

$$\begin{aligned} \frac{T_k^{n+1} - T_k^n}{\Delta t} &= -u \left(\frac{T_{k+1}^{n+1/2} - T_{k-1}^{n+1/2}}{2\Delta x} \right) + K_D \left(\frac{T_{k-1}^{n+1/2} + T_{k+1}^{n+1/2} - 2T_k^{n+1/2}}{\Delta x^2} \right) \\ &= -u(1 - \alpha) \left(\frac{T_{k+1}^n - T_{k-1}^n}{2\Delta x} \right) - u\alpha \left(\frac{T_{k+1}^{n+1} - T_{k-1}^{n+1}}{2\Delta x} \right) \\ &\quad + K_D \left((1 - \alpha) \frac{T_{k-1}^n + T_{k+1}^n - 2T_k^n}{\Delta x^2} + \alpha \frac{T_{k-1}^{n+1} + T_{k+1}^{n+1} - 2T_k^{n+1}}{\Delta x^2} \right) \end{aligned}$$

$$\frac{\partial T}{\partial t} = -u \frac{\partial T}{\partial x} + K_D \frac{\partial^2 T}{\partial x^2}$$

$$\begin{aligned} T_k^{n+1} + \Delta t u \alpha \left(\frac{T_{k+1}^{n+1} - T_{k-1}^{n+1}}{2\Delta x} \right) - \Delta t K_D \alpha \frac{T_{k-1}^{n+1} + T_{k+1}^{n+1} - 2T_k^{n+1}}{\Delta x^2} \\ = T_k^n - \Delta t u (1 - \alpha) \left(\frac{T_{k+1}^n - T_{k-1}^n}{2\Delta x} \right) + \Delta t K_D (1 - \alpha) \frac{T_{k-1}^n + T_{k+1}^n - 2T_k^n}{\Delta x^2} \end{aligned}$$

$\alpha = 0$ (FTCS), $\alpha = 1$ (Implícito), $\alpha = 0.5$ (semi-implícito, Crank Nicholson)

Na forma matricial, temos um Sistema de equações lineares para calcular a distribuição futura de T_k^{n+1} ($k = 0, \dots, N_x - 1$) $\equiv \vec{T}^{n+1}$:

$$M\vec{T}^{n+1} = \vec{b}^n$$

$$\frac{\partial T}{\partial t} = -u \frac{\partial T}{\partial x} + K_D \frac{\partial^2 T}{\partial x^2}$$

$$\begin{aligned} T_k^{n+1} + \Delta t u \alpha \left(\frac{T_{k+1}^{n+1} - T_{k-1}^{n+1}}{2\Delta x} \right) - \Delta t K_D \alpha \frac{T_{k-1}^{n+1} + T_{k+1}^{n+1} - 2T_k^{n+1}}{\Delta x^2} \\ = T_k^n - \Delta t u (1 - \alpha) \left(\frac{T_{k+1}^n - T_{k-1}^n}{2\Delta x} \right) + \Delta t K_D (1 - \alpha) \frac{T_{k-1}^n + T_{k+1}^n - 2T_k^n}{\Delta x^2} \end{aligned}$$

Ou:

$$\begin{aligned} \alpha \Delta t \left(-\frac{u}{2\Delta x} - \frac{K_D}{\Delta x^2} \right) T_{k-1}^{n+1} + \left(1 + \frac{2\alpha \Delta t K_D}{\Delta x^2} \right) T_k^{n+1} + \alpha \Delta t \left(\frac{u}{2\Delta x} - \frac{K_D}{\Delta x^2} \right) T_{k+1}^{n+1} \\ = T_k^n - \Delta t u (1 - \alpha) \left(\frac{T_{k+1}^n - T_{k-1}^n}{2\Delta x} \right) + \Delta t K_D (1 - \alpha) \frac{T_{k-1}^n + T_{k+1}^n - 2T_k^n}{\Delta x^2} \end{aligned}$$

$$M \vec{T}^{n+1} = \vec{b}^n$$

$$\begin{aligned} & \alpha \Delta t \left(-\frac{u}{2\Delta x} - \frac{K_D}{\Delta x^2} \right) T_{k-1}^{n+1} + \left(1 + \frac{2\alpha \Delta t K_D}{\Delta x^2} \right) T_k^{n+1} + \alpha \Delta t \left(\frac{u}{2\Delta x} - \frac{K_D}{\Delta x^2} \right) T_{k+1}^{n+1} \\ &= T_k^n - \Delta t u (1 - \alpha) \left(\frac{T_{k+1}^n - T_{k-1}^n}{2\Delta x} \right) + \Delta t K_D (1 - \alpha) \frac{T_{k-1}^n + T_{k+1}^n - 2T_k^n}{\Delta x^2} \end{aligned}$$

$\alpha = 0$ (FTCS), $\alpha = 1$ (Implícito), $\alpha = 0.5$ (Crank - Nicholson)

$$M\vec{T}^{n+1} = \vec{b}^n$$

$$\begin{bmatrix} \left(1 + \frac{2\alpha\lambda\Delta t}{\Delta z^2}\right) & \left(\frac{u\Delta t}{2\Delta x} - \frac{\alpha\lambda\Delta t}{\Delta z^2}\right) & \dots & \left(-\frac{u\Delta t}{2\Delta x} - \frac{\alpha\lambda\Delta t}{\Delta z^2}\right) \\ \left(-\frac{u\Delta t}{2\Delta x} - \frac{\alpha\lambda\Delta t}{\Delta z^2}\right) & \left(1 + \frac{2\alpha\lambda\Delta t}{\Delta z^2}\right) & \left(\frac{u\Delta t}{2\Delta x} - \frac{\alpha\lambda\Delta t}{\Delta z^2}\right) & \\ \vdots & & \ddots & \vdots \\ \left(\frac{u\Delta t}{2\Delta x} - \frac{\alpha\lambda\Delta t}{\Delta z^2}\right) & & \left(-\frac{u\Delta t}{2\Delta x} - \frac{\alpha\lambda\Delta t}{\Delta z^2}\right) & \left(1 + \frac{2\alpha\lambda\Delta t}{\Delta z^2}\right) \end{bmatrix} \begin{bmatrix} T_0^{n+1} \\ T_1^{n+1} \\ \vdots \\ T_{N_z-1}^{n+1} \end{bmatrix} = \vec{b}$$

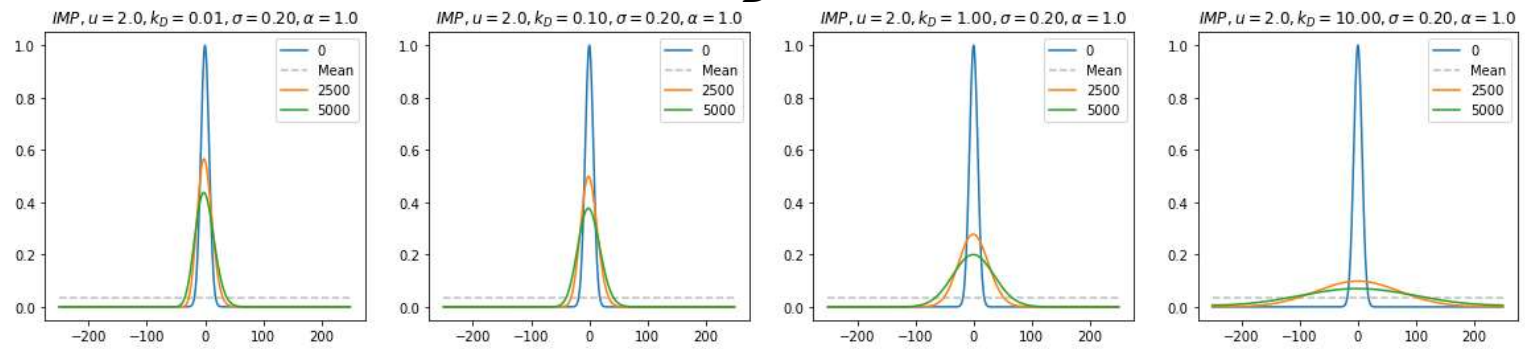
A matriz M é **esparsa** (só não são '0' a diagonal, subdiagonais e os cantos).

É uma matriz de **Toeplitz** (os termos de cada diagonal são todos iguais)

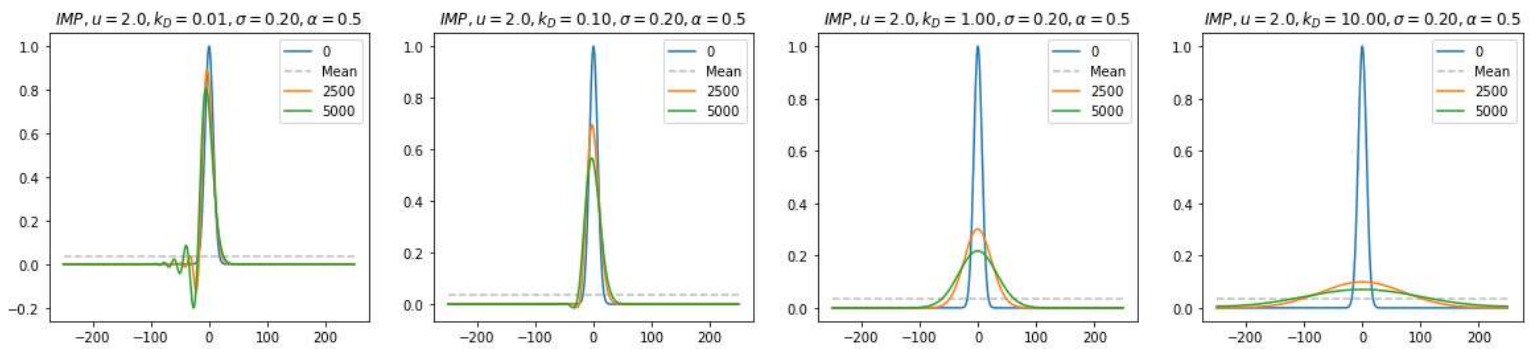
Os cantos impõem uma **condição fronteira cíclica**.

$k_D \rightarrow$

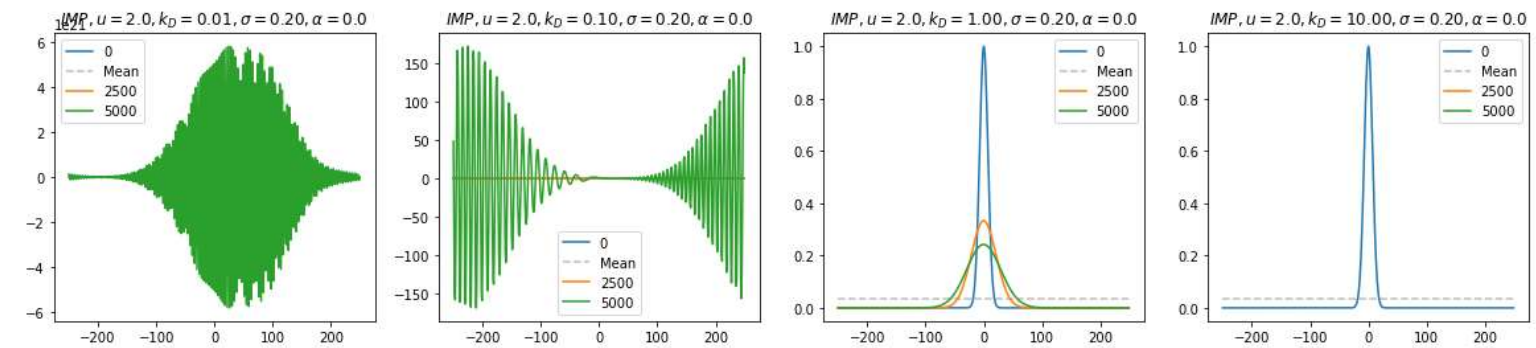
$\alpha = 1$
Implicito



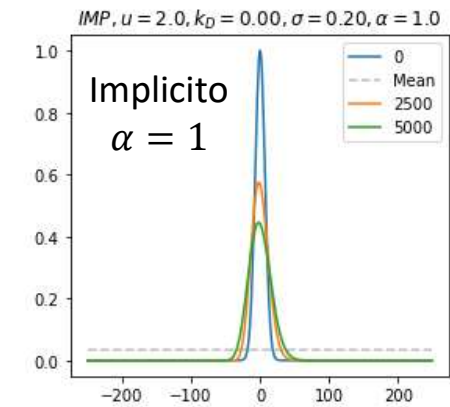
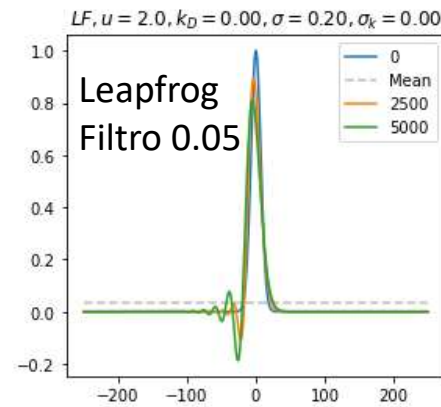
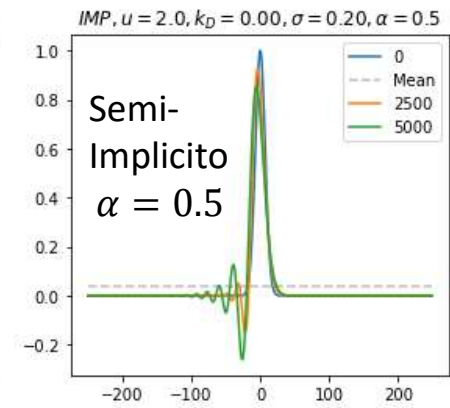
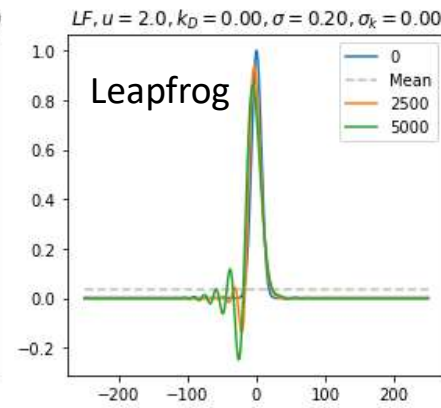
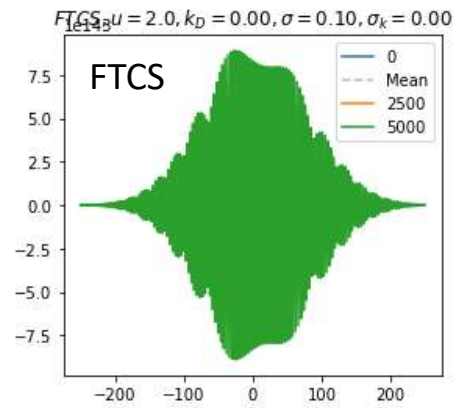
$\alpha = 0.5$



$\alpha = 0$
FTCS



$$k_D = 0$$



...

```
Wx=10;x0=0;TI=np.exp(-(x-x0)/Wx)**2); B=np.zeros(TI.shape)
T=np.copy(TI);TP=np.copy(T)
start_time=time.process_time()
M=np.zeros((nx,nx))
left=alpha*dt*(-u/(2*dx)-kD/dx**2);    right=alpha*dt*(u/(2*dx)-kD/dx**2)
center=(1+2*alpha*dt*kD/dx**2)
for ix in range(nx):
    M[ix,ix]=center
for ix in range(nx-1):
    M[ix,ix+1]=right
for ix in range(0,nx-1):
    M[ix+1,ix]=left
M[0,nx-1]=left;    M[nx-1,0]=right
```

...

```
for it in range(1,nt):
    for ix in range(nx):
        ixm=ix-1;ixp=ix+1
        if ixm<0:
            ixm=nx-1
        elif ixp>nx-1:
            ixp=0
        B[ix]=T[ix]+dt*(1-alpha)*(-u*(T[ixp]-T[ixm])/(2*dx)+kD/dx**2*(T[ixm]+T[ixp]-2*T[ix]))
    TP=np.linalg.solve(M,B)
timespent=time.process_time()-start_time
```

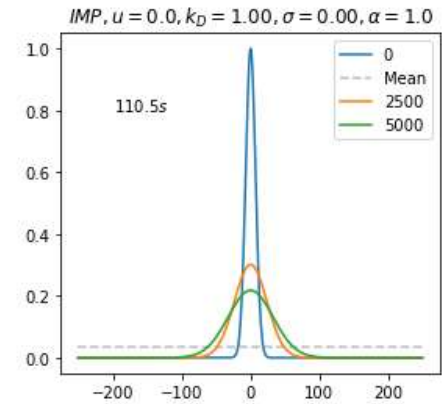
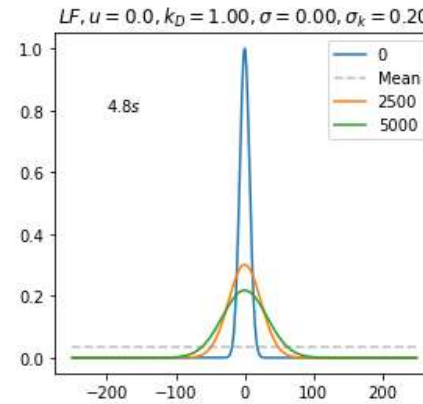
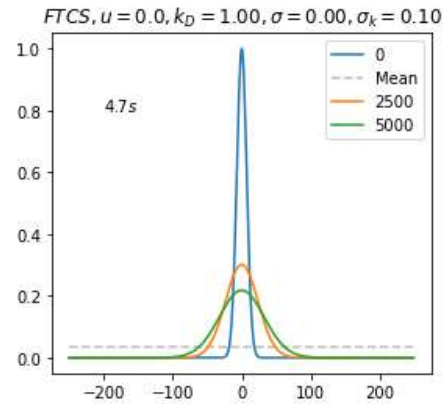
Método implícito

$$u = 0, k_D = 1$$

```
M=np.zeros((nx,nx))
```

```
...
```

```
TP=np.linalg.solve(M,B)
```



```
from scipy.sparse import lil_matrix
from scipy.sparse.linalg import spsolve
```

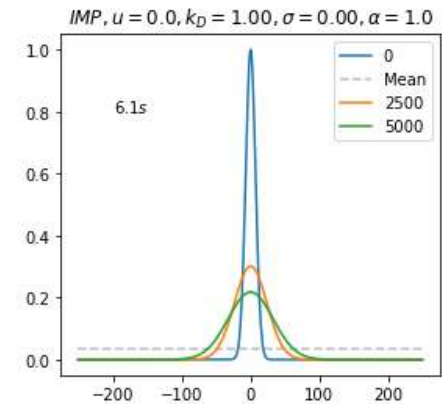
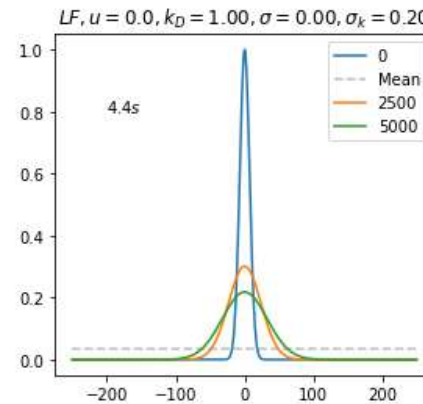
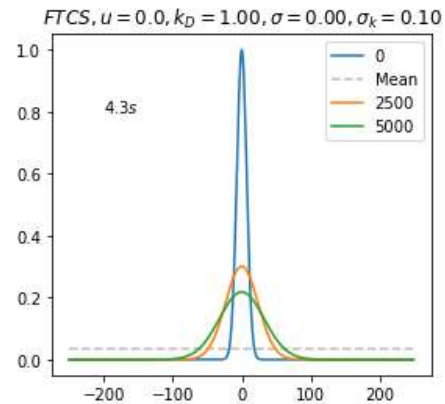
```
M=lil_matrix((nx,nx))
```

```
...
```

```
M=M.tocsr()
```

```
...
```

```
TP=spsolve(M,B)
```



```

... from scipy.sparse import lil_matrix; from scipy.sparse.linalg import spsolve
Wx=10;x0=0;TI=np.exp(-(x-x0)/Wx)**2); B=np.zeros(TI.shape)
T=np.copy(TI);TP=np.copy(T)
start_time=time.process_time()
M=lil_matrix((nx,nx)) #M=np.zeros((nx,nx))
left=alpha*dt*(-u/(2*dx)-kD/dx**2); right=alpha*dt*(u/(2*dx)-kD/dx**2)
center=(1+2*alpha*dt*kD/dx**2)
for ix in range(nx):
    M[ix,ix]=center
for ix in range(nx-1):
    M[ix,ix+1]=right
for ix in range(0,nx-1):
    M[ix+1,ix]=left
M[0,nx-1]=left; M[nx-1,0]=right
M=M.tocsr(M)
...
for it in range(1,nt):
    for ix in range(nx):
        ixm=ix-1;ixp=ix+1
        if ixm<0:
            ixm=nx-1
        elif ixp>nx-1:
            ixp=0
        B[ix]=T[ix]+dt*(1-alpha)*(-u*(T[ixp]-T[ixm])/(2*dx)+kD/dx**2*(T[ixm]+T[ixp]-2*T[ix]))
    TP=spsolve(M,B) #np.linalg.solve(M,B)
timespent=time.process_time()-start_time

```

Método
implícito
sparse

O método implícito

É absolutamente **estável** ($\alpha = 1$)

Obriga à solução de um Sistema de N_x equações, no caso 1D.

No caso multidimensional isso pode ser proibitivo.

Sendo a matriz dos coeficientes **esparsa**, existem métodos para reduzir drasticamente o custo da solução.