# CH_3D_adaptive_stepping_Method_3

March 10, 2022

## 1 Method 2 for time stepping

This proposed adaptive method of time-stepping suse a criterion related to a residual of the discrete nergy law. The method is as follows:
- step 1: compute $c^{n+1}$ and obtain: $ RE^{ n+1}=$\epsilon(\phi^{n+1}) - \epsilon(\phi^{n}) \overline{\triangle t^{n} + \int _\{\omega\}\}\vert\nabla\mu^{\{n+1 \frac{}{2\}\vert\{2\}dV\$}} t^{n+\frac{1}{2}} = (t^{n} + t^{n+1})/2$step 2: if $RE^{n+1} > resmax$ take $\triangle\{n+1\} = \triangle\{n\}/\theta\$andgotostep1step3 : if RE^{n+1} < res$

The term $\int_{\omega} \vert\nabla\mu^{n+\frac{1}{2}}\vert^{2} dV$ is computed as follows in Fourier space: - if istep > 1 :

- $\nabla\mu = \nabla[\frac{\delta f}{\delta c} - \kappa\nabla^{2}c]\$$
- FFT => $\nabla\mu = (jk).[\{\frac{\delta f}{\delta c}\}_{k} + \kappa.k^{2}.\{c\}_{k}]$
- $ $\nabla\mu\{n+\frac{1}{2}\} = (\nabla\mu^{\{n-1\}+\nabla\mu\{n\}})/2\$$**3 Import**

```
[ ]: import numpy as np
import matplotlib.pyplot as plt
import time
import warnings
warnings.simplefilter("ignore", np.ComplexWarning)
import math
import pyvista as pv
import pyfftw           # use for fast fourier transform
from scipy.fft import fft, ifft
from numba import jit  # use to speed up
import scipy.stats as st
import time
from scipy.sparse import csgraph
```

## 4 Functions

```
[ ]: def free_energ(c):
    A=1.0
    dfdc =A*(2.0*c*(1-c)**2 -2.0*c**2 *(1.0-c))
    return dfdc
```

```
#-----------------------------------------------------------------------------------------------------------

def fft_(a):
    """
    return a fft object from pyfftw library that will be use to compute fft
    """
    fft_object=pyfftw.builders.fftn(a,axes=(0,1,2), threads=12)
    return fft_object()
#-----------------------------------------------------------------------------------------------------------

def ifft_(a):
    """
    return a inverse fft object from pyfftw library that will be use to compute␣
 ↪inverse fft
    """
    ifft_object=pyfftw.builders.ifftn(a,axes=(0,1,2), threads=12)
    return ifft_object()
#-----------------------------------------------------------------------------------------------------------
#@jit(nopython=True)
def micro_ch_pre(Nx,Ny,Nz,c0):
    c=np.zeros((Nx,Ny,Nz))
    noise=0
    for i_x in range(Nx):
        for i_y in range(Ny):
            for i_z in range(Nz):
                c[i_x,i_y,i_z] =c0 + noise*(0.5-np.random.rand())
    return c

# Compute energy evolution
def calculate_energ(Nx,Ny,Nz,c,grad_coef):
    energ =0.0
    # ------------Nx------------------------------
    for i in range (Nx-1):
        ip = i + 1
        #--------------Ny-------------------------
        if (Ny>1):
            for j in range (Ny-1):
                jp = j + 1
                # ----------Nz--------------------
                if (Nz>1): # 3D
                    for l in range (Nz-1):
                        lp = l + 1
                        energ += c[i,j,l]**2  *(1.0-c[i,j,l])**2  +  0.
 ↪5*grad_coef*((c[ip,j,l]-c[i,j,l])**2 \
                            +(c[i,jp,l]-c[i,j,l])**2     +␣
 ↪(c[i,j,lp]-c[i,j,l])**2)
```

```
                else: # (Nz==1) 2D
                        energ += c[i,j,0]**2  *(1.0-c[i,j,0])**2  +  0.
 ↪5*grad_coef*((c[ip,j,0]-c[i,j,0])**2 \
                        +(c[i,jp,0]-c[i,j,0])**2)
        else : # (Ny==1):
            # ----------Nz--------------------
            if (Nz>1): # 2D
                 for l in range (Nz-1):
                     lp = l + 1
                     energ += c[i,0,l]**2  *(1.0-c[i,0,l])**2  +  0.
 ↪5*grad_coef*((c[ip,0,l]-c[i,0,l])**2 \
                     + (c[i,0,lp]-c[i,0,l])**2)
            else : # (Nz==1) 1D
                energ += c[i,0,0]**2  *(1.0-c[i,0,0])**2  +  0.
 ↪5*grad_coef*(c[ip,0,0]-c[i,0,0])**2

    return energ


#-----------------------------------------------------------------------------------------------
 ↪
def infinite_norm(M):
    # suppose that Nz=1
    m=M.shape[0]
    n=M.shape[1]
    array_row_sum=[]
    for i in range(m):
        row_sum=0
        for j in range(n):
            row_sum+=np.abs(M[i,j,0])
        array_row_sum.append(row_sum)
    inf_norm=np.max(array_row_sum)
    return inf_norm
# compute 2D laplacian
def laplacian_2D(c,i,j,l,dx,dy,dz):
    ip=i+1
    im=i-1
    jp=j+1
    jm=j-1
    if (im==-1):
        im=Nx-1
    if (ip==Nx):
        ip=0
    if (jm==-1):
        jm=Ny-1
    if (jp==Ny):
        jp=0
    hne=c[ip,j,0]
    hnw=c[im,j,0]
    hns=c[i,jm,0]
    hnn=c[i,jp,0]
    hnc=c[i,j,0]
    laplacian=(hnw+hne+hns+hnn-4*hnc)/(dx*dy) # uniform mesh
    return laplacian

# compute gradient
def gradient(c,i,j,l,dx,dy,dz):
    Nx=c.shape[0]
    Ny=c.shape[1]
    Nz=c.shape[2]
    im=i-1
    jm=j-1
    lm=l-1
    if (im==-1):
        im=Nx-1
    if (jm==-1):
        jm=Ny-1
    if (lm==-1):
        lm=Nz-1

    hw=c[im,j,l]
    hs=c[i,jm,l]
    hz=c[i,j,lm]
    hc=c[i,j,l]

    grad_mu_x=(hc-hw)/dx
    grad_mu_y=(hc-hs)/dx
    grad_mu_z=(hc-hz)/dx

    return grad_mu_x,grad_mu_y,grad_mu_z
```

## 5 remind

$\frac{\nabla c}{\delta t} = \nabla M . \nabla \mu$

where \$ $\nabla \mu = \nabla [\frac{\delta f}{\delta c} - \kappa \nabla^2 c]$\$

[ ]:
```
# compute residual at each time step (if istep >1), using Fourier space
def compute_residual_fft(array_energy,dtime, array_df_dc_k,array_ck,istep,k,␣
↪kappa):
    grad_mu_minus= (1j*k)*␣
↪(array_df_dc_k[istep-1]+kappa*(k**2)*array_ck[istep-1] )
    grad_mu_plus=  (1j*k)* (array_df_dc_k[istep]+kappa*(k**2)*array_ck[istep] )
    grad_mu_mean= (grad_mu_minus+grad_mu_plus)/2
    grad_mu_mean=np.real(ifft_(grad_mu_mean))
    # residual
    A=(array_energy[istep]-array_energy[istep-1])/dtime
    B=(grad_mu_mean**2).sum()
    RES=A+B
    return RES,A,B


# ---------------------------------------------------------------------
def compute_residual_fd(dtime, array_energy,array_dfdc,array_c, kappa,istep):
    sum_L2_square=0
    grad_mu=np.zeros((3,1))
    dfdc=array_dfdc[istep]
    dfdc_1=array_dfdc[istep-1]
    c=array_c[istep]
    c_1=array_c[istep-1]
    Nx=c.shape[0]
    Ny=c.shape[1]
    Nz=c.shape[2]
    mu=np.zeros((Nx,Ny,Nz))
    mu_p=np.zeros((Nx,Ny,Nz))
    mu_m=np.zeros((Nx,Ny,Nz))
    # compute \mu
    for i in range(Nx):
        for j in range(Ny):
            for l in range(Nz):
                mu_p[i,j,l]=dfdc[i,j,l]-kappa*laplacian_2D(c,i,j,l,dx_s,dy_s,dz_s)
                mu_m[i,j,l]=dfdc_1[i,j,l]-kappa*laplacian_2D(c_1,i,j,l,dx_s,dy_s,dz_s)
    mu=(mu_p+ mu_m)/2

    # compute Nabla(\mu) at each point grid and the associated L2 norm **2
    for i in range(Nx):
        for j in range(Ny):
            for l in range(Nz):
                grad_mu_x,grad_mu_y,grad_mu_z=gradient(mu,i,j,l,dx_s,dy_s,dz_s)
                grad_mu=np.array([grad_mu_x,grad_mu_y,grad_mu_z])
                sum_L2_square+=np.linalg.norm(grad_mu, ord=2)**2
    # A: energy derivative
    A=(array_energy[istep]-array_energy[istep-1])/dtime
    B=sum_L2_square
    RES=A+B

    return RES, A, B
```

```
[ ]: @jit(nopython=True)
     def prepar_fft(Nx,dx,Ny,dy,Nz,dz,opt):
         """
         Compute spatial frequence term and derivative
         """
         # variable initialisation
         lin_x=np.zeros(Nx)
         lin_y=np.zeros(Ny)
         lin_z=np.zeros(Nz)

         k=np.zeros((3,Nx,Ny,Nz))
         k2=np.zeros((Nx,Ny,Nz))
         k4=np.zeros((Nx,Ny,Nz))

         """
         # Method 1 to compute k  (3D)
         if (Nx % 2) == 1 : # = number odd if remainers is one
             lin_x[:int((Nx-1)/2.0+1)]=np.arange(0, int((Nx-1)/2.0+1), 1)*2*np.pi/
       ↪(Nx*dx)
             lin_x[int((Nx-1)/2.0+1):]=np.arange(int(-(Nx+1)/2.0 +1), 0, 1)*2*np.pi/
       ↪(Nx*dx)
         if (Ny % 2) == 1 :
             lin_y[:int((Ny-1)/2.0+1)]=np.arange(0, int((Ny-1)/2.0+1), 1)*2*np.pi/
       ↪(Ny*dy)
             lin_y[int((Ny-1)/2.0+1):]=np.arange(int(-(Ny+1)/2.0 +1), 0, 1)*2*np.pi/
       ↪(Ny*dy)
         if (Nz % 2) == 1 :
             lin_z[:int((Nz-1)/2.0+1)]=np.arange(0, int((Nz-1)/2.0+1), 1)*2*np.pi/
       ↪(Nz*dz)
             lin_z[int((Nz-1)/2.0+1):]=np.arange(int(-(Nz+1)/2.0 +1), 0, 1)*2*np.pi/
       ↪(Nz*dz)
         if (Nx % 2) == 0 : # = number even if remainers is zero
             lin_x[0:int(Nx/2.0)]=np.arange(0, int(Nx/2.0), 1)*2*np.pi/(Nx*dx)
             lin_x[int(Nx/2.0 + 1):]=np.arange(int(-Nx/2.0 + 1), 0, 1)*2*np.pi/
       ↪(Nx*dx)
         if (Ny % 2) == 0 :
             lin_y[0:int(Ny/2.0)]=np.arange(0, int(Ny/2.0), 1)*2*np.pi/(Ny*dy)
             lin_y[int(Ny/2.0 + 1):]=np.arange(int(-Ny/2.0 + 1), 0, 1)*2*np.pi/
       ↪(Ny*dy)
         if (Nz % 2) == 0 :
             lin_z[0:int(Nz/2.0)]=np.arange(0, int(Nz/2.0), 1)*2*np.pi/(Nz*dz)
             lin_z[int(Nz/2.0 + 1):]=np.arange(int(-Nz/2.0 + 1), 0, 1)*2*np.pi/
       ↪(Nz*dz)
         # grid
         for i in range(Nx):
             for j in range(Ny):
```

```
            for l in range(Nz):
                k[0,i,j,l]= lin_x[i]
                k[1,i,j,l]= lin_y[j]
                k[2,i,j,l]= lin_z[l]
     """
    # Method 2 to compute k
    Lx=Nx*dx
    x=np.linspace(-0.5*Lx+dx,0.5*Lx,Nx)

    Ly=Ny*dy
    y=np.linspace(-0.5*Ly+dy,0.5*Ly,Ny)

    Lz=Nz*dz
    z=np.linspace(-0.5*Lz+dz,0.5*Lz,Nz)


    xx=2*np.pi/Lx*np.concatenate((np.arange(0,Nx/2+1), np.arange(-Nx/
 ↪2+1,0)),axis=0)
    yy=2*np.pi/Ly*np.concatenate((np.arange(0,Ny/2+1), np.arange(-Ny/
 ↪2+1,0)),axis=0)
    zz=2*np.pi/Lz*np.concatenate((np.arange(0,Nz/2+1), np.arange(-Nz/
 ↪2+1,0)),axis=0)

    for i in range(Nx):
        for j in range(Ny):
            for l in range(Nz):
                k[0,i,j,l]= xx[i]
                k[1,i,j,l]= yy[j]
                k[2,i,j,l]= zz[l]

    k2=k[0]**2+k[1]**2+k[2]**2

    k4=k2**2

    return k,k2,k4,x,y,z
```

[ ]:
```
# plot micro
def plot_micro(c,opt,ttime):
    # 1D case
    if (opt=='1D'):
        plt.plot(c[:, :, 0])
        plt.xlabel('x')
        plt.ylabel('concentration')
        plt.title('initial concentration')

    else:
        # 2D or 3D cases--------------------------------------------------
        import sys
        grid  = pv.UniformGrid()
        grid.spacing=np.array([dx,dx,dx])*1E9
        grid.dimensions = np.array([Nx,Ny,Nz])#+1
        grid.point_arrays[r'c'] = np.transpose(np.resize(c,[Nx,Ny,Nz])).
↪flatten()


        # Set a custom position and size
        sargs = dict(fmt="%.1f", color='black')

        p = pv.Plotter()
        pv.set_plot_theme("ParaView")
        p.set_background("white")
        p.add_mesh(grid,show_scalar_bar=False,label='title')
        p.add_scalar_bar('Concentration', color='black',label_font_size=12,␣
↪width=0.1, height=0.7, position_x=1,position_y=0.16,vertical= True,␣
↪interactive=False)
        if (ttime==0):
            p.add_text('Initial Microstructure␣
↪',position='upper_edge',color='black',font= 'times',font_size=12)
        else:
            p.add_text('Microstructure at dimensionless time '+str('{0:.2f}'.
↪format(ttime) ),color='black',font= 'times',font_size=12)

        p.show_bounds(all_edges=True,font_size=24,bold=True, xlabel="X␣
↪[nm]",ylabel="Y [nm]",zlabel="Z [nm]",color='black')
        #p.add_title('Microstructure at dimensionless time '+str('{0:.2f}'.
↪format(ttime) ))
        p.camera_position = [1, 1, 1]
        if (opt=='2D'):
            if (ttime==0):
                p.show(screenshot='Initial microstructure.png',cpos="xy") #␣
↪cpos="xy" in case of 2D (Nz=1)
            else:
                p.show(screenshot='Microstructure at dimensionless time␣
↪'+str('{0:.2f}'.format(ttime) )+ '.png',cpos="xy") #
        elif (opt=='3D'):
            if (ttime==0):
                p.show(screenshot='Initial microstructure.png') # cpos="xy" in␣
↪case of 2D (Nz=1)
            else:
                p.show(screenshot='Microstructure at dimensionless time␣
↪'+str('{0:.2f}'.format(ttime) )+ '.png') #

        p.close()
```

[ ]:
```
def plot_micro_mayavi(c,ttime):
    from mayavi import mlab
    #mlab.clf()
    X, Y, Z = np.meshgrid(x,y,z)
    values = c
    fig = mlab.figure(figure=None, fgcolor=(0, 0, 0), bgcolor=(1,1,1),␣
↪engine=None, size=(500, 500))
    mlab.contour3d(values,colormap='hot')
    mlab.axes(xlabel='Z', ylabel='Y', zlabel='X')
    mlab.colorbar(title='Concentration',orientation='vertical', nb_labels=5)
    if (ttime==0):
        name ='Initial microstructure'
    else:
        name='Microstructure at dimensionless time '+str('{0:.2f}'.
↪format(ttime))
    mlab.title(name)
    #mlab.text(6, -2.5, '', z=-4, width=0.14)
    mlab.orientation_axes([0,0.5,0.5 ])
    mlab.savefig(name+'.png')
    mlab.show(stop=True)
```

[ ]:
```
def micro_numba(c0,r,ox,oy,oz,Nx,Ny,Nz):
    """
    Microstructure initialization:
    inputs: the position and radius of sphere that represents the precipitate␣
↪of
    composition X0_pre for a matrix of compositon X0_mat
    outpus: value of the variable eta and X_mat for a given grid
    """

    c   = np.zeros((Nx,Ny,Nz))
    x      = np.arange(Nx)*dx
    y      = np.arange(Ny)*dy
    z      = np.arange(Nz)*dz

    for i_x in range(Nx):
        for i_cir in range(len(r)):
            norm=np.sqrt( (ox[i_cir]-x[i_x])**2)

            if norm<=r[i_cir]:
                c[i_x][0][0]  =1

    return c
```

## 6 Input Data

[ ]:
```
Nx=64 ; Ny=64; Nz=1
c0=0.4  # initial concentration
# spacing
dx=10e-10 # [m]
dy=10e-10 # [m]
dz=10e-10 # [m]

# convert into adimensional grid
dx_s=dx/dx
dy_s=dy/dy
dz_s=dz/dz

# get x,y,z (to plot microstructure)
k,k2,k4,x,y,z=prepar_fft(Nx,dx_s,Ny,dy_s,Nz,dz_s,opt="3d")
```

[ ]:
```
# input parameters are defined in the form of array for sensitivty analysis␣
 ↪(loop on each paramter )
array_dt_init=[0.1]      #  normalized time [-]
array_resmin=[0.1]
array_resmax=[30]  #np.arange(2,12,2)
array_theta=[1.1 ]
```

[ ]:
```
mobility =1.0
coefA = 1.0
grad_coef=0.5



"""
#uncomment if necessary
# For comparison purposes: load the same initial microtructure as Matlab
# retrieving data from file.
loaded_arr = np.loadtxt("3D_micro_init.txt")

# This loadedArr is a 2D array, therefore
# we need to convert it to the original
# array shape.reshaping to get original
# matrice with original shape.
load_original_arr = loaded_arr.reshape(
loaded_arr.shape[0], loaded_arr.shape[1] // c.shape[2], c.shape[2])

c=load_original_arr
"""
```

[ ]:
```
'\n#uncomment if necessary\n# For comparison purposes: load the same initial
microtructure as Matlab\n# retrieving data from file.\nloaded_arr =
np.loadtxt("3D_micro_init.txt")\n\n# This loadedArr is a 2D array, therefore\n#
```

```
we need to convert it to the original\n# array shape.reshaping to get
original\n# matrice with original shape.\nload_original_arr =
loaded_arr.reshape(\nloaded_arr.shape[0], loaded_arr.shape[1] // c.shape[2],
c.shape[2])\n\nc=load_original_arr\n'
```

## 7 plot initial microstructure

### 7.1 plot using Mayavi

### 7.2 Geomtry used in case of coarseing growth

[ ]:
```
# to use a different microstructure (precipitates) in case of study of the␣
↪coarsening of precipitates
ox  = np.array([16,30,45,65,81,91])*1e-9
oy= np.array([20,20,20,20,20,20])*1e-9
oz = np.array([0,0,0,0,0,0])*1e-9
r=  np.array([6,4,4,6,4,4])*1e-9
```

[ ]:
```
"""
c=micro_numba(c,r,ox,oy,oz,Nx,Ny,Nz)
plt.plot(c[:,0,0])
c_0=c
"""
```

[ ]:
```
'\nc=micro_numba(c,r,ox,oy,oz,Nx,Ny,Nz)\nplt.plot(c[:,0,0])\nc_0=c\n'
```

### 7.3 Geomtry for spinodal decomposition

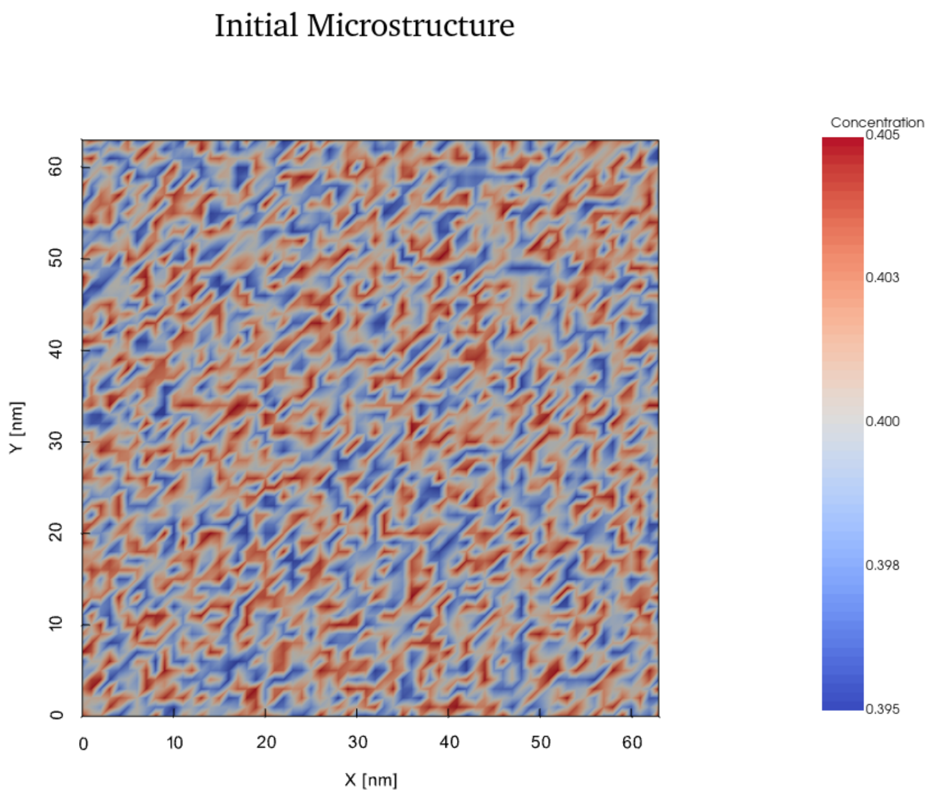
[ ]:
```
#initialize microstructure
c0=0.4  # initial concentration
c= micro_ch_pre(Nx,Ny,Nz,c0)
c0_save=c
```

[ ]:
```
original_c = np.loadtxt("c0_save.txt").reshape(Nx, Ny)
c[:, :, 0]=original_c
```

[ ]:
```
ttime=0
#plot_micro_mayavi(c,ttime)
# nb: in interactive mode, close Mayavi plot before stop interaction
```

### 7.4 plot using Pyvista

[ ]:
```
ttime=0
plot_micro(c,"2D",ttime)
```

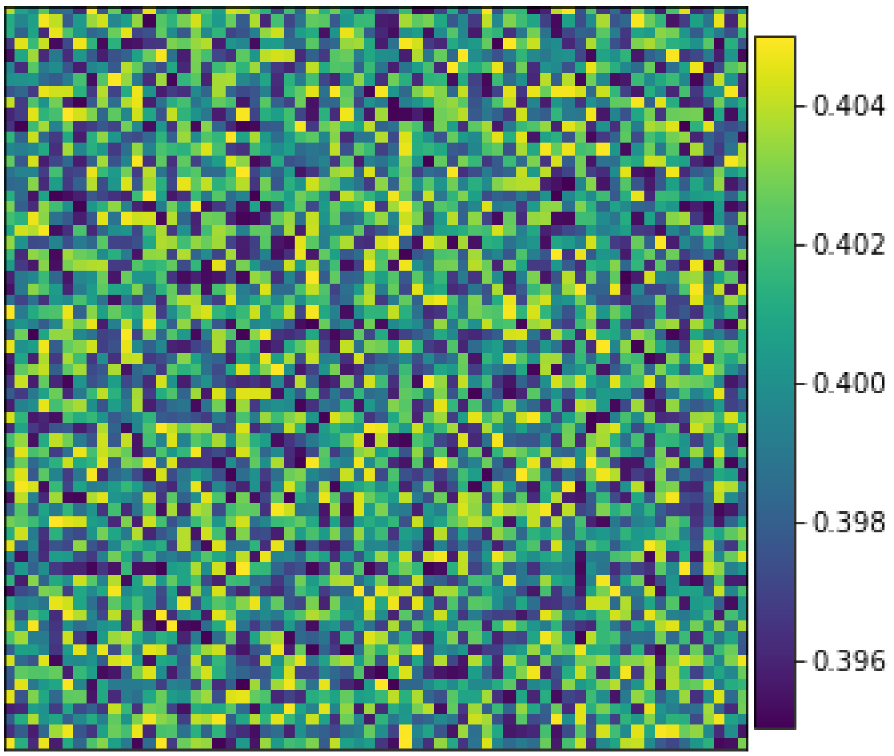


-

[ ]:
```
from pymks import (
    generate_checkerboard,
    plot_microstructures,
    PrimitiveTransformer,
    TwoPointCorrelation
)
```

[ ]:
```
plot_microstructures(c)
```

```
C:\Users\seifa\miniconda3\lib\site-packages\pymks\fmks\plot.py:12:
MatplotlibDeprecationWarning:
The colNum attribute was deprecated in Matplotlib 3.2 and will be removed two
minor releases later. Use ax.get_subplotspec().colspan.start instead.
  axis.set_title(titles[axis.colNum])
C:\Users\seifa\miniconda3\lib\site-packages\pymks\fmks\plot.py:14:
MatplotlibDeprecationWarning:
The colNum attribute was deprecated in Matplotlib 3.2 and will be removed two
minor releases later. Use ax.get_subplotspec().colspan.start instead.
  arrs[axis.colNum],
```



## 8 Loop on time steps

[ ]:
```
f = open("log.txt", "w") # to print residual evolution and follow iterations
f_dtime = open("dtime.txt", "w") # to print times steps during simulation
# loop to change time step (dtime) and compute associated energy dissipation␣
 ↪for CH equation (at each time step)
for index in range(len(array_resmin)):     # to make possible the change of ␣
 ↪simulation parameters (resmin, resmax or theta) if needed,=> for index in   ␣
 ↪
                                        # range(len(array_resmax))
    # start simulation
    f.write('start simulation\n')

    t_start = time.time()

    theta=array_theta[0]
    resmin=array_resmin[index]  # the parameter to vary in sensitivity analysis
    resmax=array_resmax[0]
    dt_init=array_dt_init[0]

    #c=c0_save  # take the same microstructure
```

```
# time step and constant values
ttime=0 # for each simulation
dtime=dt_init
#------------------
# time steps and print parameters
Nt=10 # trial
nstep=10000 #int(round(Nt/dtime)) #
endstep=nstep  # stop criteria
nprint=100; # step to print
# set fourier coefficient
# compute the spatial frequency term from fft
k,k2,k4,x,y,z=prepar_fft(Nx,dx_s,Ny,dy_s,Nz,dz_s,opt="3d")



array_time=np.zeros(nstep)  # to save time steps
array_dtime=np.zeros(nstep)

array_c=np.zeros((nstep,Nx, Ny, Nz)) # to save concentration values for␣
↪each time steps
array_c_k=np.zeros((nstep,Nx, Ny, Nz)) # to save concentration value in␣
↪Fourier space for each time step; needed to compute residual
array_df_dc_k=np.zeros((nstep,Nx, Ny, Nz))# to save energy derivative␣
↪values in Fourier space, for each time step; needed to compute residual
array_df_dc=np.zeros((nstep,Nx, Ny, Nz))  # to save energy derivative␣
↪values in real space, for each time step; needed to compute    residual
dfdc=np.zeros((Nx,Ny,Nz))

array_energy=np.zeros(nstep)  # to save energy value at each time step
array_residus=np.zeros(nstep)  # to store residual and its associated terms
array_residus_fd=np.zeros(nstep) # computed by finite difference
array_energy_deriv=np.zeros(nstep)
array_energy_deriv_fd=np.zeros(nstep)
array_energy_potentiel_grad=np.zeros(nstep)
array_energy_potentiel_grad_fd=np.zeros(nstep)
array_residual_deriv=np.zeros(nstep)



residual_deriv=1  # default valuefor the stop criteria
flag=0   # to stop simulation

t_start = time.time() # to compute CPU for each simulation
endstep=nstep
flag=0
#--------------------------------------------------
for istep in range(nstep):
    #---------------------------------------------------
        f.write('istep '+ str(istep)+'\n')

        if (flag==1):
            print('stop criteria reached')
            break # break the for loop


        iter=1  # iterations made when res > resmax  (see adaptive time␣
↪stepping lines below)
        while True:
                if iter >1:
                    f.write('istep '+ str(istep) + ' is redone : iteration nř '␣
↪+ str(iter) +'\n')
                # compute free energy
                dfdc=free_energ(c)

                dfdck=fft_(dfdc)
                ck=fft_(c)

                # Time integration
                numer=dtime*mobility*k2*dfdck
                denom = 1.0 + dtime*coefA*mobility*grad_coef*k4
                ck =(ck-numer)/denom

                c=np.real(ifft_(ck))

                # for small deviations
                c[np.where(c >= 0.9999)]= 0.9999
                c[np.where(c <= 0.00001)]=0.00001

                # store computed variables
                energy=calculate_energ(Nx,Ny,Nz,c,grad_coef)
                if energy<50: #(ttime>268):
                    print('break simulation')
                    endstep=istep
                    flag=1
                    break # break the while loop

                array_energy[istep]=energy
                array_df_dc[istep]=dfdc
                array_df_dc_k[istep]=dfdck
                array_c[istep]=c
                array_c_k[istep]=ck
                ttime = ttime + dtime  # ttime is the cumulative simulation␣
↪time
```

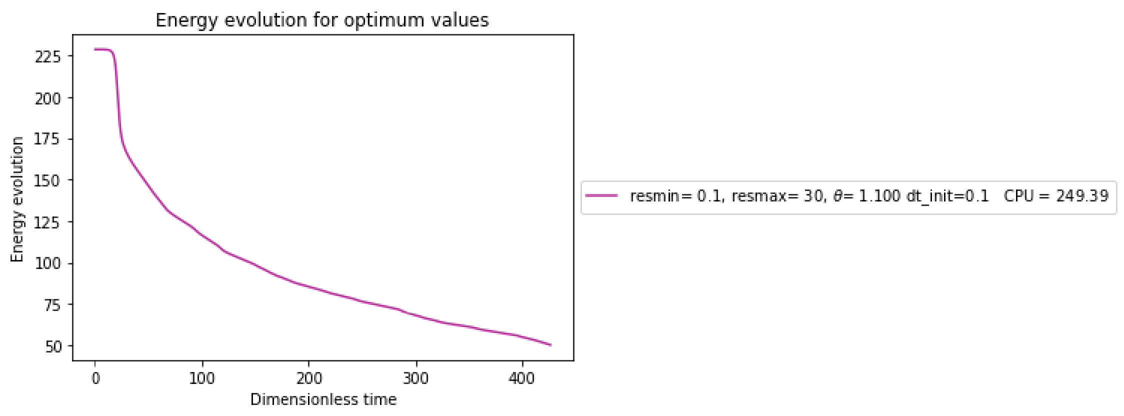
```
                array_dtime[istep]=dtime # to store dtime values => plot␣
↪evolution
                array_time[istep]=ttime

               ␣
↪#--------------------------------------------------------------------------------------------------
↪
                # -------------------------adaptive time stepping␣
↪--------------------------------------------
               ␣
↪#--------------------------------------------------------------------------------------------------
↪
                if (istep==0):
                    break # break the while loop (nothing to do)
                if (istep>0):
                   ␣
↪#RE,energy_deriv,potentiel_grad=compute_residual_fft(array_energy,array_dtime[istep-1],␣
↪array_df_dc_k,array_c_k,istep,k, grad_coef) #  Fourier transform
                   ␣
↪RE_fd,energy_deriv_fd,potentiel_grad_fd=compute_residual_fd(dtime,array_energy,array_df_dc,
↪grad_coef,istep)
                    #array_residus[istep]=RE
                    #array_energy_deriv[istep]=energy_deriv
                    #array_energy_potentiel_grad[istep]=potentiel_grad
                    array_energy_deriv_fd[istep]=energy_deriv_fd
                    array_energy_potentiel_grad_fd[istep]=potentiel_grad_fd
                    array_residus_fd[istep]=RE_fd
                    RE=RE_fd
                    potentiel_grad=potentiel_grad_fd
                    energy_deriv=energy_deriv_fd

                    # criteria based on derivative of the energy residual
                   ␣
↪residual_deriv=(array_residus[istep]-array_residus[istep-1])/
↪array_dtime[istep]
                    array_residual_deriv[istep]=residual_deriv

                    # stop criteria ==> break the while loop ==> break the main␣
↪loop

                    #print(residual_deriv_mean)
                    """
                    if (np.abs(np.sqrt(potentiel_grad_fd))<0.01) :
                        print(istep,np.sqrt(potentiel_grad_fd))
                        flag=1
                        endstep=istep
```

```
                            break # break the while loop
                        """

                       ␣
↪#RE,A,B=compute_residual_FD(array_energy,array_dtime[istep-1],␣
↪array_df_dc,array_c,istep, grad_coef) # Finite difference

                        if (RE>resmax):
                            f.write('RE>resmax\n')
                            dtime=dtime/theta
                            f_dtime.write('iteration '+ str(iter)+'        ')
                            iter +=1
                            # compute energy derivative with respect to time
                           ␣
↪energy_deriv=(array_energy[istep]-array_energy[istep-1])/array_dtime[istep]

                            if (iter>10):
                                        energy_derivative=(np.
↪array(array_energy)[istep]-np.array(array_energy)[istep-1])/dtime
                                        alpha=array_theta[0]
                                        dt_min=array_dt_init[0]
                                        dt_max=10*dt_min
                                        dtime=np.max([dt_min,dt_max/np.
↪sqrt(1+alpha*(energy_derivative**2))])
                                        f.write ('Residual = '+ str('{0:.2f}'.
↪format(RE)) + ','+ ' A= ' + str('{0:.2f}'.format(energy_deriv))+ ','+ ' B=␣
↪'+str('{0:.2f}'.format(potentiel_grad))+ ',' + 'Energy=                    ␣
↪   '+ str('{0:.2f}'.format(energy) )+'\n')
                                        break  # break the while loop => go to next␣
↪"for loop" iteration with a new dtime  c and RE


                            f.write ('Residual = '+ str('{0:.2f}'.format(RE)) +␣
↪','+ ' A= ' + str('{0:.2f}'.format(energy_deriv))+ ','+ ' B= '+str('{0:.2f}'.
↪format(potentiel_grad))+ ',' + 'Energy=                  '+ str('{0:.
↪2f}'.format(energy) )+'\n')
                            #f.write('restarting the actual istep '+ str(istep)+␣
↪'\n')
                            continue   # continue the while loop =>  restart the␣
↪"for loop" actual step with a new dtime=> recompute c and RE

                        elif (RE<resmax) and (RE>resmin) :
                            f.write(' We get  (resmin<RE<resmax) ;  go to step␣
↪'+str(istep+1)+'\n')
```

```
                        f.write ('Residual = '+ str('{0:.2f}'.format(RE)) +␣
↪','+ ' A= ' + str('{0:.2f}'.format(energy_deriv))+ ','+ ' B= '+str('{0:.2f}'.
↪format(potentiel_grad))+ ',' + 'Energy=                         '+ str('{0:.
↪2f}'.format(energy) )+'\n'+'\n')

                        break # break the while loop => go to next "for loop"␣
↪iteration with a new dtime

                    else: # (RE<resmin):
                        energy_derivative=(np.array(array_energy)[istep]-np.
↪array(array_energy)[istep-1])/dtime
                        alpha=array_theta[0]
                        dt_min=array_dt_init[0]
                        dt_max=10*dt_min
                        dtime=np.max([dt_min,dt_max/np.
↪sqrt(1+alpha*(energy_derivative**2))])
                        #dtime=dtime*theta
                        f.write(' We get  (RE < resmin);  go to step with new␣
↪time step: '+str('{0:.2f}'.format(dtime))+'\n')
                        f.write('Residual = '+ str('{0:.2f}'.format(RE)) + ','+␣
↪' A= ' + str('{0:.2f}'.format(energy_deriv))+ ','+ ' B= '+str('{0:.2f}'.
↪format(potentiel_grad))+ ',' + 'Energy=                         '+ str('{0:.
↪2f}'.format(energy) )+'\n'+'\n')

                        break # break the while loop => go to next "for loop"␣
↪iteration with a new dtime

      ␣
↪#------------------------------------------------------------------------------------------------
↪
       #-----------------------    end adaptive time stepping        ␣
↪---------------------------------
      ␣
↪#------------------------------------------------------------------------------------------------
↪
       f_dtime.write('step '+ str(istep)+ '     dtime= ' +str('{0:.2f}'.
↪format(dtime)) +'\n')
       #-----------------------------------------------------------------------␣
↪-----------------------
       """
       if (math.fmod(int(energy),20)==0):
           plot_micro(c,"2D",ttime)
       """
       """
       if (math.fmod(istep,nprint)==0) and (istep>0):  # to plot micrstructure␣
↪evolution
```

```
            y=1 #print('')  # just to say him (do nothing)
            #plot_micro(c,"2D",ttime)
            #plot_micro_mayavi(c,"3D,ttime)


            # plot actual microstructure

            import matplotlib.pylab as plt1
            # 1D case
            rgb = np.random.rand(3,)
            if (istep==100):
                plt1.plot(c0_save[:, :, 0],  color ='r', label='initial␣
↪concentration') # keep this indent
            plt1.plot(c[:, :, 0],  color =rgb, label='concentration at␣
↪dimensionless time: '+str('{0:.2f}'.format(ttime)))
            plt1.legend(loc='center left', bbox_to_anchor=(1, 0.5))
            plt1.xlabel('x')
            plt1.ylabel('Concentration')
    plt1.plot(c0_save[:, :, 0],  color ='r', label='initial concentration') #␣
↪keep this indent
    plt1.show()
    """

    #-----------------------------------------------------------------------␣
↪-----------------------

  ␣
↪#-------------------------------------------------------------------------------------
  ␣
↪#-------------------------------------------------------------------------------------
    #--------------------------   Post processing  ␣
↪-------------------------------------
  ␣
↪#-------------------------------------------------------------------------------------
  ␣
↪#-------------------------------------------------------------------------------------␣
↪
    # plot energy evolution during spinodal deomposition
  ␣
↪#-------------------------------------------------------------------------------------␣
↪
    energ = np.array(array_energy)
    array_time = np.array(array_time)
    rgb = np.random.rand(3,)
    plt.plot(array_time[:endstep],energ[:endstep],label = 'resmin=␣
↪'+str(resmin)+ ", "+ 'resmax= '+str(resmax) + ", "+r'$\theta$= '+str('{0:.
↪3f}'.format(array_theta[0]))+' dt_init='+str(dt_init) +"   CPU = "+ str('{0:.
↪2f}'.format(time.time()-t_start)),color =rgb)
    plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
    plt.xlabel('Dimensionless time')
    plt.ylabel('Energy evolution')
    #plt.show()
    name='Energy evolution ' + ".png"
    #plt.savefig(name)
    plt.title('Energy evolution for optimum values')
    #plt.show()
   ␣
↪#-------------------------------------------------------------------------------␣
↪
    #plot solution evolution in space for (y=x)
   ␣
↪#-------------------------------------------------------------------------------␣
↪
    """
    #transform array_time (time steps sauvegarded) from list to array
    array_time=np.array(array_time)

    # return index of time of plot (here the end of simulation is chossen)
    time_plot=int(np.array(np.where(abs(array_time - ttime)<0.001)))
    print(time_plot)
    #solution at the choosen instant
    sol=array_c[time_plot]
    # extract diagonal of the matrix "sol"
    x_y_solution=np.diag(sol)
    plt.xlabel('y=x')
    plt.ylabel('Concentration at the end of simulation')
    rgb = np.random.rand(3,)
    plt.plot(x_y_solution,label = "dt="+str(dtime),color =rgb)
    plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
    plt.show()
    """
   ␣
↪#-------------------------------------------------------------------------------␣
↪
    # plot evolution of infinite norm versus time
   ␣
↪#-------------------------------------------------------------------------------
    """
    infinite_norm=[]
    array_c=np.array(array_c)
    for i in range (1,nstep):
        #compute infinite norm
        c_n=array_c[i]
        c_n__1=array_c[i-1]
        infinite_norm.append(np.max(c_n-c_n__1))
    infinite_norm=np.array( infinite_norm)
    rgb = np.random.rand(3,)
    plt.plot(array_time[1:],infinite_norm,label = 'resmin= '+str(resmax)+ ", "+␣
 ↪'resmax= '+str(resmin) )
    plt.xlabel('t$^{n}$')
    plt.ylabel('||c$^{n}$ - c$^{n-1}$||$_{inf}$')
    plt.title('Infinite norm evolution during spinodal decompostion - Method 1␣
 ↪for time stepping')
    plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
    plt.show()
    """




print("simulation time : %s seconds ---" % (time.time() - t_start))
f.close()
f_dtime.close()
```

```
break simulation
stop criteria reached
simulation time : 249.4055118560791 seconds ---
```

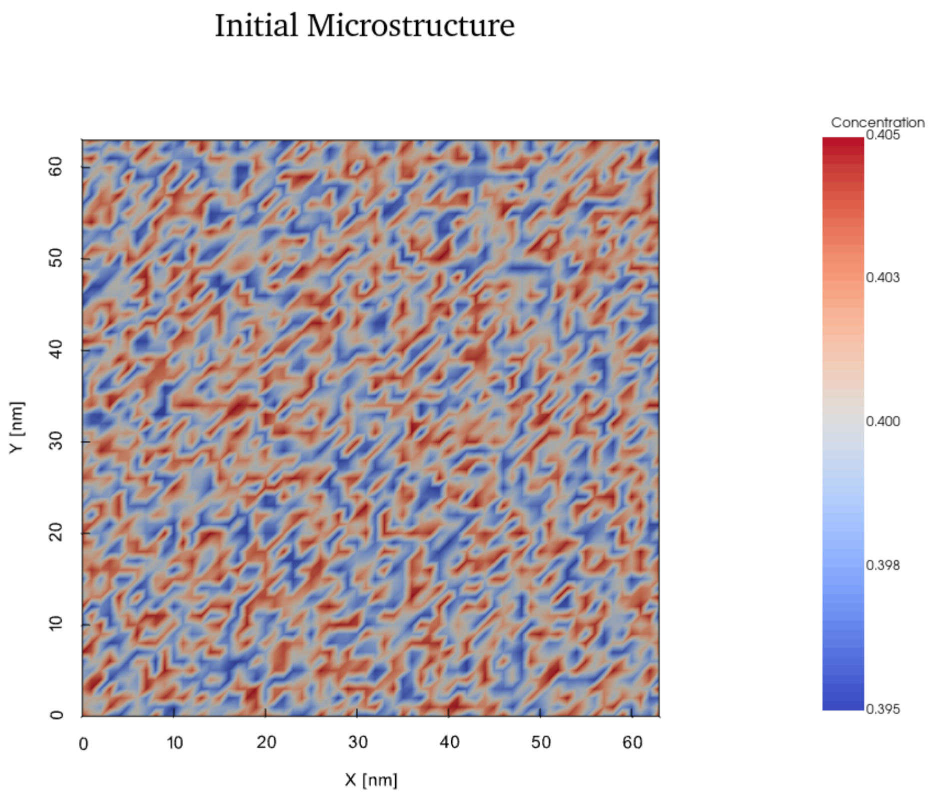


## 9 Postprocess

[ ]:
```
energ[endstep-1]
```

[ ]:
```
73.81126499496685
```

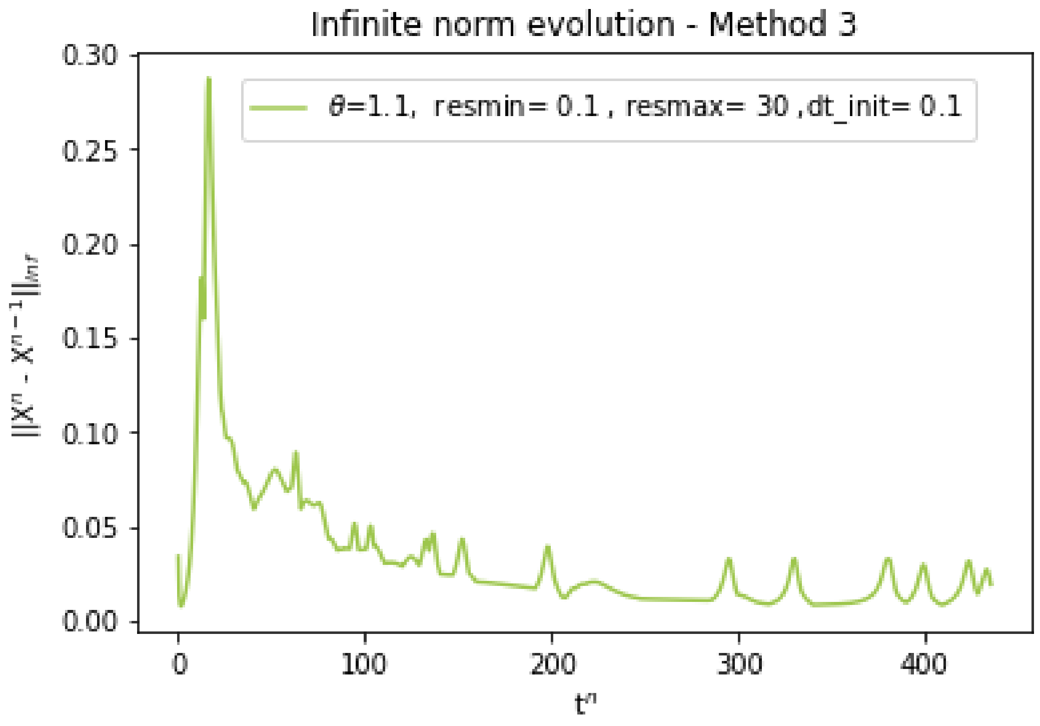
[ ]:
```
plot_micro(c,'2D',ttime)
```



### 9.1 infinity norm

[ ]:
```
array_infinite_norm=[]
array_c=np.array(array_c)
for i in range (1,endstep):
    #compute infinite norm
    c_n=np.array(array_c[i])
    c_n__1=np.array(array_c[i-1])
    array_infinite_norm.append(infinite_norm(c_n-c_n__1))
array_infinite_norm=np.array(array_infinite_norm)
rgb = np.random.rand(3,)
```

```
plt.plot(array_time[1:endstep],array_infinite_norm, label=r'$\theta$='␣
↪+str(theta) +  ", " + " resmin= "+str(resmin)+ " ," + " resmax=␣
↪"+str(resmax)+" ," + "dt_init= " + str(dt_init) ,color      =rgb)
plt.xlabel('t$^{n}$')
plt.ylabel('||X$^{n}$ - X$^{n-1}$||$_{inf}$')
plt.title('Infinite norm evolution - Method 3')
plt.legend(loc='center left', bbox_to_anchor=(0.1, 0.9))
plt.show()
```



## 9.2 save energy

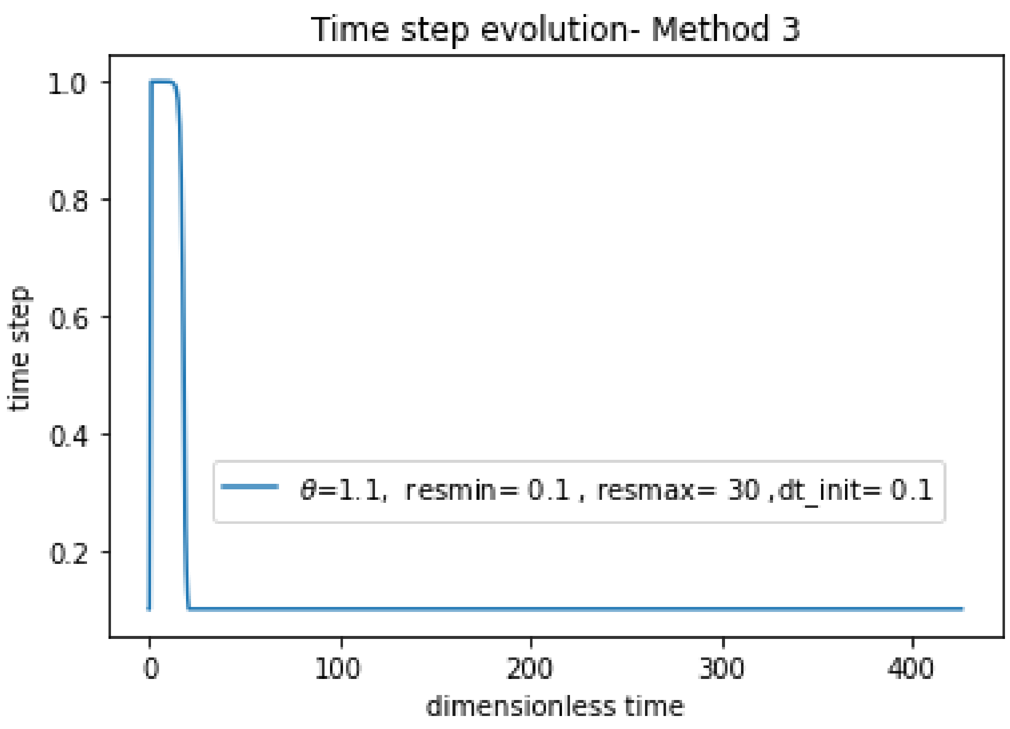
[ ]:
```
# save energy_vs_time in txt file : for comparative purposes
np.savetxt('energy_method_3.txt',energ[:endstep], fmt=' %.2f')
np.savetxt('time_method_3.txt',array_time[:endstep], fmt=' %.2f')

#energ_fd =np.loadtxt("energy_fd.txt",  delimiter=" ", unpack=False)
```

## 9.3 dtime evolution

[ ]:
```
# plot dtime versus time evolution
```

```
plt.plot(array_time[:endstep],array_dtime[:endstep],label=r'$\theta$='␣
↪+str(theta) +  ", " + " resmin= "+str(resmin)+ " ," + " resmax=␣
↪"+str(resmax)+" ," + "dt_init= " + str(dt_init))
plt.legend(loc='center left', bbox_to_anchor=(0.1, 0.25))
plt.xlabel('dimensionless time')
plt.ylabel('time step')
plt.title('Time step evolution- Method 3')
```

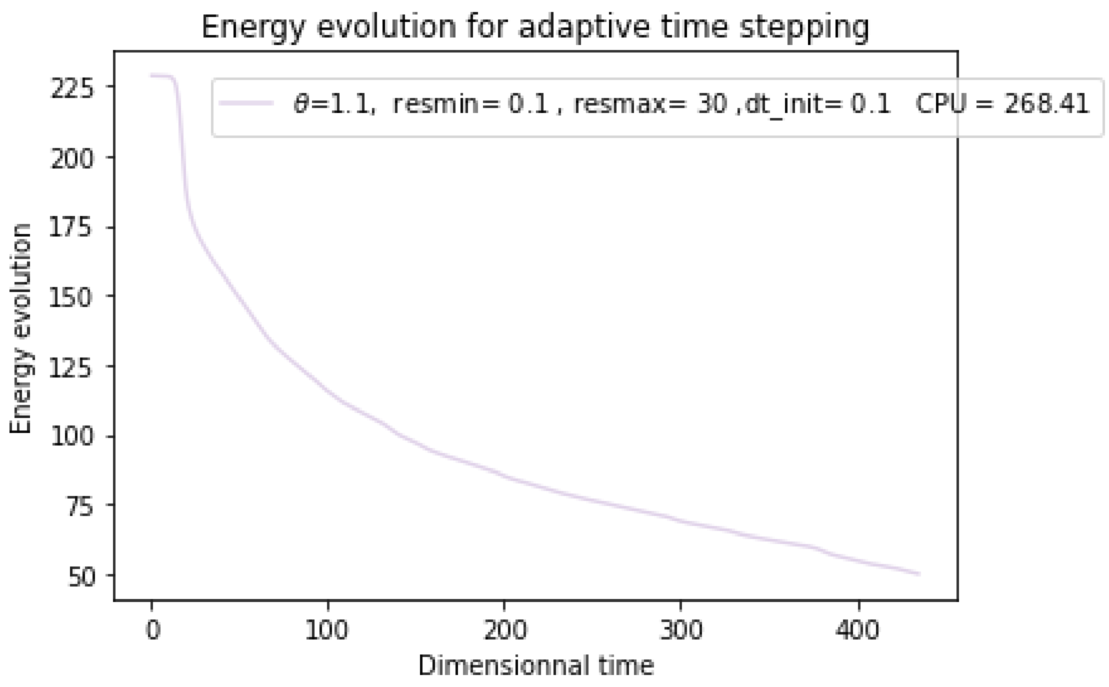
[ ]:
```
Text(0.5, 1.0, 'Time step evolution- Method 3')
```



### 9.4 energy evolution

[ ]:
```
# Energy evolution
energ = np.array(array_energy)
plt.plot(array_time[:endstep],energ[:endstep],label=r'$\theta$=' +str(theta) + ␣
↪", " + " resmin= "+str(resmin)+ " ," + " resmax= "+str(resmax)+" ," +␣
↪"dt_init= " + str(dt_init)+"    CPU = "+ str(268.41),color =rgb)
plt.legend(loc='center left', bbox_to_anchor=(0.1, 0.9))
plt.title('Energy evolution for adaptive time stepping')
plt.xlabel('Dimensionnal time')
plt.ylabel('Energy evolution')
```

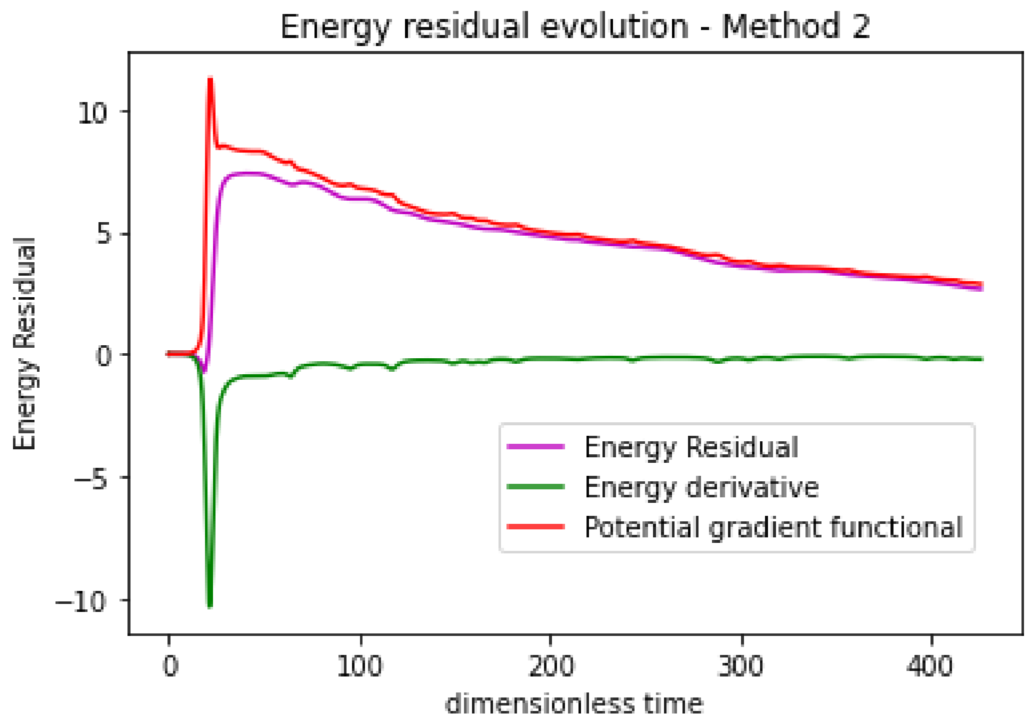
[ ]:
```
Text(0, 0.5, 'Energy evolution')
```



## 9.5 Residual evolution

[ ]:
```
# plot dtime versus time evolution
#plt.plot(array_time,array_residus, label='Residus (FFT)',c='b')
plt.plot(array_time[:endstep],array_residus_fd[:endstep], label='Energy␣
 ↪Residual',c='m')
#plt.plot(array_time,array_energy_deriv, label='Energy derivative',c='g')
plt.plot(array_time[:endstep],array_energy_deriv_fd[:endstep], label='Energy␣
 ↪derivative',c='g')
#plt.plot(array_time,array_energy_potentiel_grad, label='Potentioel gradient␣
 ↪functional',c='r')
plt.plot(array_time[:endstep],array_energy_potentiel_grad_fd[:endstep],␣
 ↪label='Potential gradient functional',c='r')
plt.legend(loc='center left', bbox_to_anchor=(0.4, 0.25))
plt.xlabel('dimensionless time')
plt.ylabel(' Energy Residual')
plt.title('Energy residual evolution - Method 2')
```

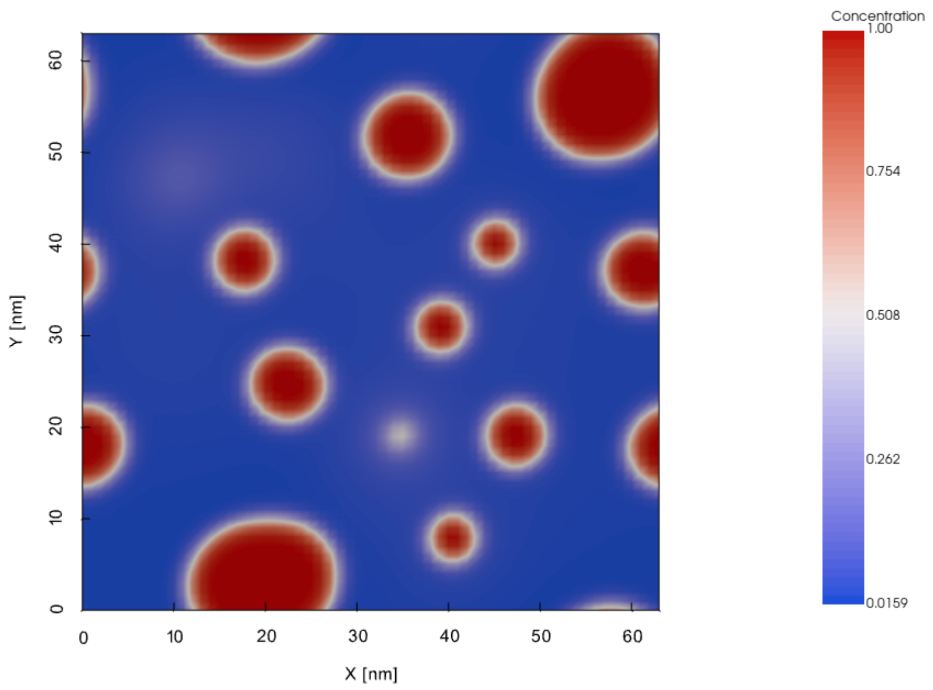
[ ]:
```
Text(0.5, 1.0, 'Energy residual evolution - Method 2')
```



### 9.6 plot actual microstructure

[ ]:
```
plot_micro(c,'2D',ttime)
```

Microstructure at dimensionless time 425.91

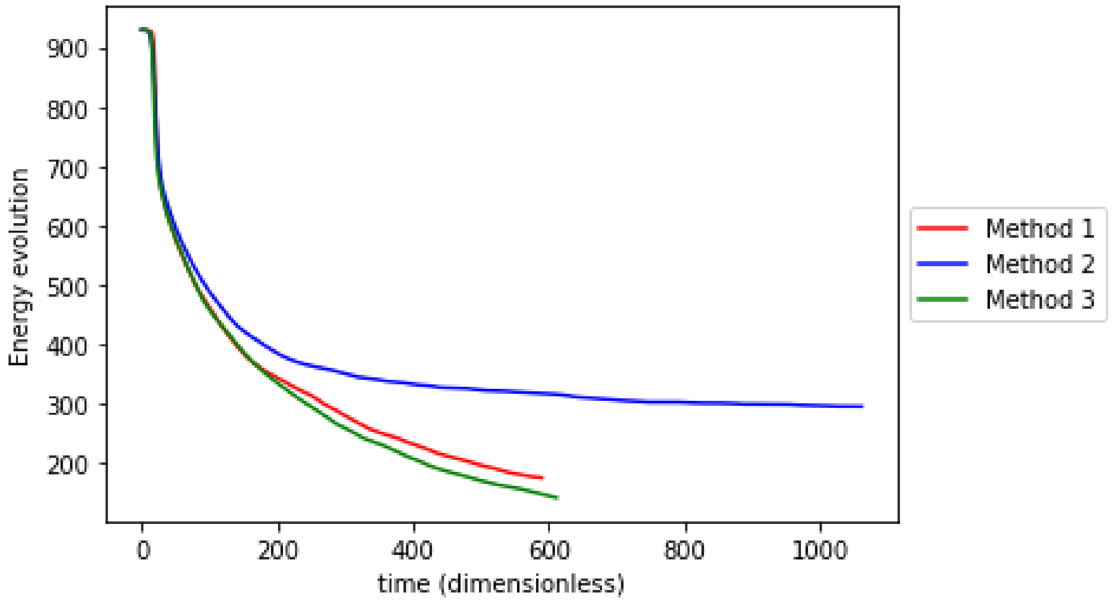


### 9.7 compare methods 1 and 2 and 3

[ ]:
```
plot_micro_mayavi(c,ttime)
```

```
No valid current object, please select an active object.
```

[ ]:
```
# save energy_vs_time in txt file : for comparative purposes
#np.savetxt('energy_method_2.txt',energ, fmt='%.2f')
#np.savetxt('time_method_2.txt',array_time, fmt=' %.2f')
energ_1 =np.loadtxt("energy_method_1.txt",   unpack=False)
energ_2 =np.loadtxt("energy_method_2.txt", unpack=False)
energ_3 =np.loadtxt("energy_method_3.txt", unpack=False)
time_1 =np.loadtxt("time_method_1.txt", unpack=False)
time_2 =np.loadtxt("time_method_2.txt", unpack=False)
time_3 =np.loadtxt("time_method_3.txt", unpack=False)
plt.plot(time_1,energ_1,label = 'Method 1', c='r')
plt.plot(time_2[:500],energ_2[0:500],label = 'Method 2',c='b')
plt.plot(time_3,energ_3,label = 'Method 3',c='g')
plt.xlabel('time (dimensionless)')
plt.ylabel('Energy evolution')
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.show()
```

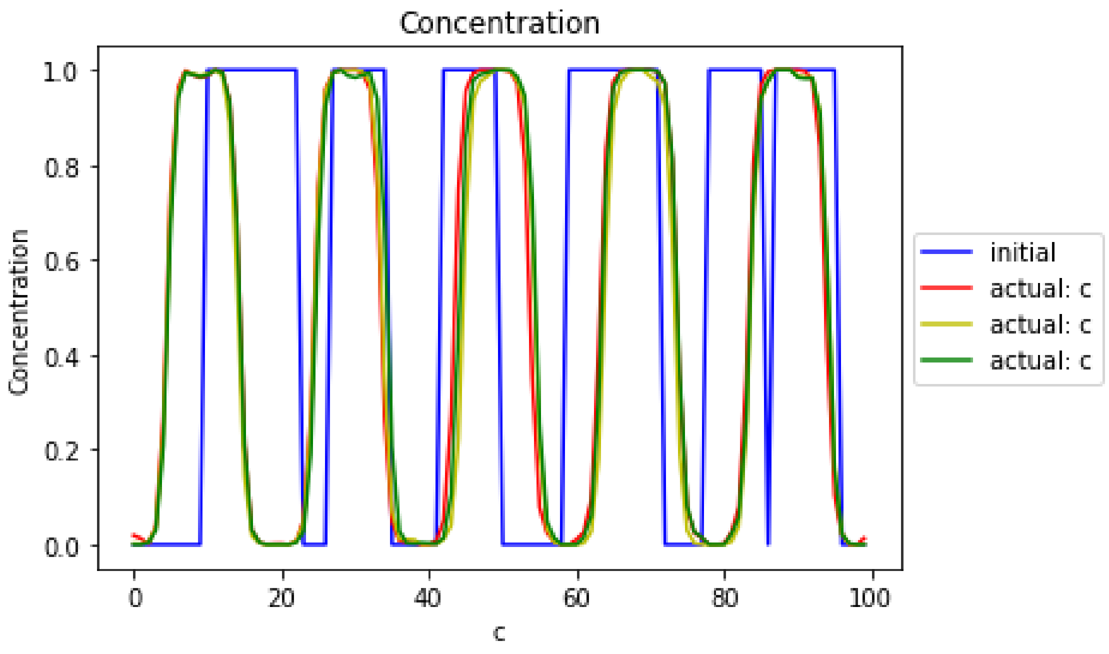


## 9.8 Case of coarsening of precipitates study

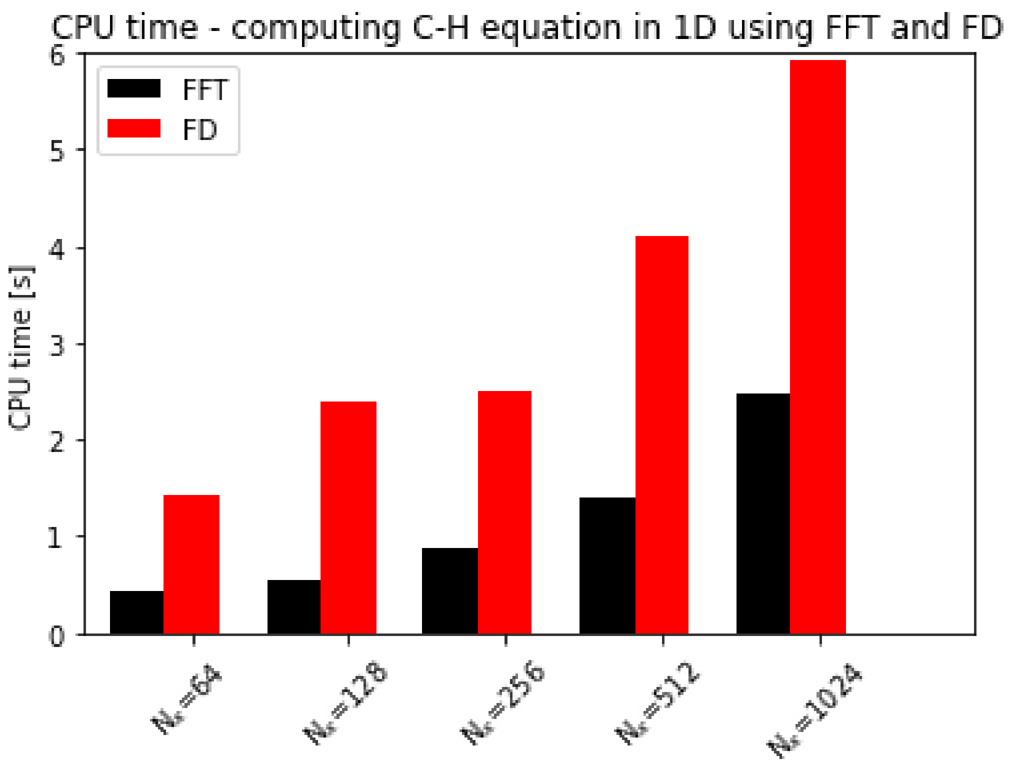
[ ]:
```
c_1=c[:,0,0]
```

[ ]:
```
c_2=c[:,0,0]
```

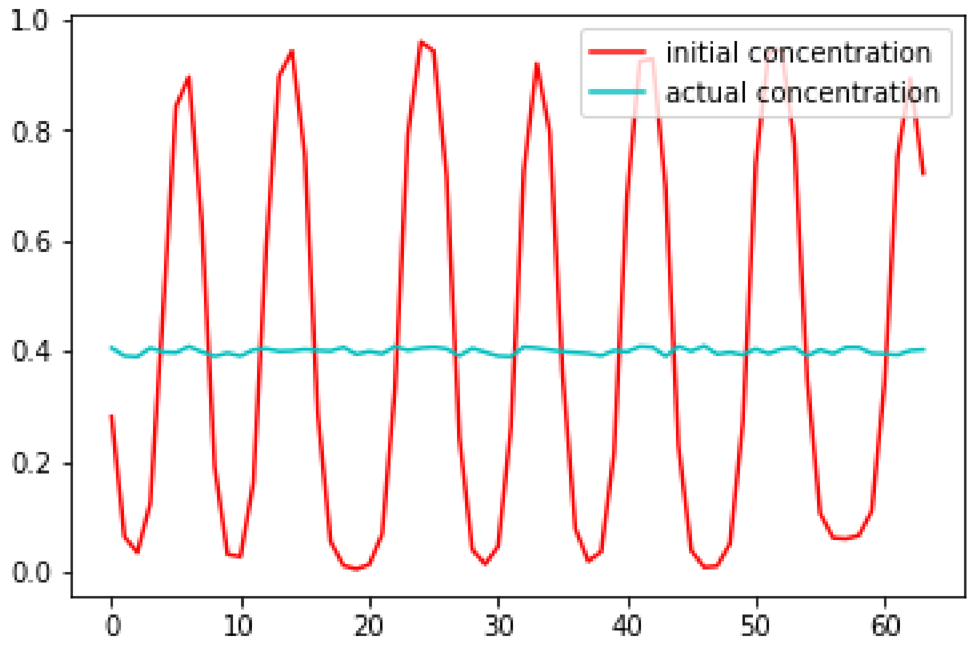
[ ]:
```
plt.plot(c_0[:,0,0],label='initial',c='b')
plt.plot(c_1,label='actual: c',c='r')
plt.plot(c_2,label='actual: c',c='y')
plt.plot(c[:,0,0],label='actual: c',c='g')
#plt.plot(X_al_out[:,0,0],label='actual: Si in matrix',c='g')
#plt.plot(X_th_out[:,0,0],label='actual: Si in precipitates',c='m')
plt.xlabel("c")
plt.ylabel("Concentration")
plt.title('Concentration')
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.show()
```



[ ]:
```
# plot histogram (to compare CPU time when using FFT or FD to compute CH␣
↪equation in 1D)
#makes the data
fig = plt.figure()
ax = fig.add_subplot(111)

## the data
N = 5
fft = [0.42,0.53,0.87,1.39,2.48]
fd =   [1.43,2.38,2.51,4.1,5.93]



## necessary variables
ind = np.arange(N)                # the x locations for the groups
width = 0.35                      # the width of the bars

rects1 = ax.bar(ind, fft, width,
                color='black',
                error_kw=dict(elinewidth=2,ecolor='red'))

rects2 = ax.bar(ind+width, fd, width,
                    color='red',
                    error_kw=dict(elinewidth=2,ecolor='black'))
# axes and labels
ax.set_xlim(-width,len(ind)+width)
ax.set_ylim(0,6)
ax.set_ylabel('CPU time [s]')
ax.set_title('CPU time - computing C-H equation in 1D using FFT and FD')
xTickMarks = ['N$_x$='+str(i) for i in [64,128,256,512,1024]]
ax.set_xticks(ind+width)
xtickNames = ax.set_xticklabels(xTickMarks)
plt.setp(xtickNames, rotation=45, fontsize=10)

## add a legend
ax.legend( (rects1[0], rects2[0]), ('FFT', 'FD') )

plt.show()
```

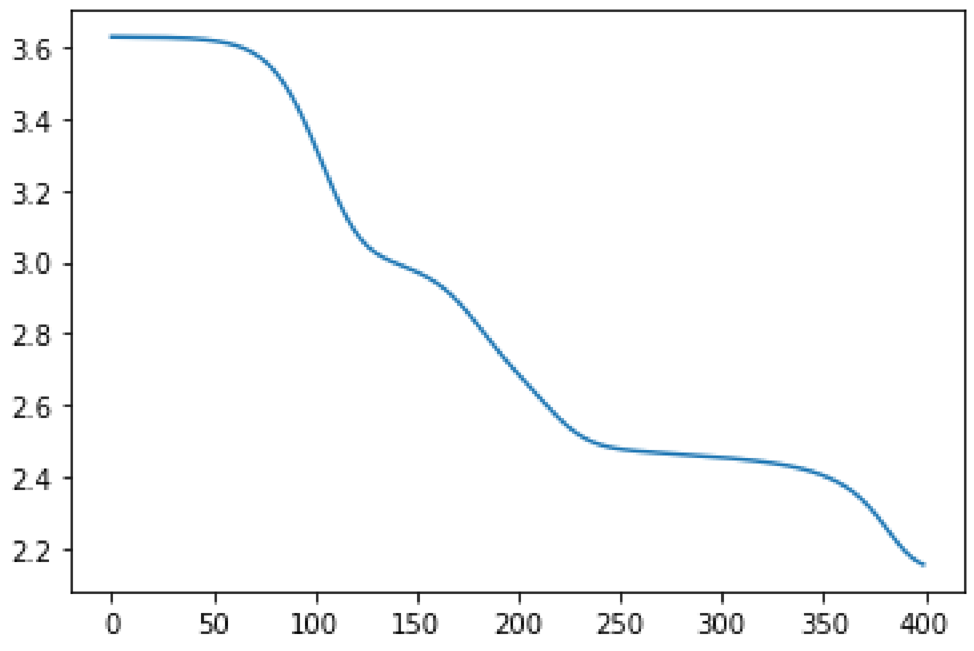


[ ]:
```
# 1D case
fig, ax = plt.subplots()
ax.plot(c[:, :, 0],  color ='r', label='initial concentration')
ax.plot(c0_save[:, :, 0],  color ='c', label='actual concentration')
leg = ax.legend()
#ax.xlabel('x')
#ax.ylabel('concentration')
#ax.title('initial and actual concentration after spinodal decomposition')
```



```
[ ]: plt.plot(energ)
     print(energ.shape)
```

```
(400,)
```



[ ]:
```
# save energy_vs_time in txt file : for comparative purposes
n_lines=energ.shape[0]
energy_time_adap=np.ones((n_lines,2))
energy_time_adap[:,0]=timesteps
energy_time_adap[:,1]=energ

np.savetxt('energy_versus_time_adaptive.txt', energy_time_adap, fmt='%.2f')
```

## 10 plot microstructure

import sys

## 11 grid2 : visualize c variable

grid = pv.UniformGrid() grid.spacing=np.array([dx,dy,dz])*1E9 grid.dimensions = np.array(c.shape) grid.point_arrays[r'Concentration'] = c.flatten(order="F") # Flatten the array!

pv.set_plot_theme("document") # = theme cmap = plt.cm.get_cmap("coolwarm", 150) # = color map

## 12 contours for c variable = 0.001 and 0.99

contours = grid.contour(isosurfaces=2,rng=([0.01,0.99])) #[0.5, 1] p = pv.Plotter()

p.camera_position = [0, -.75, -1] p.add_mesh(grid,cmap=cmap, show_scalar_bar=True,opacity=1.,clim=[0.5,1])#)#, p.add_mesh(contours,cmap=cmap, show_scalar_bar=True,color="black") #color="black",,clim=[1.,1.] p.show_bounds(all_edges=True,xlabel="x [nm]",ylabel="y [nm]",zlabel="z [nm]") sargs = dict(height=0.1, vertical=False, position_x=0.20, position_y=-0.01)

#p.show(cpos="xy") # projection plotter.show grid.plot(show_edges=True)

[ ]:
```

```