Diffusion equation in TCLB solver

In this workshop we will cover basic conceptions related to TCLB solver. We will not dive into detail of TCLB compilation or model development - it is out of scope of this tutorial and is covered in other materials.

The d2q9_reaction_diffusion_system_XXXX models

This TCLB model is a collection of Reaction-Partial/Ordinary differential equations systems. Basically, the model is build to solve systems in form:

$$\frac{\partial \mathbf{DRE}_1(x,t)}{\partial t} = \mathrm{Diffusivity\_DRE_1} \nabla \mathbf{DRE}_1(x,t) + R_1(\mathrm{RHS})$$

$$\cdots$$

$$\frac{\partial \mathbf{DRE}_i(x,t)}{\partial t} = \mathrm{Diffusivity\_DRE_i} \nabla \mathbf{DRE}_i(x,t) + R_i(\mathrm{RHS})$$

$$\frac{d\mathbf{ODE}_1(x,t)}{dt} = F_1(\mathrm{RHS})$$

$$\cdots$$

$$\frac{d\mathbf{ODE}_i(x,t)}{dt} = F_i(\mathrm{RHS})$$

Where $DRE_i(x,t)$ is spatially variable field, solution of first Diffusion-Reaction equation, and $ODE_i(x,t)$ is solution of Ordinary Differential Equation at point x. Both equations are solved using second order, implicit midpoint scheme. Spatial discretisation of DRE is performed using LBM method - details could be found in [X]. The right hend side vector is equall

$$\mathrm{RHS} = [DRE_i(x,t), ODE_i(x,t)]$$

Most of the models have meaningfull names for $\mathbf{DRE}_i$ variables and params, provided below.

At point of writing, supported model are:

d2q9_reaction_diffusion_system_SimpleDiffusion

$$\frac{\partial \mathbf{PHI}(x,t)}{\partial t} = \mathbf{Diffusivity\_PHI} \nabla \mathbf{PHI}(x,t)$$

or

$$\frac{\partial \phi(x,t)}{\partial t} = \nu \nabla \phi(x,t)$$

d2q9_reaction_diffusion_system_AllenCahn

$$\frac{\partial \mathbf{PHI}(x,t)}{\partial t} = \mathbf{Diffusivity\_PHI} \nabla \mathbf{PHI}(x,t) + \mathbf{Lambda} * \mathbf{PHI}(x,t) * (1 - \mathbf{PHI}(x,t))$$

or

$$\frac{\partial \phi(x,t)}{\partial t} = \nu \nabla \phi(x,t) + C\phi(1-\phi)$$

d2q9_reaction_diffusion_system_SIR_SimpleLaplace

This simple spatial extension of SIR model, by addition of diffusivity

$$\nabla(S, I, R)$$

to every term

$$\frac{\partial}{\partial t}\mathbf{S} = -\mathbf{Beta} * \mathbf{S} * \mathbf{I} + \mathbf{Diffusivity\_S} \nabla \mathbf{S}$$

$$\frac{\partial}{\partial t}\mathbf{I} = \mathbf{Beta} * \mathbf{S} * \mathbf{I} - \mathbf{Gamma} * \mathbf{I} + \mathbf{Diffusivity\_I} \nabla \mathbf{I}$$

$$\frac{\partial}{\partial t}\mathbf{R} = \mathbf{Gamma} * \mathbf{I} + \mathbf{Diffusivity\_R} \nabla \mathbf{R}$$

or

$$\frac{\partial}{\partial t}S = -\beta \frac{S}{N} I + \nu_S \nabla S$$

$$\frac{\partial}{\partial t}I = \beta \frac{S}{N} I - \gamma I + \nu_I \nabla I$$

$$\frac{\partial}{\partial t}R = \gamma I + \nu_R \nabla R$$

for $N = 1$

d2q9_reaction_diffusion_system_SIR_ModifiedPeng

or the WSIR model, already referenced in this workshop

$$\frac{\partial}{\partial t}\mathbf{W} = \mathbf{Beta_w} * [(\mathbf{I} - \mathbf{W})] + \mathbf{Diffusivity\_W} \nabla \mathbf{W}$$

$$\frac{\partial}{\partial t}\mathbf{S} = -\mathbf{Beta} * \frac{\mathbf{S} * \mathbf{W}}{\mathbf{N}} *$$

$$\frac{\partial}{\partial t}\mathbf{I} = \mathbf{Beta} * \frac{\mathbf{S} * \mathbf{W}}{\mathbf{N}} - \mathbf{Gamma} * \mathbf{I}$$

$$\frac{\partial}{\partial t}\mathbf{R} = \mathbf{Gamma} * \mathbf{I}$$

or

$$\frac{\partial}{\partial t}W = \beta_W \left[\frac{r^2}{8} W + (I - W)\right]$$

$$\frac{\partial}{\partial t}S = -\beta \frac{S}{N} W$$

$$\frac{\partial}{\partial t}I = \beta \frac{S}{N} W - \gamma I$$

$$\frac{\partial}{\partial t}R = \gamma I$$

Keep in mind that for consistency, it's recomended to set

$$\mathbf{Diffusivity\_W} = \mathbf{Beta_w} * \frac{r^2}{8}$$

Additionaly, list of models could be extracted via:

In [1]:
```
! tclbmake d2q9_reaction_diffusion_system/list
```

```
TCLB_PATH:  /home/mdzik/_TCLB/TCLB
                                                 AllenCahn SIR_ModifiedPeng
d2q9_reaction_diffusion_system_AllenCahn             X              -
d2q9_reaction_diffusion_system_SIR_ModifiedPeng      -              X
d2q9_reaction_diffusion_system_SIR_SimpleLaplace     -              -
d2q9_reaction_diffusion_system_SimpleDiffusion       -              -
                                                 SIR_SimpleLaplace
d2q9_reaction_diffusion_system_AllenCahn                 -
d2q9_reaction_diffusion_system_SIR_ModifiedPeng          -
d2q9_reaction_diffusion_system_SIR_SimpleLaplace         X
d2q9_reaction_diffusion_system_SimpleDiffusion           -
                                                 SimpleDiffusion
d2q9_reaction_diffusion_system_AllenCahn                 -
d2q9_reaction_diffusion_system_SIR_ModifiedPeng          -
d2q9_reaction_diffusion_system_SIR_SimpleLaplace         -
d2q9_reaction_diffusion_system_SimpleDiffusion           X
```

What is included in this environment

To run TCLB model us ipython shell binding:

```
! tclb ModelName ConfigurationFile.xml
```

This will effectivelu run (in the curren working directory)

```
$TCLB_PATH/CLB/ModelName/main ConfigurationFile.xml
```

in your Jupyter/Binder. We will use

```
! tclb ModelName ConfigurationFile.xml > /dev/null && echo "DONE!"
```

to supress output in most cases.

TCLB solver

As you might noticed TCLB is a set of models (like d2q9). TCLB uses XML as source of configuration plus limited numebr of command line options which will be covered later. There is a python library that helps you build XML on-the-fly if You like.

In [2]:
```python
import h5py
import numpy as np
import matplotlib.pyplot as plt
from display_xml import XML
```

Basic configuration file

Lets solve diffusion equation, on 100x100 domain with diffusivity $\nu = 1/6$

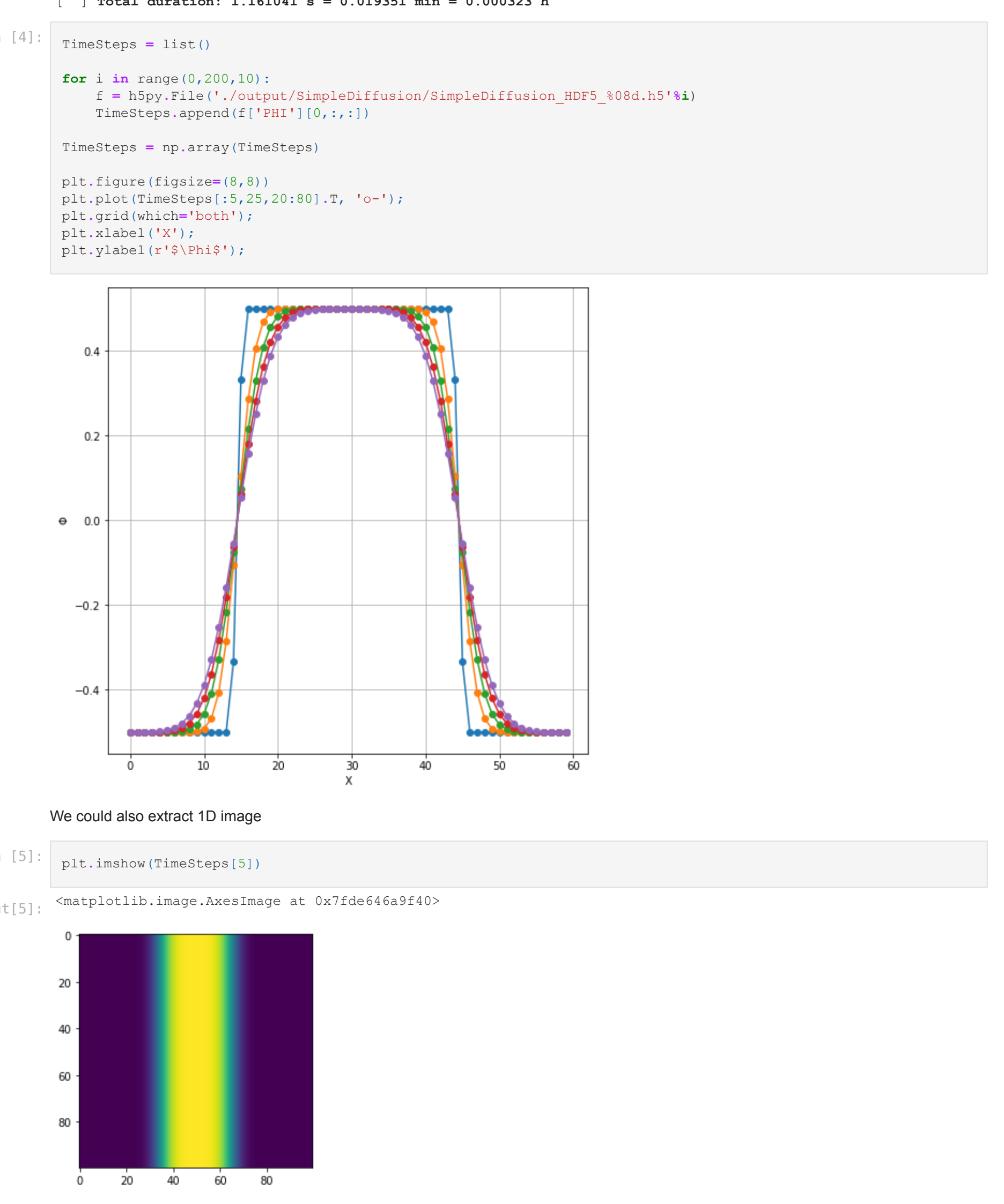
```xml
<CLBConfig version="2.0" output="output/SimpleDiffusion/"> <!-- The root xml element -->
    <Geometry nx="100" ny="100"> <!-- Mesh size, by default nz=1. MPI divisions are along X -->
        <None name="city"> <!--Named zone or BC, part of the mesh that could be referenced in Model section -->
            <Box dx="35" nx="30"/> <!-- Markers/geometrical descriptions of the parent zone -->
        </None>
    </Geometry>
    <Model> <!-- Here we set the model parameters, like viscosity -->
        <Param name="Diffusivity_DRE_1" value="0.1666"/> <!-- or Diffusivity for Diffusive-Reactive-Equation #1 -->
        <Param name="Init_DRE_1" value="-0.5"/> <!-- Initial value for Diffusive-Reactive-Equation #1  -->
        <Param name="Init_DRE_1" value="0.5" zone="city"/> <!-- Initial value for Diffusive-Reactive-Equation #1 in Zone City -->
    </Model>
    <HDF5/> <!-- Save at t=0 -->
    <Solve Iterations="200"> <!-- Iterate 100 iterations -->
        <HDF5 Iterations="10"/> <!-- Save HDF5 every 10, HDF5 could be replaced by VTK -->
    </Solve>
</CLBConfig>
```

and let's run it:

In [3]:
```
! tclb d2q9_reaction_diffusion_system_SimpleDiffusion SimpleDiffusion.xml
```

```
MPMD: TCLB: local:0/1 work:0/1 --- connected to:
[  ] -------------------------------------------------------------------------
[  ] -  CLB version:            v6.5.0-71-g352b9281                          -
[  ] -        Model:  d2q9_reaction_diffusion_system_SimpleDiffusion
[  ] -------------------------------------------------------------------------
[  ] Setting output path to: SimpleDiffusion
[  ] Discarding 1 comments
[  ] Running on CPU
[ 0] WARNING: No "Units" element in config file
[  ] Mesh size in config file: 100x100x1
[  ] Global lattice size: 100x100x1
[  ] Max region size: 10000. Mesh size 10000. Overhead:  0%
[  ] Local lattice size: 100x100x1
Hello allocator!
[  ]     Threads  |       Action
[  ]       1x1    | Primal , NoGlobals , InitFromExternal
[  ]       1x1    | Tangent , NoGlobals , InitFromExternal
[  ]       1x1    | Optimize , NoGlobals , InitFromExternal
[  ]       1x1    | SteadyAdjoint , NoGlobals , InitFromExternal
[  ]       1x1    | Primal , IntegrateGlobals , InitFromExternal
[  ]       1x1    | Tangent , IntegrateGlobals , InitFromExternal
[  ]       1x1    | Optimize , IntegrateGlobals , InitFromExternal
[  ]       1x1    | SteadyAdjoint , IntegrateGlobals , InitFromExternal
[  ]       1x1    | Primal , OnlyObjective , InitFromExternal
[  ]       1x1    | Tangent , OnlyObjective , InitFromExternal
[  ]       1x1    | Optimize , OnlyObjective , InitFromExternal
[  ]       1x1    | SteadyAdjoint , OnlyObjective , InitFromExternal
[  ]       1x1    | Primal , NoGlobals , BaseIteration
[  ]       1x1    | Tangent , NoGlobals , BaseIteration
[  ]       1x1    | Optimize , NoGlobals , BaseIteration
[  ]       1x1    | SteadyAdjoint , NoGlobals , BaseIteration
[  ]       1x1    | Primal , IntegrateGlobals , BaseIteration
[  ]       1x1    | Tangent , IntegrateGlobals , BaseIteration
[  ]       1x1    | Optimize , IntegrateGlobals , BaseIteration
[  ]       1x1    | SteadyAdjoint , IntegrateGlobals , BaseIteration
[  ]       1x1    | Primal , OnlyObjective , BaseIteration
[  ]       1x1    | Tangent , OnlyObjective , BaseIteration
[  ]       1x1    | Optimize , OnlyObjective , BaseIteration
[  ]       1x1    | SteadyAdjoint , OnlyObjective , BaseIteration
[  ]       1x1    | Primal , NoGlobals , BaseInit
[  ]       1x1    | Tangent , NoGlobals , BaseInit
[  ]       1x1    | Optimize , NoGlobals , BaseInit
[  ]       1x1    | SteadyAdjoint , NoGlobals , BaseInit
[  ]       1x1    | Primal , IntegrateGlobals , BaseInit
[  ]       1x1    | Tangent , IntegrateGlobals , BaseInit
[  ]       1x1    | Optimize , IntegrateGlobals , BaseInit
[  ]       1x1    | SteadyAdjoint , IntegrateGlobals , BaseInit
[  ]       1x1    | Primal , OnlyObjective , BaseInit
[  ]       1x1    | Tangent , OnlyObjective , BaseInit
[  ]       1x1    | Optimize , OnlyObjective , BaseInit
[  ]       1x1    | SteadyAdjoint , OnlyObjective , BaseInit
[  ] [0] Cumulative allocation of 1619520 b (1.6 MB)
[  ] Creating geom size:10000
[  ] Setting output path to: SimpleDiffusion
[  ] Setting output path to: output/SimpleDiffusion/SimpleDiffusion
[  ] loading geometry ...
[  ] Setting number of zones to 2
[  ] Setting Diffusivity_PHI to 0.1666 (0.166600)
[  ] [0] Settings [Diffusivity for _PHI] to 0.166600
[  ] Setting Init_PHI in zone  (-1) to -0.5 (-0.500000)
[  ] Setting Init_PHI in zone city (1) to 0.5 (0.500000)
[  ] Initializing Lattice ...
[  ] Callback HDF5 with no Iterations attribute==] 2373h  2m
[  ] Negotiated HDF5 chunks: 1x100x100[x3]
[  ]          0 it writing hdf5
[  ] Setting action Solve at 200.000000 iterations
[  ] Setting callback HDF5 at 10.000000 iterations
[  ] Negotiated HDF5 chunks: 1x100x100[x3]
[  ] Adding HDF5 to the solver hands
[  ]       53.0 MLBUps      8.74 GB/s [=====================================]2m
[  ]         10 it writing hdf5
[  ]       53.9 MLBUps      8.74 GB/s [=====================================]
[  ]         20 it writing hdf5
[  ]       17.8 MLBUps      2.89 GB/s [=====================================]
[  ]         30 it writing hdf5
[  ]       17.7 MLBUps      2.86 GB/s [=====================================]
[  ]         40 it writing hdf5
[  ]       17.8 MLBUps      2.88 GB/s [=====================================]
[  ]         50 it writing hdf5
[  ]       17.5 MLBUps      2.84 GB/s [=====================================]
[  ]         60 it writing hdf5
[  ]       17.4 MLBUps      2.83 GB/s [=====================================]
[  ]         70 it writing hdf5
[  ]       16.2 MLBUps      2.62 GB/s [=====================================]
[  ]         80 it writing hdf5
[  ]       17.5 MLBUps      2.84 GB/s [=====================================]
[  ]         90 it writing hdf5
[  ]        7.4 MLBUps      1.20 GB/s [=====================================]
[  ]        100 it writing hdf5
[  ]       16.8 MLBUps      2.72 GB/s [=====================================]
[  ]        110 it writing hdf5
[  ]       18.0 MLBUps      2.92 GB/s [=====================================]
[  ]        120 it writing hdf5
[  ]       18.1 MLBUps      2.93 GB/s [=====================================]
[  ]        130 it writing hdf5
[  ]       18.2 MLBUps      2.95 GB/s [=====================================]
[  ]        140 it writing hdf5
[  ]       18.8 MLBUps      3.05 GB/s [=====================================]
[  ]        150 it writing hdf5
[  ]       18.8 MLBUps      3.05 GB/s [=====================================]
[  ]        160 it writing hdf5
[  ]        8.3 MLBUps      1.35 GB/s [=====================================]
[  ]        170 it writing hdf5
[  ]       18.5 MLBUps      2.99 GB/s [=====================================]
[  ]        180 it writing hdf5
[  ]       17.8 MLBUps      2.88 GB/s [=====================================]
[  ]        190 it writing hdf5
[  ]       18.4 MLBUps      2.98 GB/s [=====================================]
[  ]        200 it writing hdf5
[  ] Total duration: 1.161041 s = 0.019351 min = 0.000323 h
```

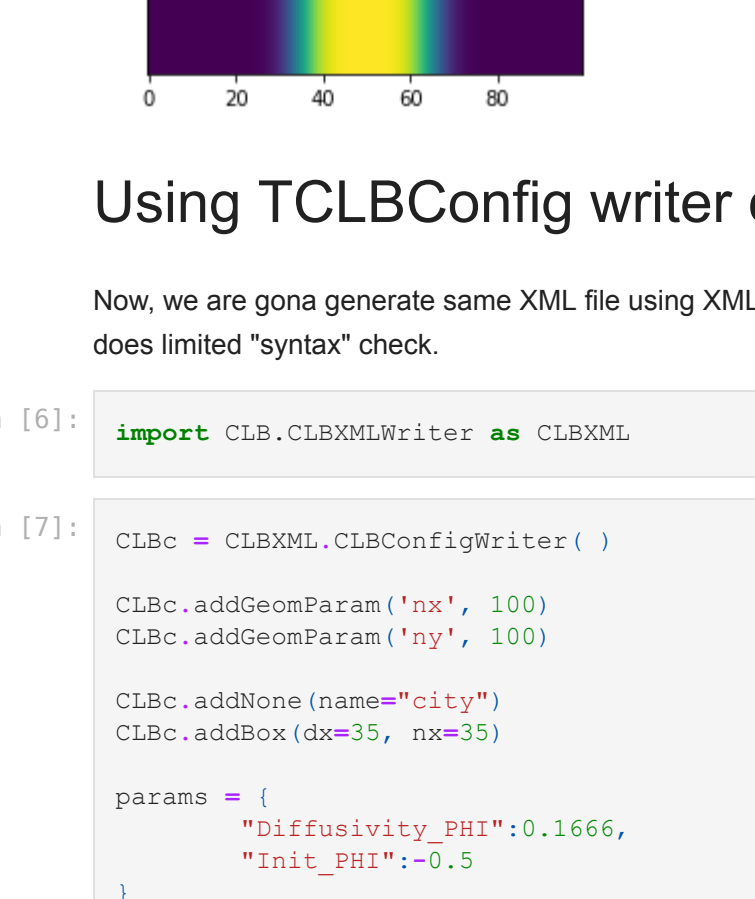
In [4]:
```python
TimeSteps = list()

for i in range(0,200,10):
    f = h5py.File('./output/SimpleDiffusion/SimpleDiffusion_HDF5_%08d.h5'%i)
    TimeSteps.append(f['PHI'][0,:,:])

TimeSteps = np.array(TimeSteps)

plt.figure(figsize=(6,6))
plt.plot(TimeSteps[:5,25,20:80].T, 'o-');
plt.grid(which='both');
plt.xlabel('X');
plt.ylabel(r'$\Phi$');
```



We could also extract 1D image

In [5]:
```python
plt.imshow(TimeSteps[5])
```

Out[5]:
```
<matplotlib.image.AxesImage at 0x7fde646a9f40>
```



Using TCLBConfig writer class

Now, we are gona generate same XML file using XML library. A nice think is that we could use it to do some parametric studies. It also does limited "syntax" check.

In [6]:
```python
import CLB.CLBXMLWriter as CLBXML
```

In [7]:
```python
CLBc = CLBXML.CLBConfigWriter( )

CLBc.addGeomParam('nx', 100)
CLBc.addGeomParam('ny', 100)

CLBc.addNone(name="city")
CLBc.addBox(dx=35, nx=35)

params = {
        "Diffusivity_PHI":0.1666,
        "Init_PHI":-0.5
}
CLBc.addModelParams(params)

params = {
        "Init_PHI":0.5
}

CLBc.addHDF5()
CLBc.addModelParams(params, zone='city')
solve = CLBc.addSolve(iterations=200)
CLBc.addHDF5(iterations=10, parent=solve)

CLBc.write('SimpleDiffusionByCLBXMLWriter.xml')
```

Apart from float representation, the resulting file is identical

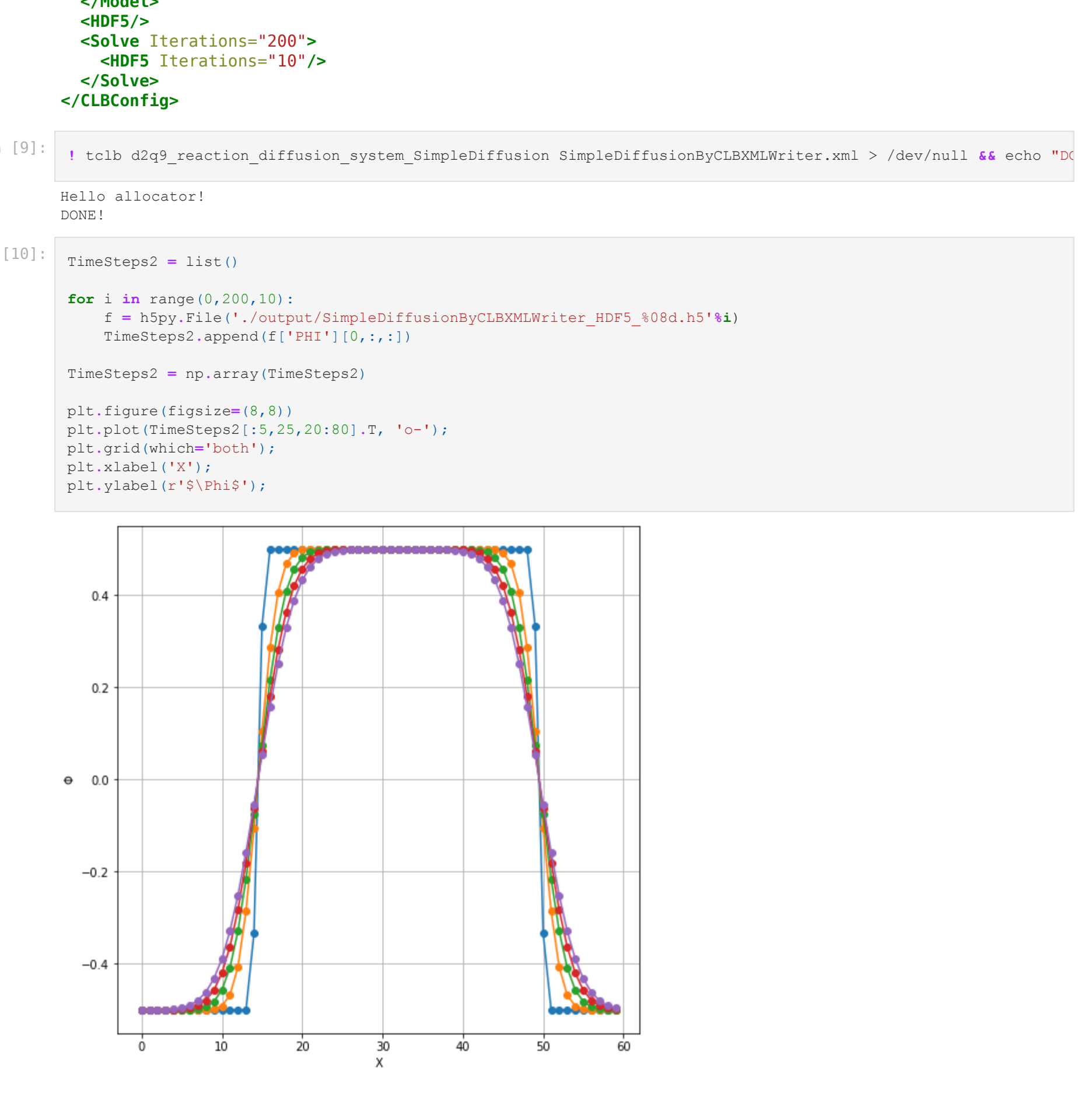
In [8]:
```python
f = open('SimpleDiffusionByCLBXMLWriter.xml', 'r')
XML(''.join(f.readlines()))
```

Out[8]:
```xml
<CLBConfig version="2.0" output="output/">
    <!--Created using CLBConfigWriter-->
    <Geometry predef="none" model="MRT" nx="100.0000000000000000" ny="100.0000000000000000">
        <None name="city">
            <Box dx="35" nx="35"/>
        </None>
    </Geometry>
    <Model>
        <Param name="Diffusivity_PHI" value="0.1666000000000000"/>
        <Param name="Init_PHI" value="-0.5000000000000000"/>
        <Param name="Init_PHI" value="0.5000000000000000" zone="city"/>
    </Model>
    <HDF5/>
    <Solve Iterations="200">
        <HDF5 Iterations="10"/>
    </Solve>
</CLBConfig>
```

In [9]:
```
! tclb d2q9_reaction_diffusion_system_SimpleDiffusion SimpleDiffusionByCLBXMLWriter.xml > /dev/null && echo "DONE!"
```

```
Hello allocator!
DONE!
```

In [10]:
```python
TimeSteps2 = list()

for i in range(0,200,10):
    f = h5py.File('./output/SimpleDiffusionByCLBXMLWriter_HDF5_%08d.h5'%i)
    TimeSteps2.append(f['PHI'][0,:,:])

TimeSteps2 = np.array(TimeSteps2)

plt.figure(figsize=(6,6))
plt.plot(TimeSteps2[:5,25,20:80].T, 'o-');
plt.grid(which='both');
plt.xlabel('X');
plt.ylabel(r'$\Phi$');
```



RInside: periodic IC and comparison with Finite Difference

Lets create initial condition. We will start in python

R inside block is build as

```python
CLBc.addRunR(eval=\
"""
some <- r_code
""")
```

which will result in XML as:

```xml
<RunR>
<![CDATA[
    some <- r_code
]]>
</RunR>
```

Notice, that `<` in some cases got converted into `<`. This is XML character escaping. Keep the CDATA element and all be OK :)

Outmost usable part of R-TCLB integration are accessors to internal Fields:

```r
Solver.Fields.FIELDNAME[] = SAMESHAPEVARIABLE;
```

and Actions/Stages:

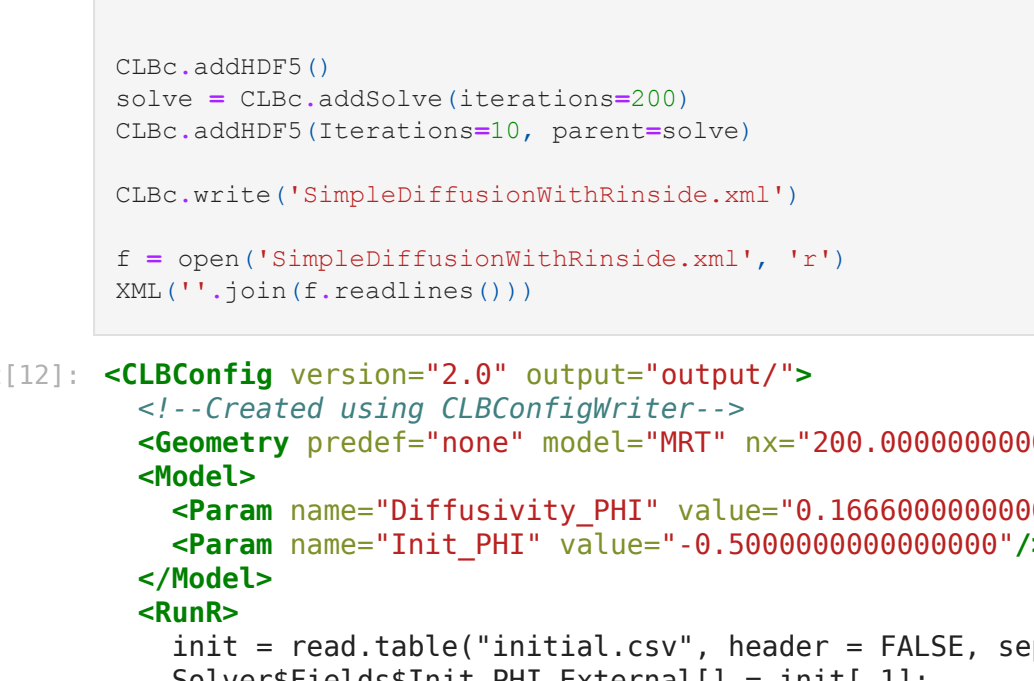
```
Solver.Actions.InitFromExternalAction();
```

You could also call standard R functions inside (Full R should be available - it's embeded interpreter, see RInside upstream documentation for details/limitations if you need):

```r
init = read.table("initial.csv", header = FALSE, sep = "", dec = ".");
```

Let's create initial "data file"

In [11]:
```python
u_ic = np.zeros(200)
u_ic[75:125] = 1
plt.plot(u_ic)
np.savetxt("initial.csv", u_ic, delimiter=",")
```



Now the XML configuration

In [12]:
```python
CLBc = CLBXML.CLBConfigWriter( )

CLBc.addGeomParam('nx', 200)
CLBc.addGeomParam('ny', 100)

CLBc.addRunR(eval=\
"""
    init = read.table("initial.csv", header = FALSE, sep = "", dec = ".");
    Solver$Fields$Init_PHI_External[] = init[1,1];
    Solver$Actions$InitFromExternalAction();
""")

params = {
        "Diffusivity_PHI":0.1666,
        "Init_PHI":-0.5
}

CLBc.addModelParams(params)

CLBc.addHDF5()
solve = CLBc.addSolve(iterations=200)
CLBc.addHDF5(iterations=10, parent=solve)

CLBc.write('SimpleDiffusionWithRinside.xml')

f = open('SimpleDiffusionWithRinside.xml', 'r')
XML(''.join(f.readlines()))
```

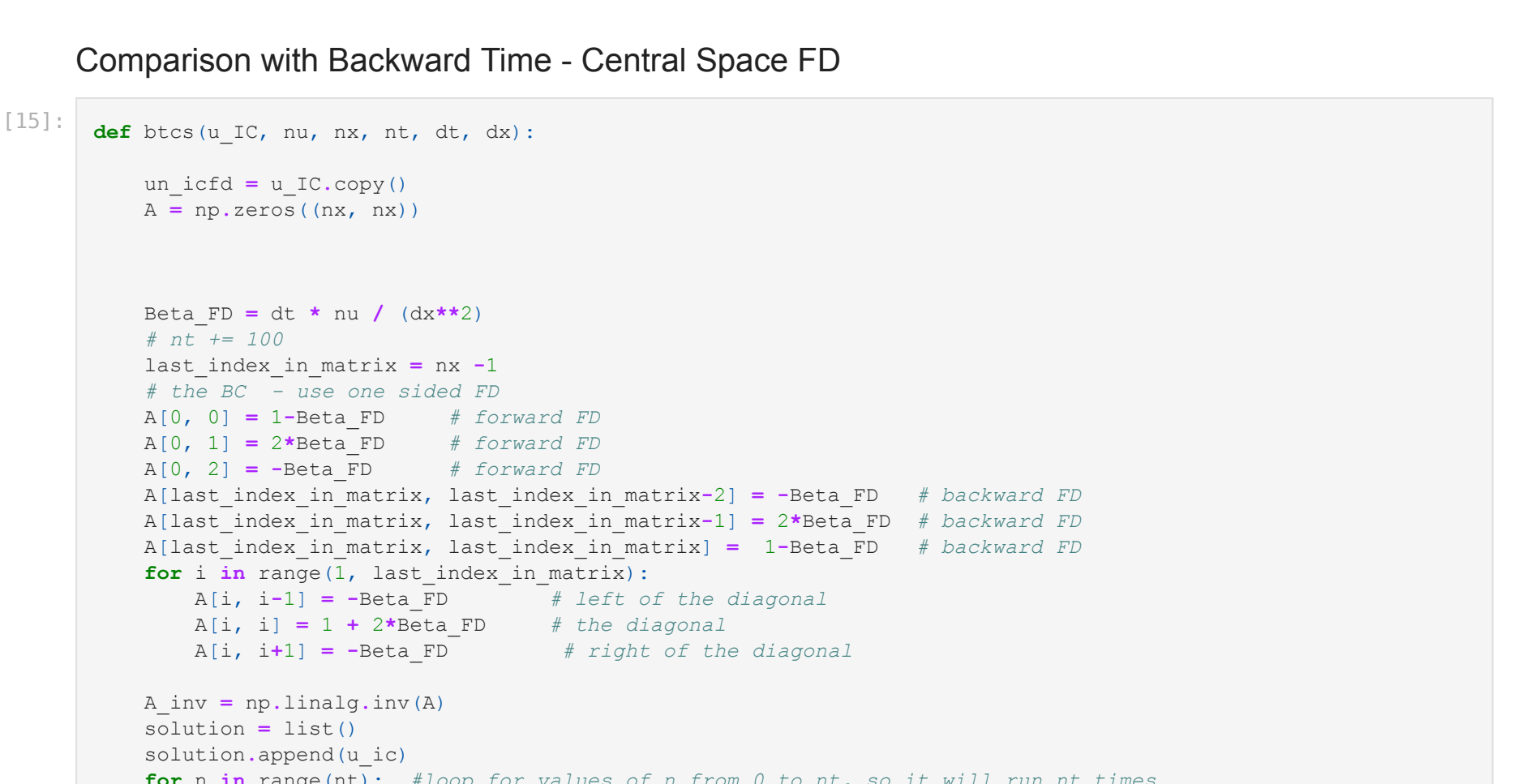
Out[12]:
```xml
<CLBConfig version="2.0" output="output/">
    <!--Created using CLBConfigWriter-->
    <Geometry predef="none" model="MRT" nx="200.0000000000000000" ny="100.0000000000000000"/>
    <Model>
        <Param name="Diffusivity_PHI" value="0.1666000000000000"/>
        <Param name="Init_PHI" value="-0.5000000000000000"/>
    </Model>
    <RunR>
        init = read.table("initial.csv", header = FALSE, sep = "", dec = ".");
        Solver$Fields$Init_PHI_External[] = init[1,1];
        Solver$Actions$InitFromExternalAction();
    </RunR>
    <HDF5/>
    <Solve Iterations="200">
        <HDF5 Iterations="10"/>
    </Solve>
</CLBConfig>
```

In [13]:
```
! tclb d2q9_reaction_diffusion_system_SimpleDiffusion SimpleDiffusionWithRinside.xml > /dev/null && echo "DONE!"
```

```
Hello allocator!
DONE!
```

Solution obtained from TCLB

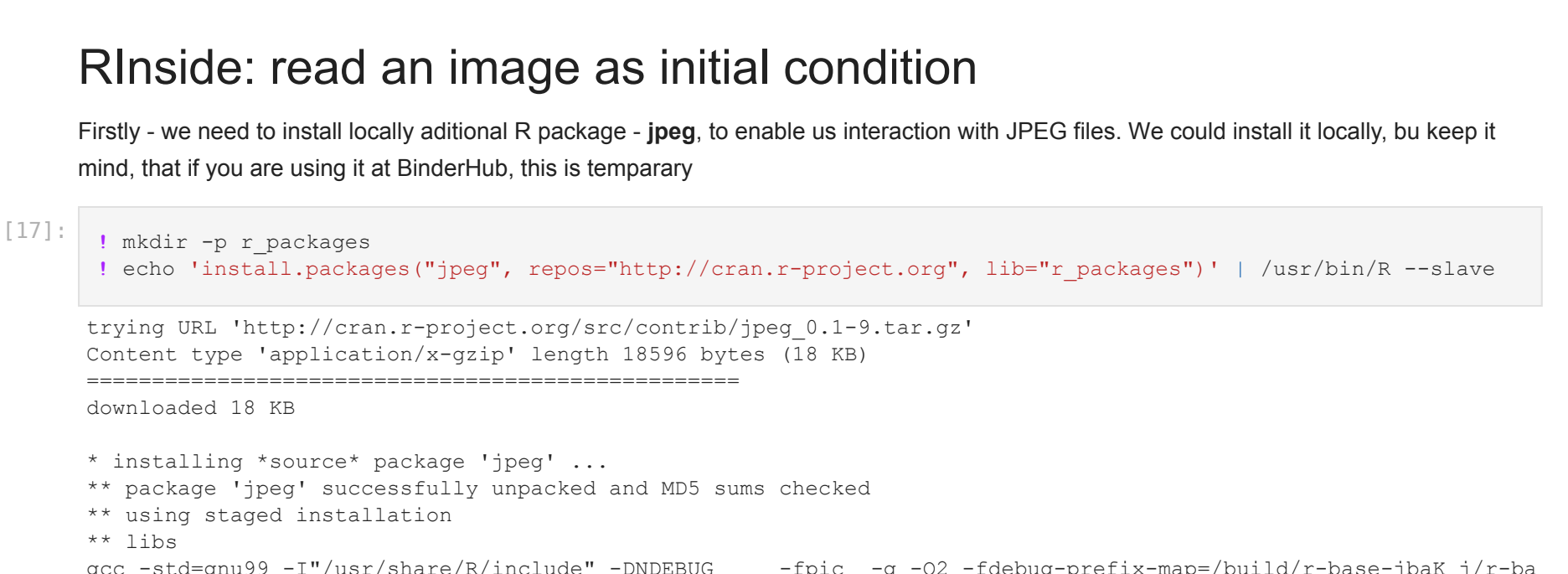
In [14]:
```python
TimeSteps2 = list()

for i in range(0,200,10):
    f = h5py.File('./output/SimpleDiffusionWithRinside_HDF5_%08d.h5'%i)
    TimeSteps2.append(f['PHI'][0,:,:])

TimeSteps2 = np.array(TimeSteps2)

plt.figure(figsize=(6,6))
plt.plot(TimeSteps2[5,25,:].T, '-');
plt.grid(which='both');
plt.xlabel('X');
plt.ylabel(r'$\Phi$');
```



Comparison with Backward Time - Central Space FD

In [15]:
```python
def btcs(u_IC, nu, nx, nt, dt, dx):

    un_icfd = u_IC.copy()
    A = np.zeros((nx, nx))

    Beta_FD = dt * nu / (dx**2)
    # nt += 100
    last_index_in_matrix = nx -1
    # for the BC - use one sided FD
    A[0, 0] = 1-Beta_FD      # forward FD
    A[0, 1] = 2*Beta_FD      # forward FD
    A[0, 2] = -Beta_FD       # forward FD
    A[last_index_in_matrix, last_index_in_matrix-2] = -Beta_FD   # backward FD
    A[last_index_in_matrix, last_index_in_matrix-1] = 2*Beta_FD  # backward FD
    A[last_index_in_matrix, last_index_in_matrix] = 1-Beta_FD    # backward FD
    for i in range(1, last_index_in_matrix):
        A[i, i-1] = -Beta_FD     # left of the diagonal
        A[i, i] = 1 + 2*Beta_FD  # the diagonal
        A[i, i+1] = -Beta_FD     # right of the diagonal

    A_inv = np.linalg.inv(A)
    solution = list()
    solution.append(u_icfd)
    for n in range(nt):  #loop for values of n from 0 to nt, so it will run nt times
        un_icfd = A_inv@un_icfd
        solution.append(un_icfd)

    return np.array(solution)

solution = btcs(u_IC, 0.1666, u_ic.shape[0], 200, 1, 1)
```

In [16]:
```python
plt.figure(figsize=(10,5))
plt.plot(TimeSteps2[5,25,:].T, 'k-', label="TCLB");
plt.plot(solution[0,:], label='Initial Condition')
plt.plot(solution[50,:], "--", label='Implicit Time, Central Space FD')
plt.legend()
plt.grid(which='both')
```



RInside: read an image as initial condition

Firstly - we need to install locally aditional R package - **jpeg**, to enable us interaction with JPEG files. We could install it locally, bu keep it mind, that if you are using it at BinderHub, this is temporary

In [17]:
```
! mkdir -p r_packages
! echo 'install.packages("jpeg", repos="http://cran.r-project.org", lib="r_packages")' | /usr/bin/R --slave
```

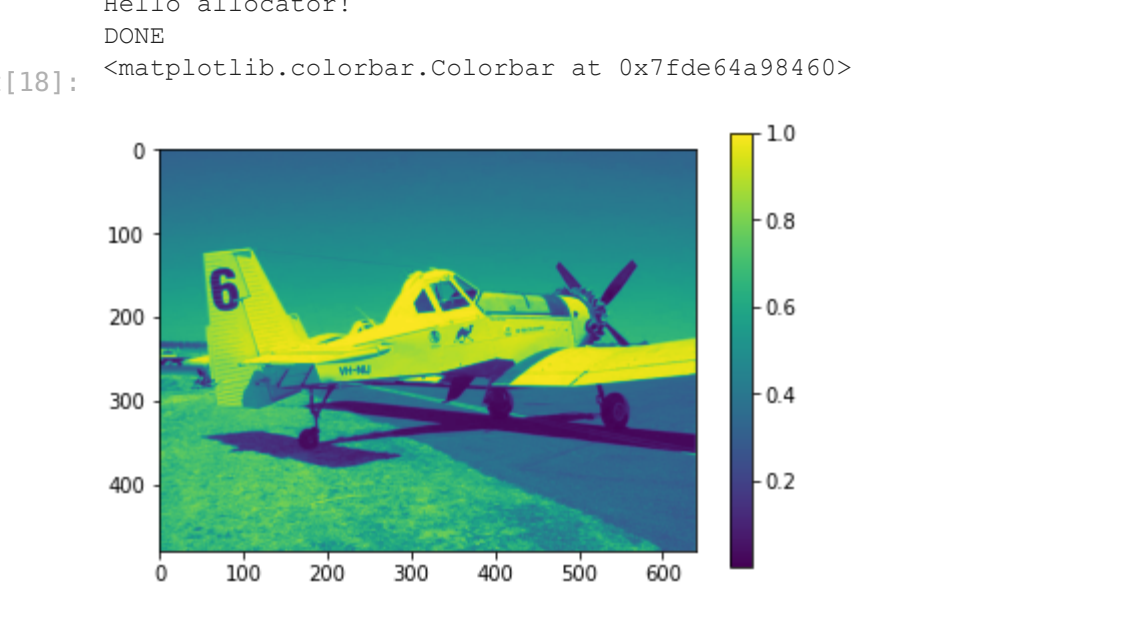
```
trying URL 'http://cran.r-project.org/src/contrib/jpeg_0.1-9.tar.gz'
Content type 'application/x-gzip' length 18596 bytes (18 KB)
==================================================
downloaded 18 KB

* installing *source* package 'jpeg' ...
** package 'jpeg' successfully unpacked and MD5 sums checked
** using staged installation
** libs
gcc -std=gnu99 -I"/usr/share/R/include" -DNDEBUG     -fpic  -g -O2 -fdebug-prefix-map=/build/r-base-jbaX_j/r-ba
se-3.6.3=. -fstack-protector-strong -Wformat -Werror=format-security -Wdate-time -D_FORTIFY_SOURCE=2 -g  -c rea
d.c -o read.o
gcc -std=gnu99 -I"/usr/share/R/include" -DNDEBUG     -fpic  -g -O2 -fdebug-prefix-map=/build/r-base-jbaX_j/r-ba
se-3.6.3=. -fstack-protector-strong -Wformat -Werror=format-security -Wdate-time -D_FORTIFY_SOURCE=2 -g  -c re
g.c -o reg.o
gcc -std=gnu99 -I"/usr/share/R/include" -DNDEBUG     -fpic  -g -O2 -fdebug-prefix-map=/build/r-base-jbaX_j/r-ba
se-3.6.3=. -fstack-protector-strong -Wformat -Werror=format-security -Wdate-time -D_FORTIFY_SOURCE=2 -g  -c wri
te.c -o write.o
gcc -std=gnu99 -shared -L/usr/lib/R/lib -Wl,-Bsymbolic-functions -Wl,-z,relro -o jpeg.so read.o reg.o write.o -
ljpeg -L/usr/lib/R/lib -lR
installing to /home/mdzik/_TCLB/TCLB_binder/IDUB/workshops/40_draft_IntroTCLB/r_packages/00LOCK-jpeg/00new/jpe
g/libs
** R
** inst
** byte-compile and prepare package for lazy loading
** help
*** installing help indices
** building package indices
** testing if installed package can be loaded from temporary location
** checking absolute paths in shared objects and dynamic libraries
** testing if installed package can be loaded from final location
** testing if installed package keeps a record of temporary installation path
* DONE (jpeg)

The downloaded source packages are in
        '/tmp/RtmpY6tcDo/downloaded_packages'
```

Let's check if it work - we use an image of a M-18A Dromader airplane as initial condition :)

In [18]:
```python
CLBc = CLBXML.CLBConfigWriter( )

CLBc.addGeomParam('nx', 640)
CLBc.addGeomParam('ny', 480)

CLBc.addRunR(eval=\
"""
    library("jpeg", lib="r_packages")

    myurl <- "https://upload.wikimedia.org/wikipedia/commons/thumb/a/a5/M-18A_Dromader_CALM.jpg/640px-M-18A_Dro
    z <- tempfile()
    download.file(myurl,z,mode="wb", quiet=TRUE);
    pic <- readJPEG(z);
    file.remove(z) # cleanup

    Solver$Fields$Init_PHI_External[] = t(pic[,,1]);
    Solver$Actions$InitFromExternalAction();
""")

params = {
        "Diffusivity_PHI":0.1666,
        "Init_PHI":-0.5
}
CLBc.addModelParams(params)

CLBc.addHDF5()
CLBc.write('SimpleDiffusionOfDromader.xml')

! tclb d2q9_reaction_diffusion_system_SimpleDiffusion SimpleDiffusionOfDromader.xml > /dev/null && echo "DONE"

i = 0
f = h5py.File('./output/SimpleDiffusionOfDromader_HDF5_%08d.h5'%i)
plt.imshow(f['PHI'][0,:,:])
plt.colorbar()
```

```
Hello allocator!
DONE
```

Out[18]:
```
<matplotlib.colorbar.Colorbar at 0x7fde64a98460>
```



The CLBc object could be reused (something could be appended to it after save, parameters could be overwritten)

XML for diffusion of the example image will look like that:

In [19]:
```python
solve = CLBc.addSolve(iterations=200)
CLBc.addHDF5(iterations=10, parent=solve)
CLBc.write('SimpleDiffusionOfDromader_withIterations.xml')
f = open('SimpleDiffusionOfDromader_withIterations.xml', 'r')
XML(''.join(f.readlines()))
```

Out[19]:

```
<CLBConfig version="2.0" output="output/">
  <!--Created using CLBConfigWriter-->
  <Geometry predef="none" model="MRT" nx="640.0000000000000000" ny="480.0000000000000000"/>
  <Model>
    <Param name="Diffusivity_PHI" value="0.1666000000000000"/>
    <Param name="Init_PHI" value="-0.5000000000000000"/>
  </Model>
  <RunR>
    library('jpeg', lib="r_packages")

    myurl &lt;- "https://upload.wikimedia.org/wikipedia/commons/thumb/a/a5/M-18A_Dromader_CALM.jpg/
640px-M-18A_Dromader_CALM.jpg"
    z &lt;- tempfile()
    download.file(myurl,z,mode="wb", quiet=TRUE);
    pic &lt;- readJPEG(z);
    file.remove(z) # cleanup

    Solver$Fields$Init_PHI_External[] = t(pic[,,1]);
    Solver$Actions$InitFromExternalAction();
  </RunR>
  <HDF5/>
  <Solve Iterations="200">
    <HDF5 Iterations="10"/>
  </Solve>
</CLBConfig>
```

In [20]:

```
! tclb d2q9_reaction_diffusion_system_SimpleDiffusion SimpleDiffusionOfDromader_withIterations.xml > /dev/null
```

```
Hello allocator!
DONE
```

In [21]:

```
for i in range(0,200,50):
    plt.figure()
    f = h5py.File("./output/SimpleDiffusionOfDromader_withIterations_HDF5_%08d.h5"%i)
    plt.imshow(f["PHI"][0,:,:])
```