In [271…
```
import numpy as np
from matplotlib import pyplot as plt
```

Q2

a)

The below function returns the greens function for a grid of dimensions ndim and size of each dimension n

In [272…
```
def greens(n, ndim=2):
    dx=np.arange(n)
    dx[n//2:]=dx[n//2:]-n
    if ndim==2:
        pot=np.zeros([n,n])
        xmat,ymat=np.meshgrid(dx,dx)
        dr=np.sqrt(xmat**2+ymat**2)
        dr[0,0]=1
        pot=-np.log(dr)/2/np.pi
        pot[0,0]=pot[1,0] + 0.25
        return pot
```

I make a grid of 100X100. I initially set dr[0,0]=1 so that log of dr does not give an error at (0,0). Since the potential goes as -log(r) for 2D point charge and we set epsilon to 1, the potential at every point is just -log(r)/2*pi*. *Potential at (0,0) can be found by using the formula v(0,0) = charge(0,0) + V_avg_neighbours. Since we are considering charge at (0,0) to be 1, and since the neighbours of (0,0) are (1,0), (0,1), (-1,0), (0,-1) which all have the same potential, this gives the V at (0,0) to be (4*V(1,0)/4) + 0.25 (as Laplacian in 2D picks up rho/4 at zero point)

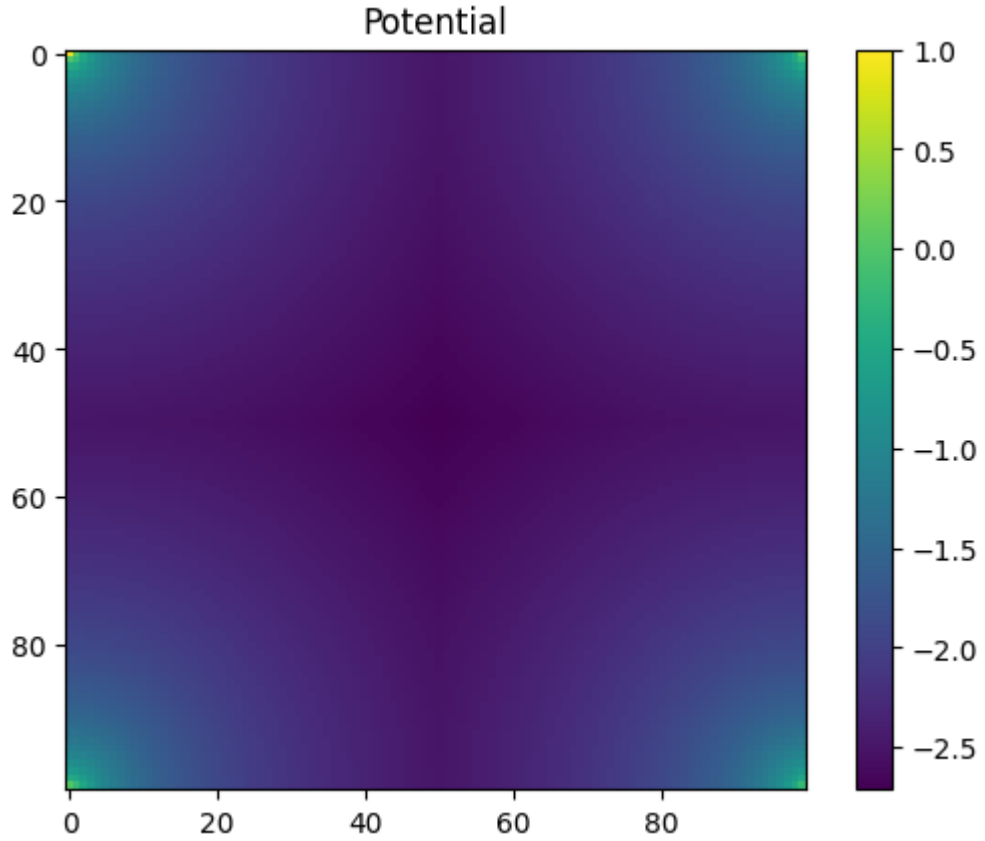
In [273…
```
pot = greens(100,2)
print("Potential at (0,0) is {}".format(pot[0,0]))
```

```
Potential at (0,0) is 0.25
```

To get V at (0,0) to be 1, I rescale the potential -- multiply it by 4

In [274…
```
pot = 4*pot
plt.imshow(pot)
plt.colorbar()
plt.title("Potential")
```

Out[274]:
```
Text(0.5, 1.0, 'Potential')
```



In [275…
```
print("V at (1,0) = {}\nV at (2,0) = {}\nV at (5,0) = {}\n".format(pot[1,0],
```

```
V at (1,0) = -0.0
V at (2,0) = -0.4412712003053032
V at (5,0) = -1.0245999974535522
```

As can be seen, this almost satisfies the sanity check for V at (5,0)!

b)

Some helper functions

Function which will convolve the green's function with the charge denisty to give the potential

In [276…
```
def rho2pot(rho,kernelft):
    tmp=rho.copy()
    tmp=np.pad(tmp,(0,tmp.shape[0]))

    tmpft=np.fft.rfftn(tmp)
    tmp=np.fft.irfftn(tmpft*kernelft)
    tmp=tmp[:rho.shape[0],:rho.shape[1]]
    return tmp
```

The function calls the rho2pot function with the charge only on the boundary and

returns the corresponding potential from the charge on the boundary

In [277…
```
def rho2pot_masked(rho,mask,kernelft,return_mat=False):
    rhomat=np.zeros(mask.shape)
    rhomat[mask]=rho
    potmat=rho2pot(rhomat,kernelft)
    if return_mat:
        return potmat
    else:
        return potmat[mask]
```

Function which does the conjugate gradient to solve Ax=b where A is the Laplacian. Since we want to find the charge distribution, the potential V will be b and the charge density rho will be the x

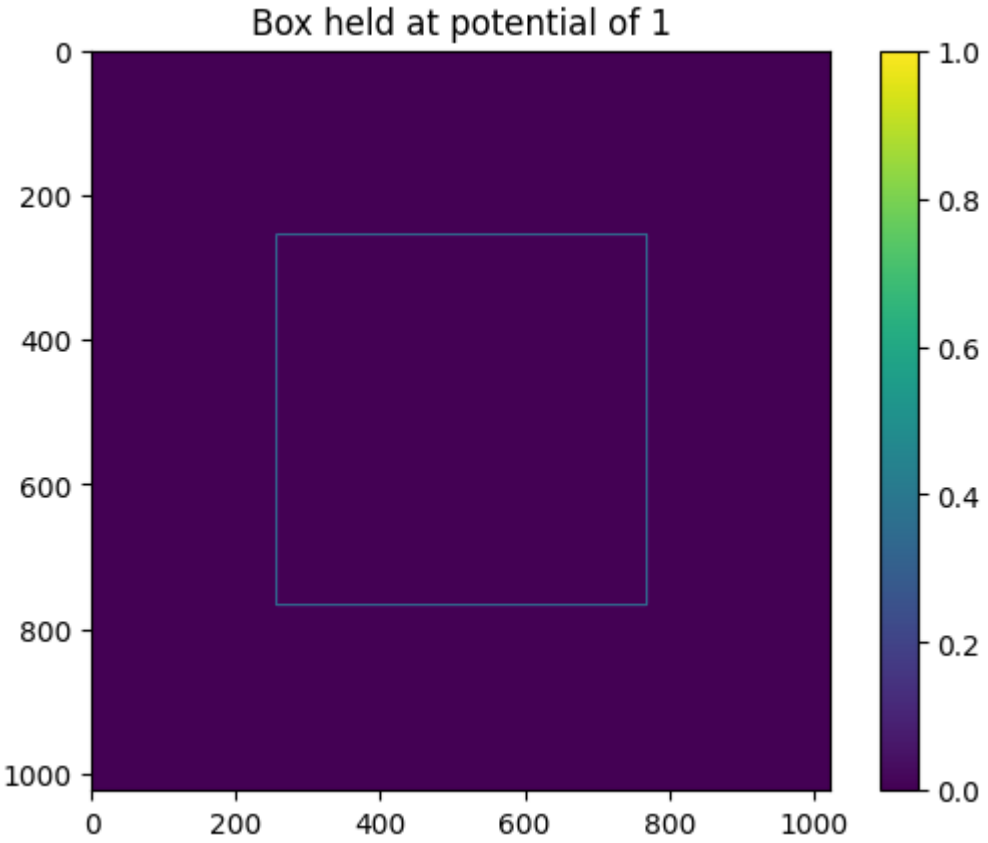
In [278…
```
def cg(rhs,x0,mask,kernelft,niter,fun=rho2pot_masked,show_steps=False,step_p
    Ax=fun(x0,mask,kernelft)
    r=rhs-Ax
    p=r.copy()
    x=x0.copy()
    rsqr=np.sum(r*r)
    print('starting rsqr is ',rsqr)
    for k in range(niter):

        Ap=fun(p,mask,kernelft)
        alpha=np.sum(r*r)/np.sum(Ap*p)
        x=x+alpha*p
        if show_steps:
            tmp=fun(x,mask,kernelft,True)
            plt.imshow(tmp,vmin=-2.1,vmax=2.1)
            plt.colorbar()
            plt.title('rsqr='+repr(rsqr)+' on iter '+repr(k+1))
            plt.savefig('laplace_iter_1024_'+repr(k+1)+'.png')
            plt.pause(step_pause)
        plt.show()
        r=r-alpha*Ap
        rsqr_new=np.sum(r*r)
        beta=rsqr_new/rsqr
        p=r+beta*p
        rsqr=rsqr_new
    print('final rsqr is ',rsqr)
    return x
```

Given the appropriate boundary conditions, the above functions will solve for the charge on the boundary given the potential on the boundary. Defining the boundary as a square box held at a potential of 1:

In [279…
```
n=1024
bc=np.zeros([n,n])
mask=np.zeros([n,n],dtype='bool')
mask[0,:]=True
mask[-1,:]=True
mask[:,0]=True
```

```
mask[:,-1]=True
bc[0,0]=0.0
bc[0,-1]=0.0
bc[-1,0]=0.0
bc[-1,-1]=0.0
#This adds a bar in the interior held at fixed potential
bc[n//4:3*n//4,n//4]=1.0
mask[n//4:3*n//4,n//4]=True
bc[n//4:3*n//4,3*n//4]=1.0
mask[n//4:3*n//4,3*n//4]=True
bc[n//4,n//4:3*n//4]=1.0
mask[n//4,n//4:3*n//4]=True
bc[3*n//4,n//4:3*n//4]=1.0
mask[3*n//4,n//4:3*n//4]=True
plt.imshow(bc)
plt.colorbar()
plt.title("Box held at potential of 1")
```

Out[279]: Text(0.5, 1.0, 'Box held at potential of 1')

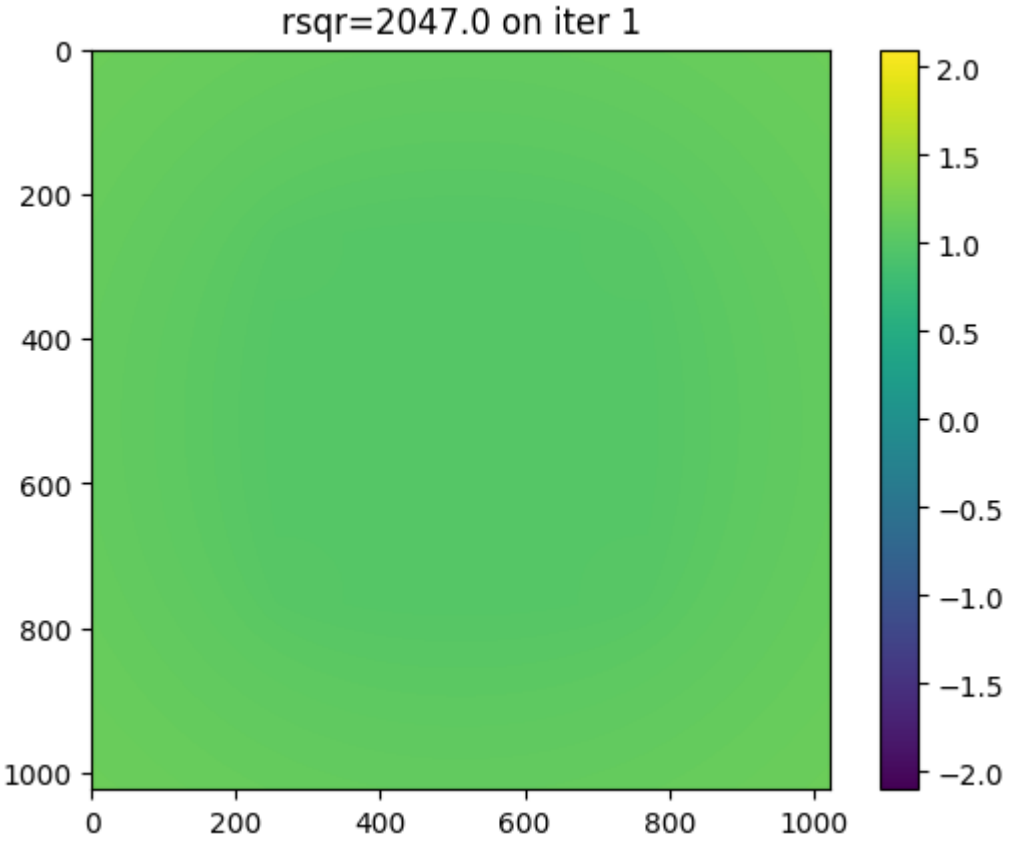


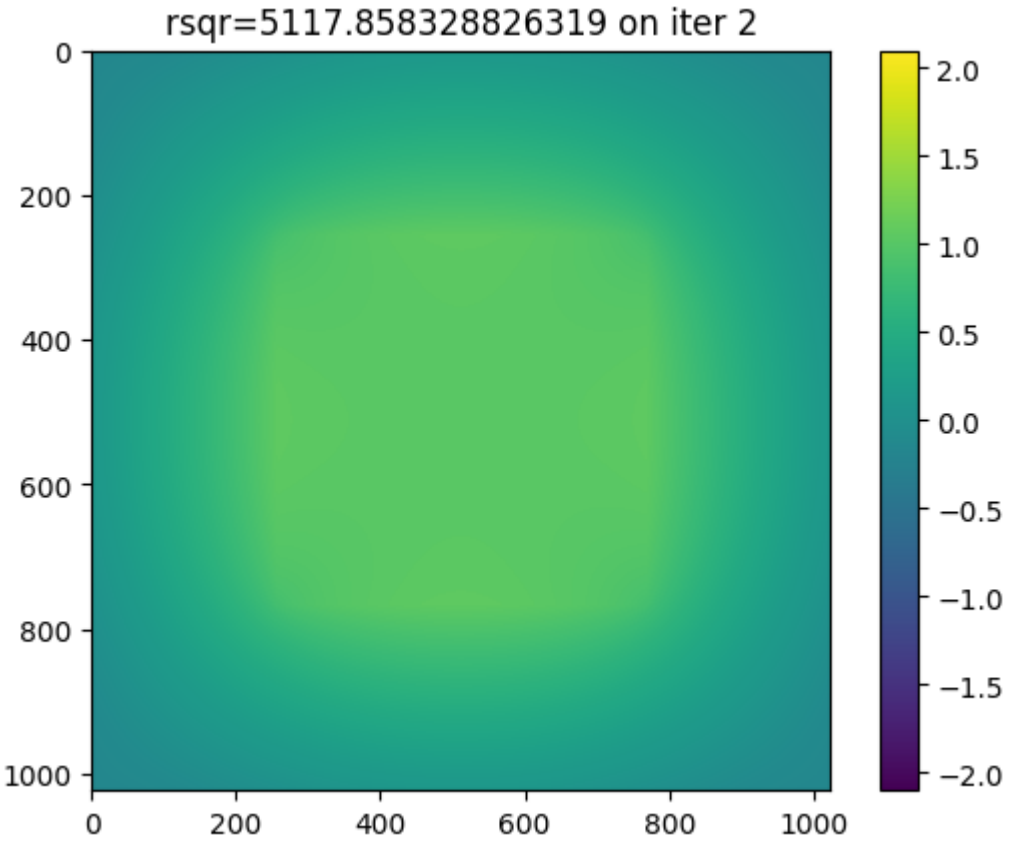
First getting the green's function for the appropriate dimensions. Then defining the b of Ax=b (rhs) as the potential on the boundary. And solving for rho:

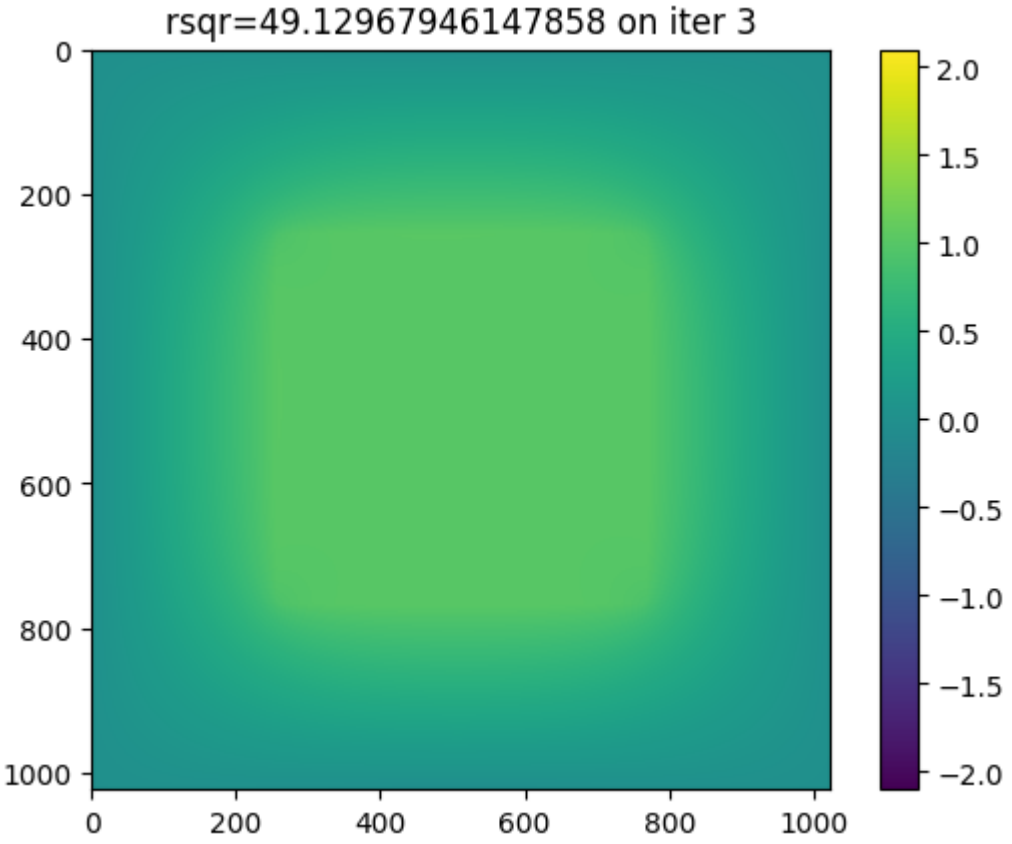
In [280…

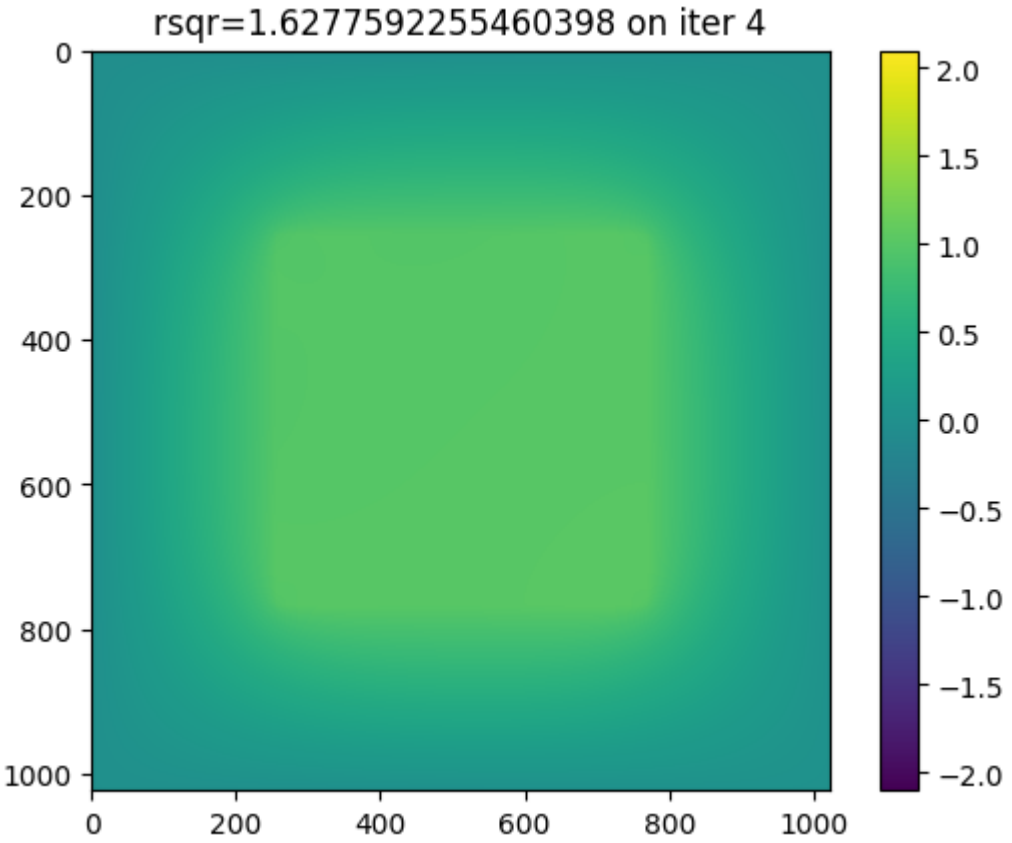
```
kernel=greens(2*n,2)
kernelft=np.fft.rfft2(kernel)
rhs=bc[mask]
x0=0*rhs
rho_out=cg(rhs,x0,mask,kernelft,40,show_steps=True,step_pause=0.25)
```

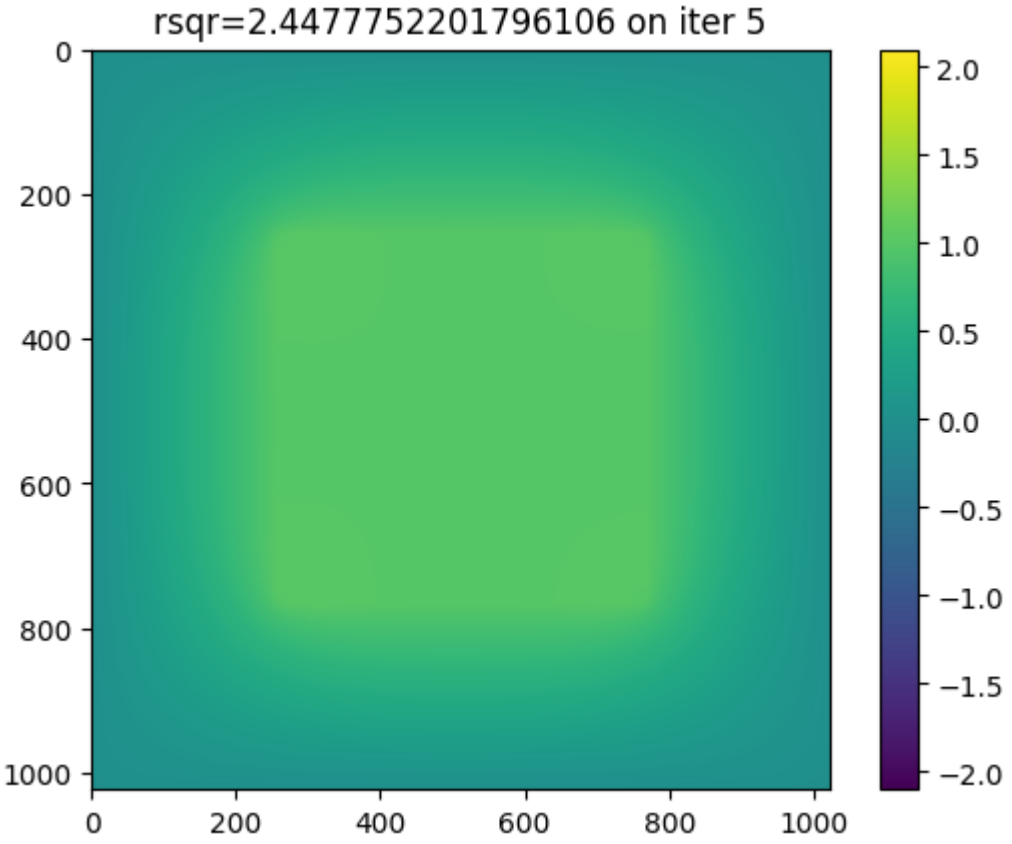
```
starting rsqr is  2047.0
```

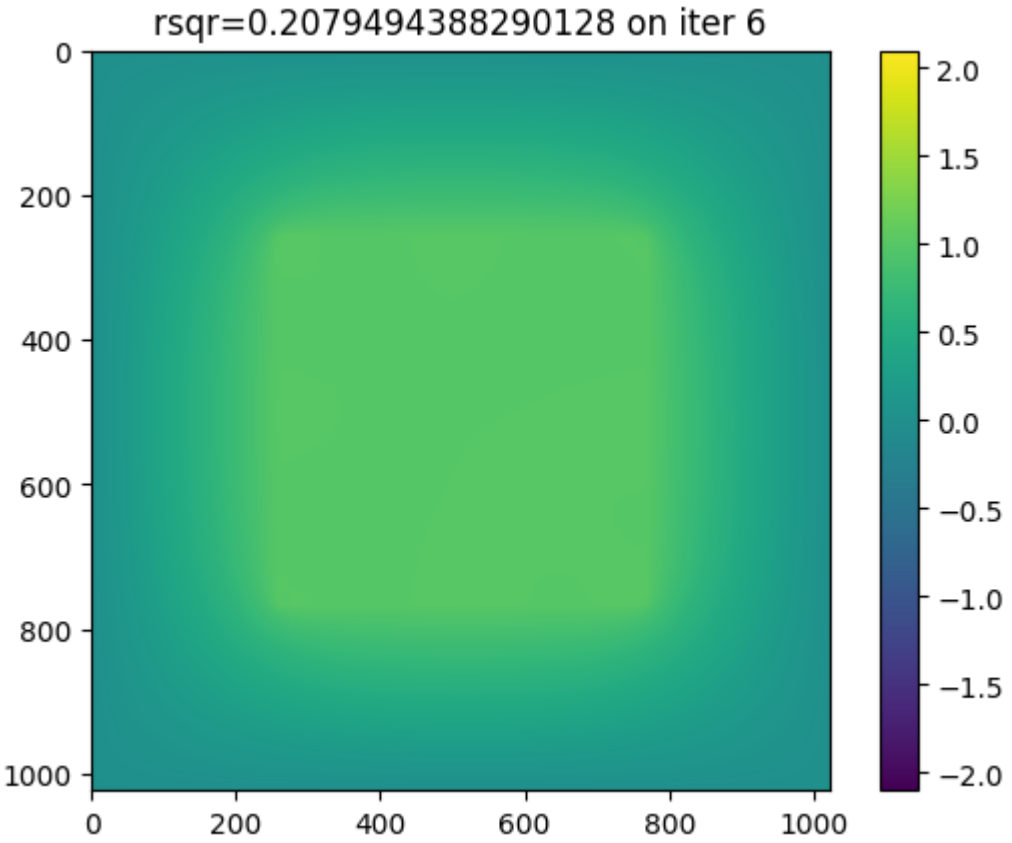

rsqr=2047.0 on iter 1
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

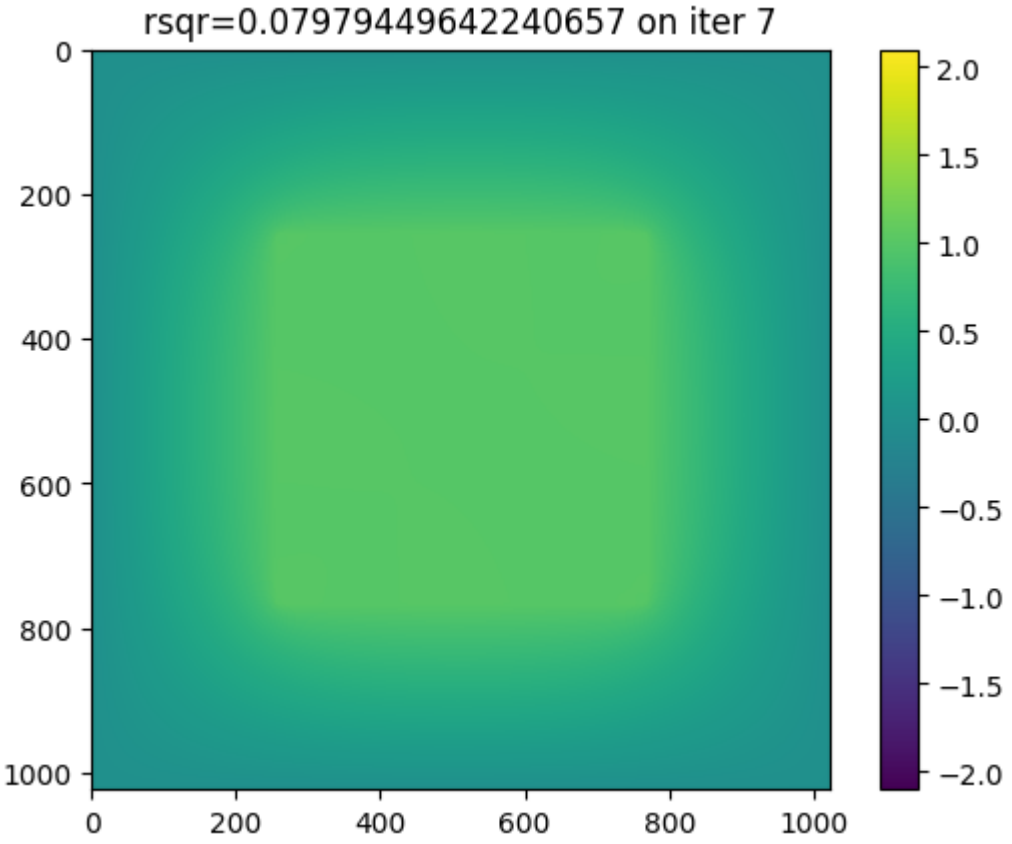

rsqr=5117.858328826319 on iter 2
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

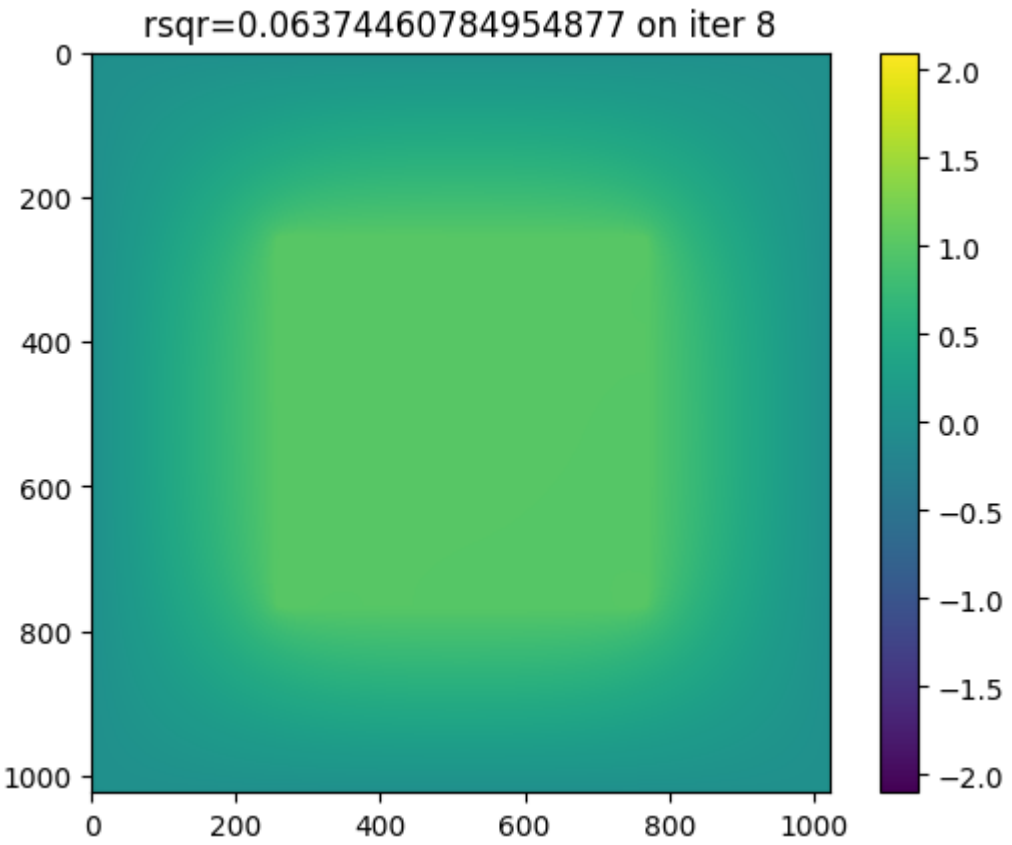

rsqr=49.12967946147858 on iter 3
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

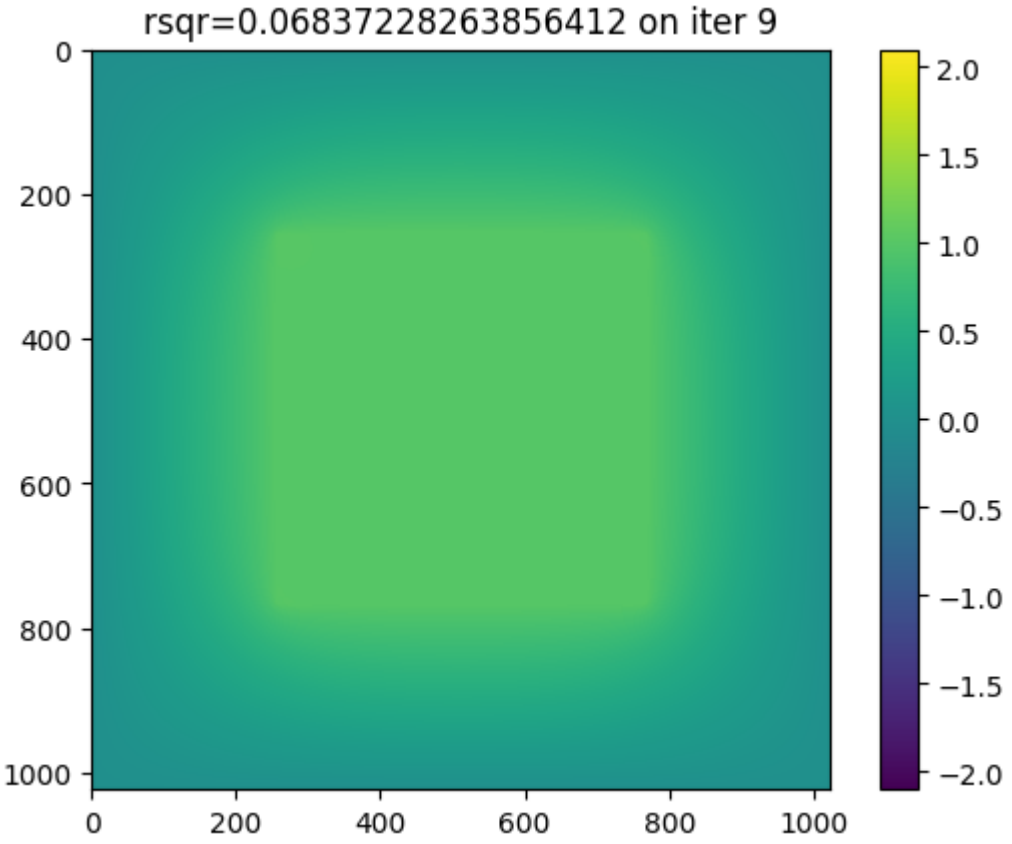

rsqr=1.6277592255460398 on iter 4
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

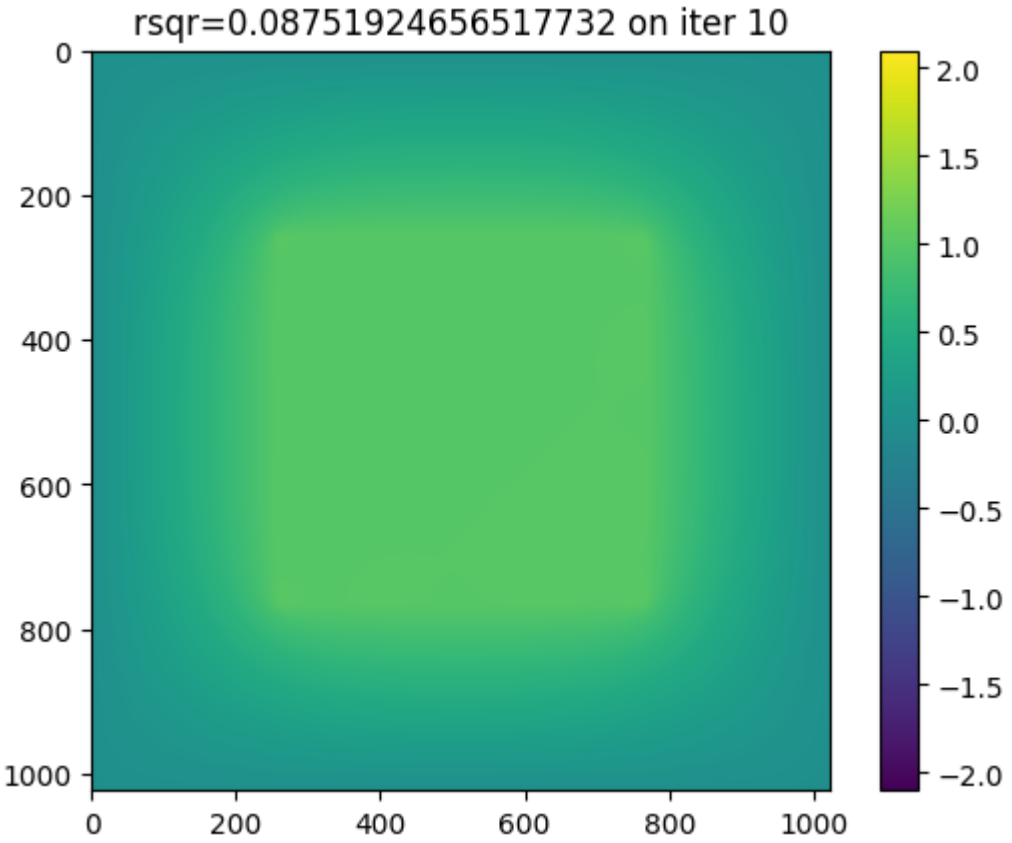

rsqr=2.4477752201796106 on iter 5
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

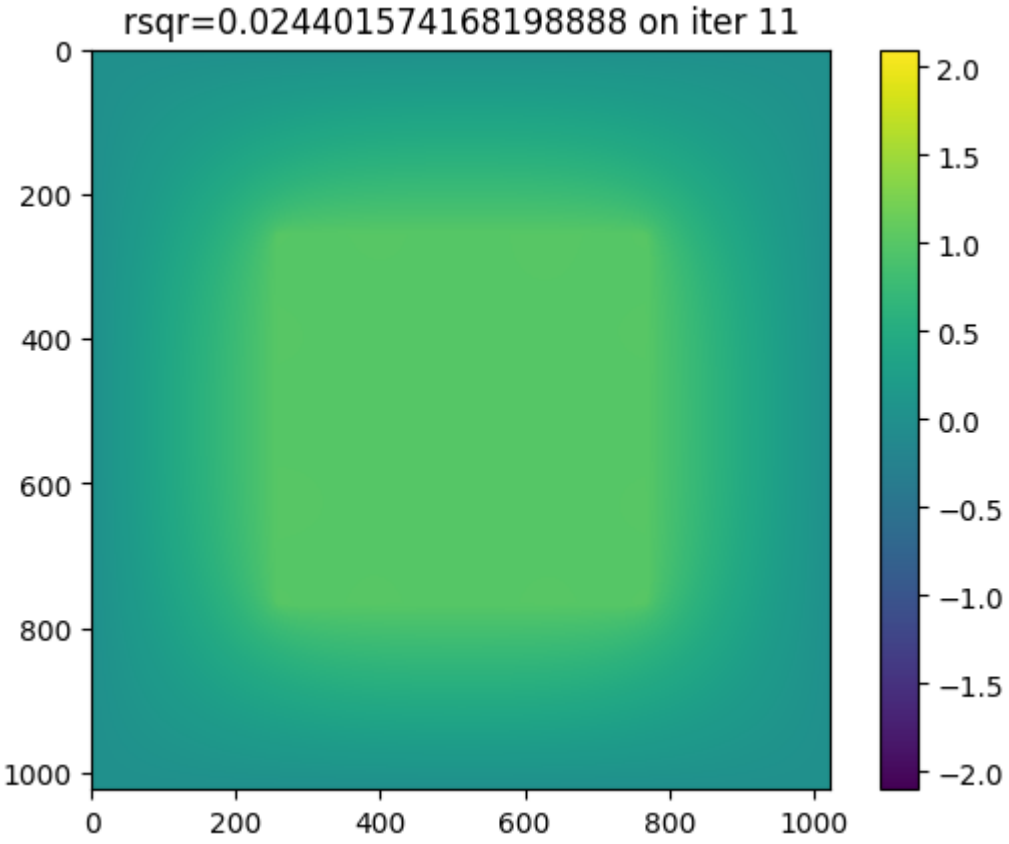

rsqr=0.2079494388290128 on iter 6
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

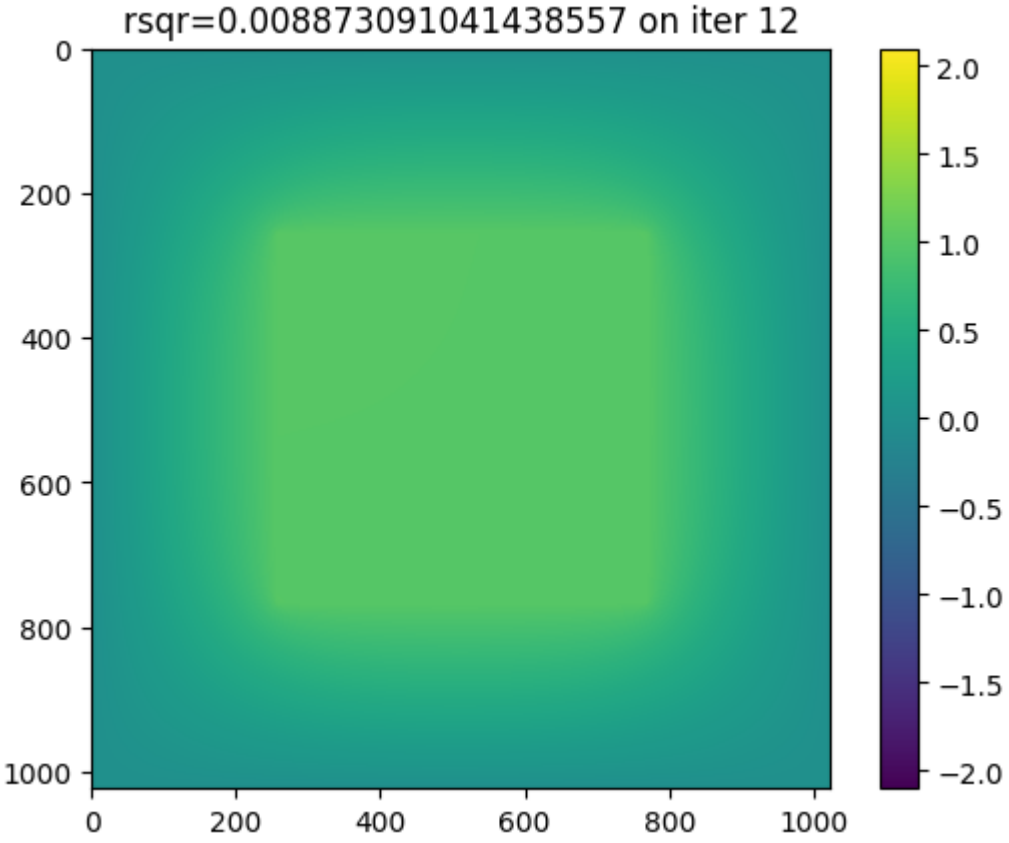

rsqr=0.07979449642240657 on iter 7
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

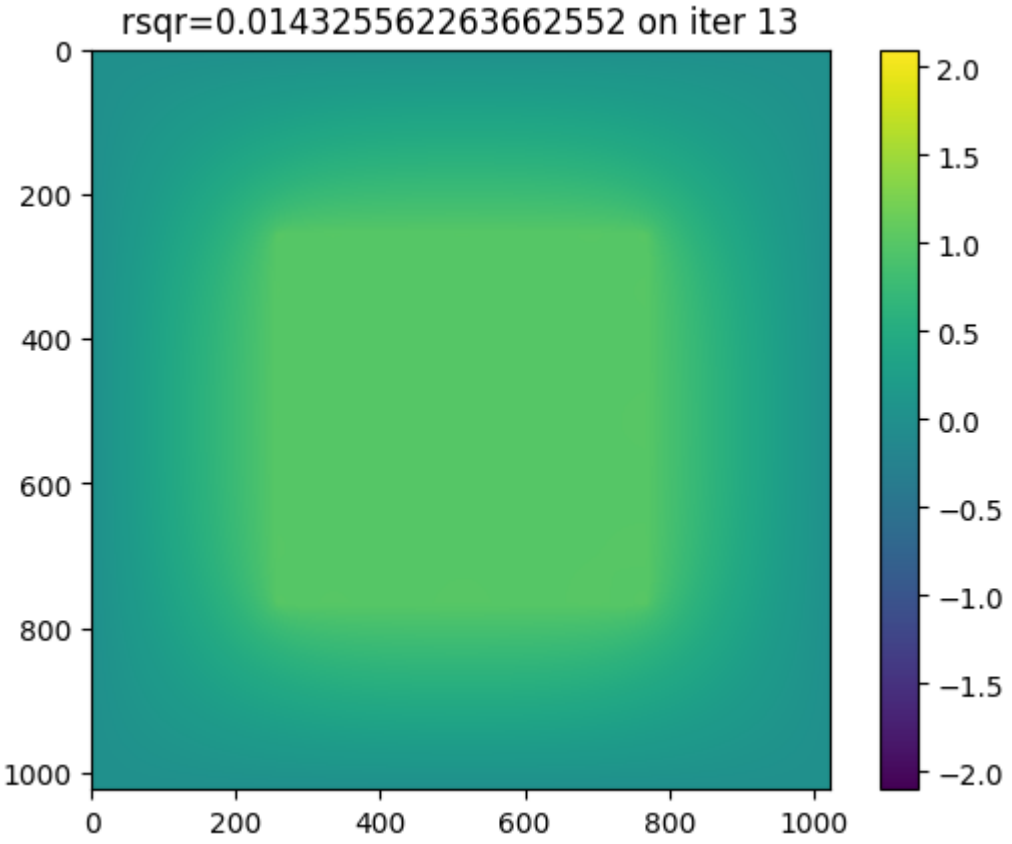

rsqr=0.06374460784954877 on iter 8
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

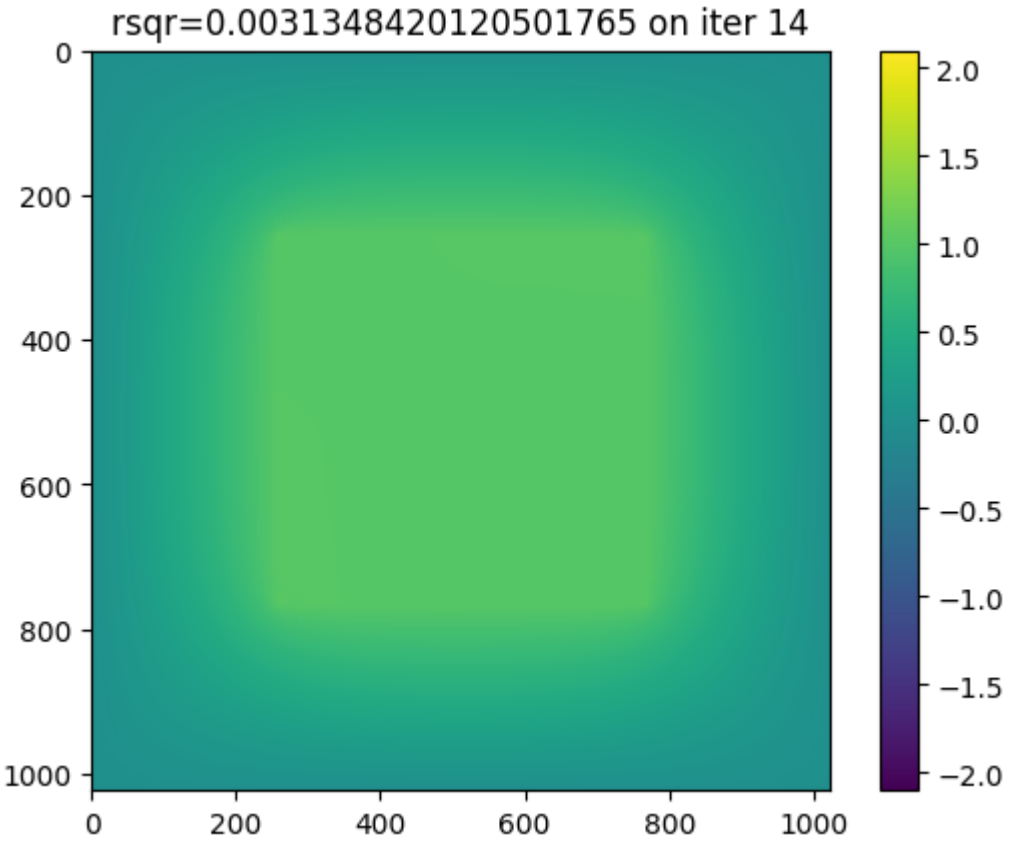

rsqr=0.06837228263856412 on iter 9
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

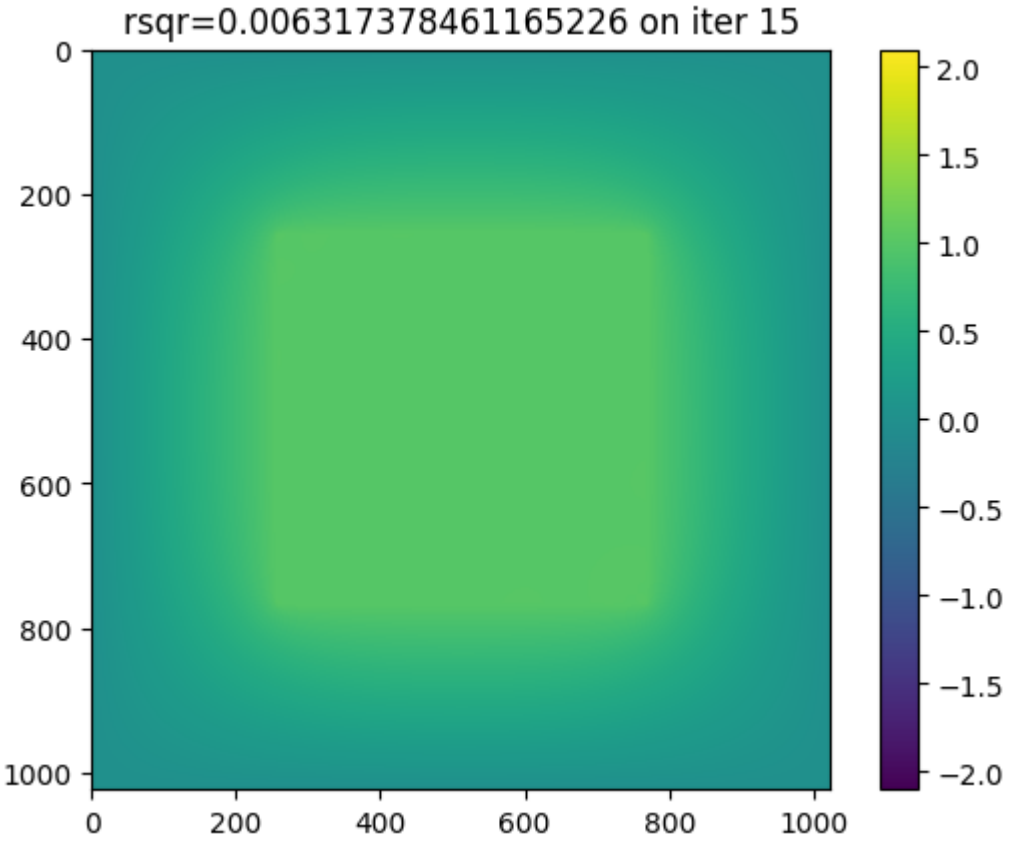

rsqr=0.08751924656517732 on iter 10
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

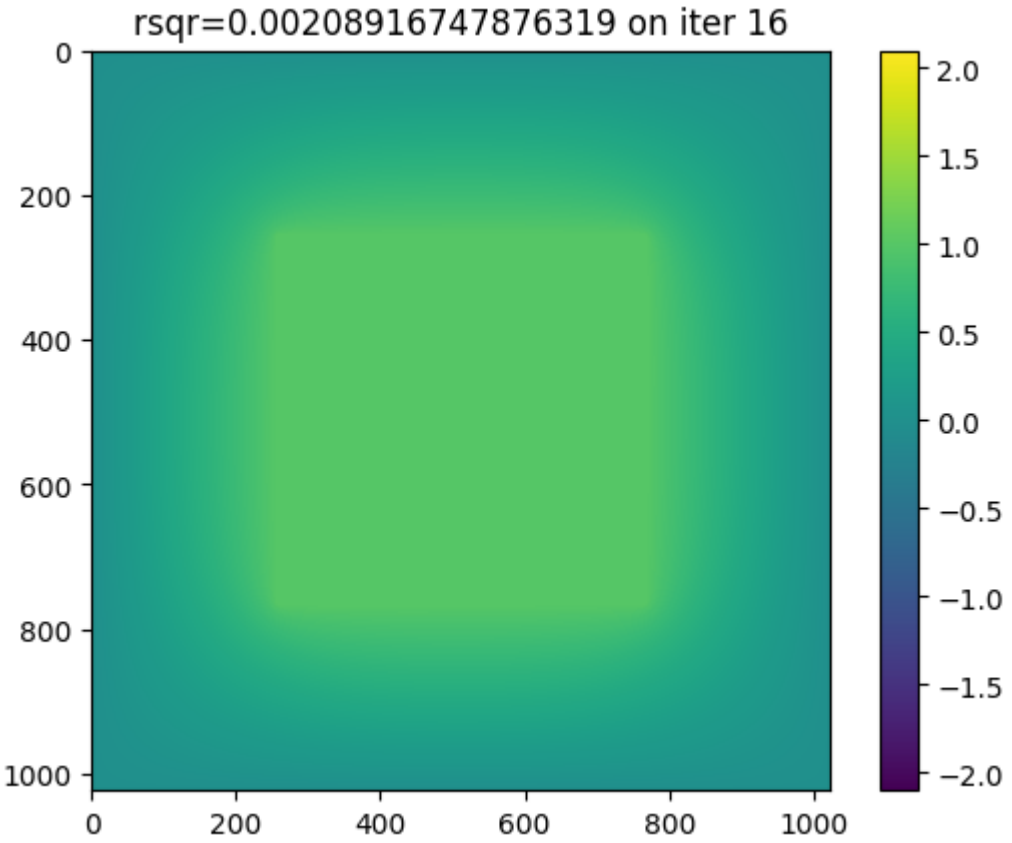

rsqr=0.0244015741681988888 on iter 11
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

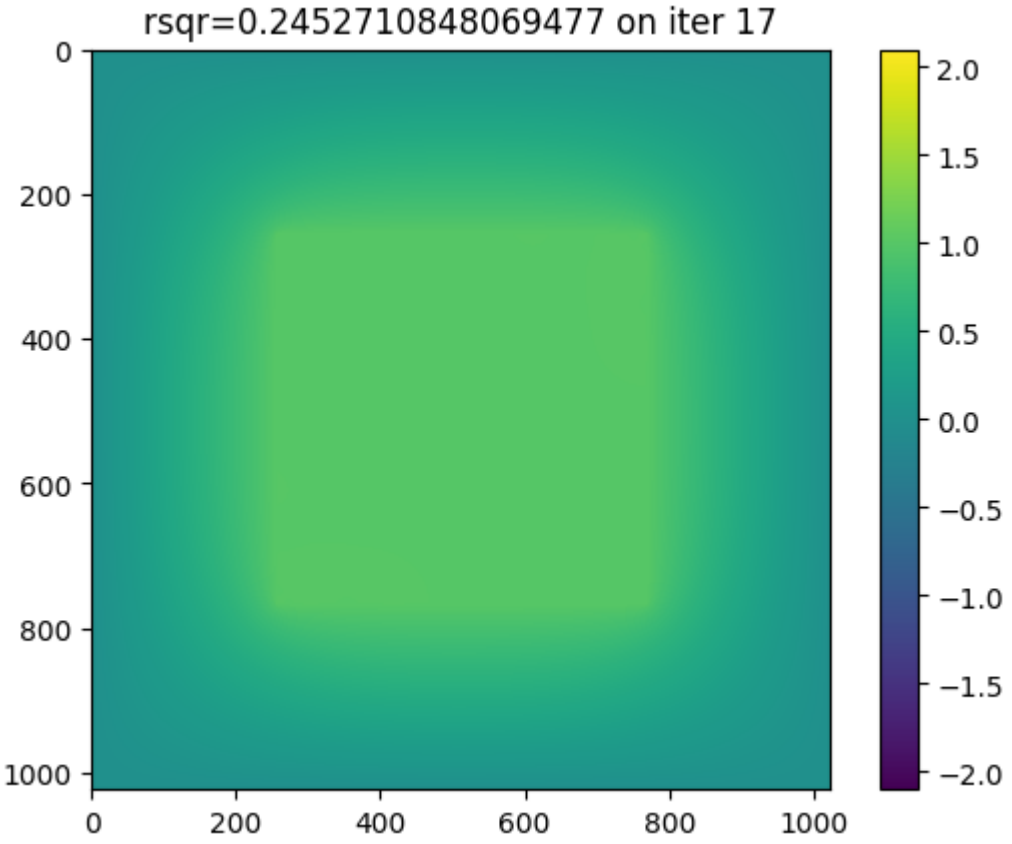

rsqr=0.008873091041438557 on iter 12
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

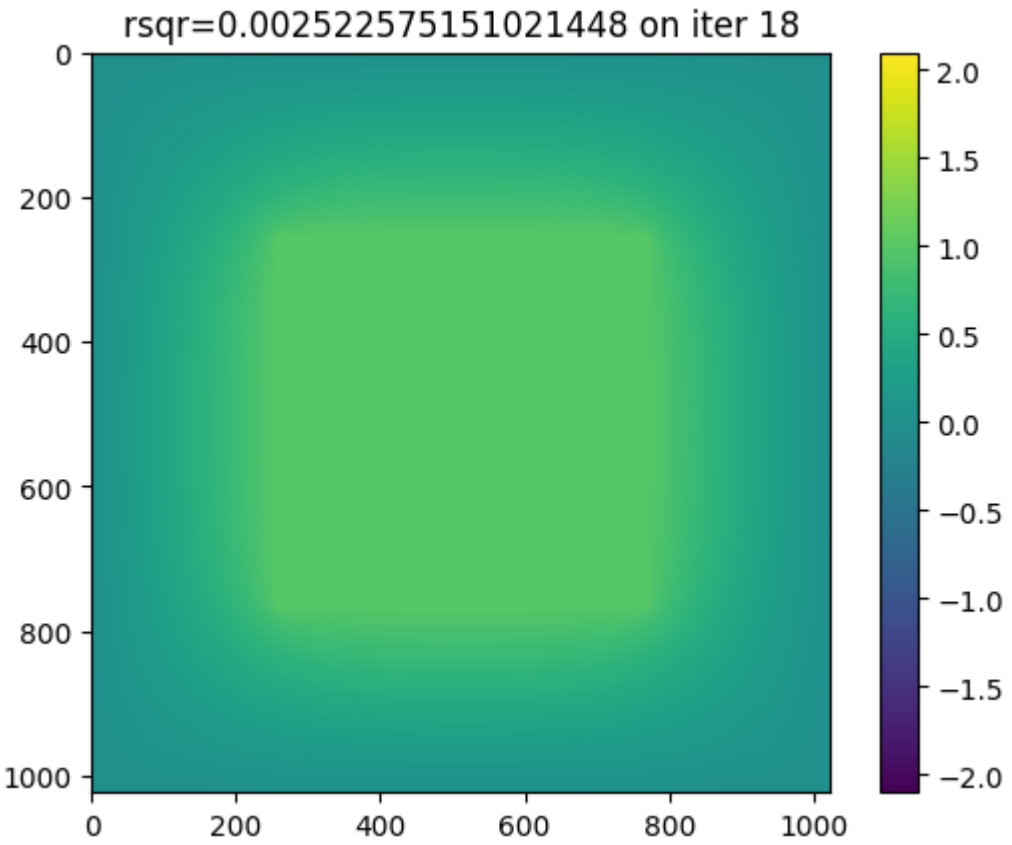

rsqr=0.014325562263662552 on iter 13
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

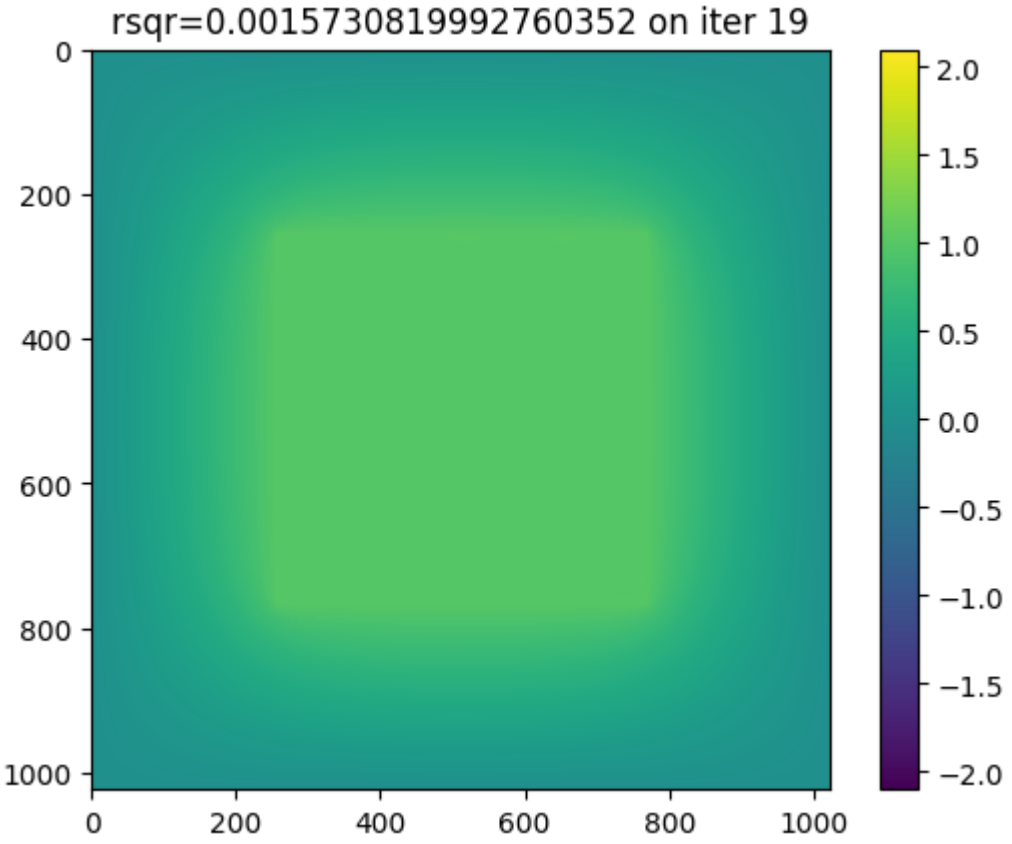

rsqr=0.0031348420120501765 on iter 14
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

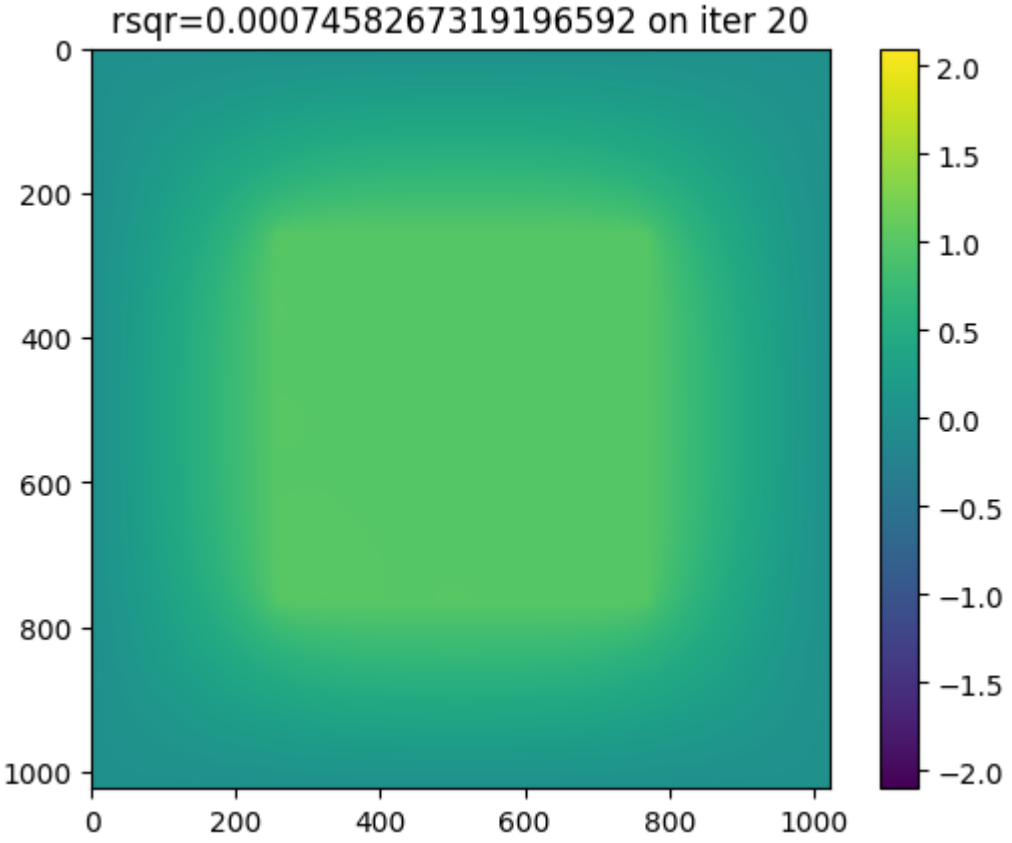

rsqr=0.006317378461165226 on iter 15
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

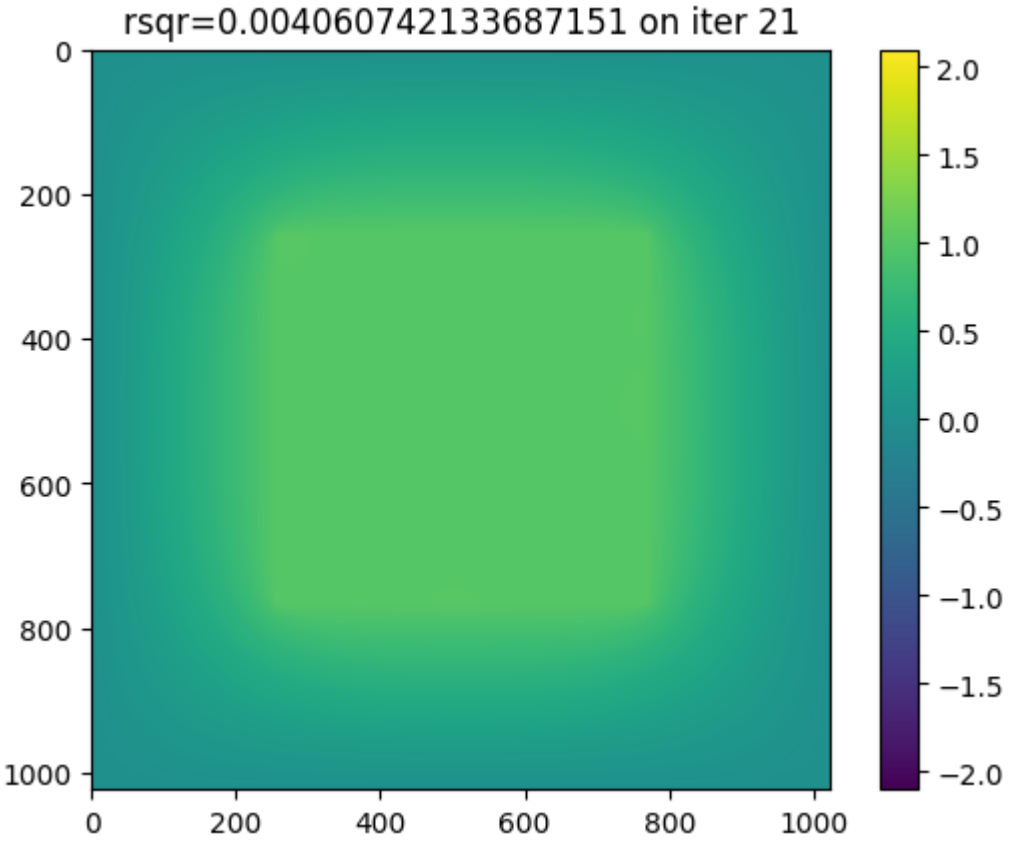

rsqr=0.002089167478763 19 on iter 16
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

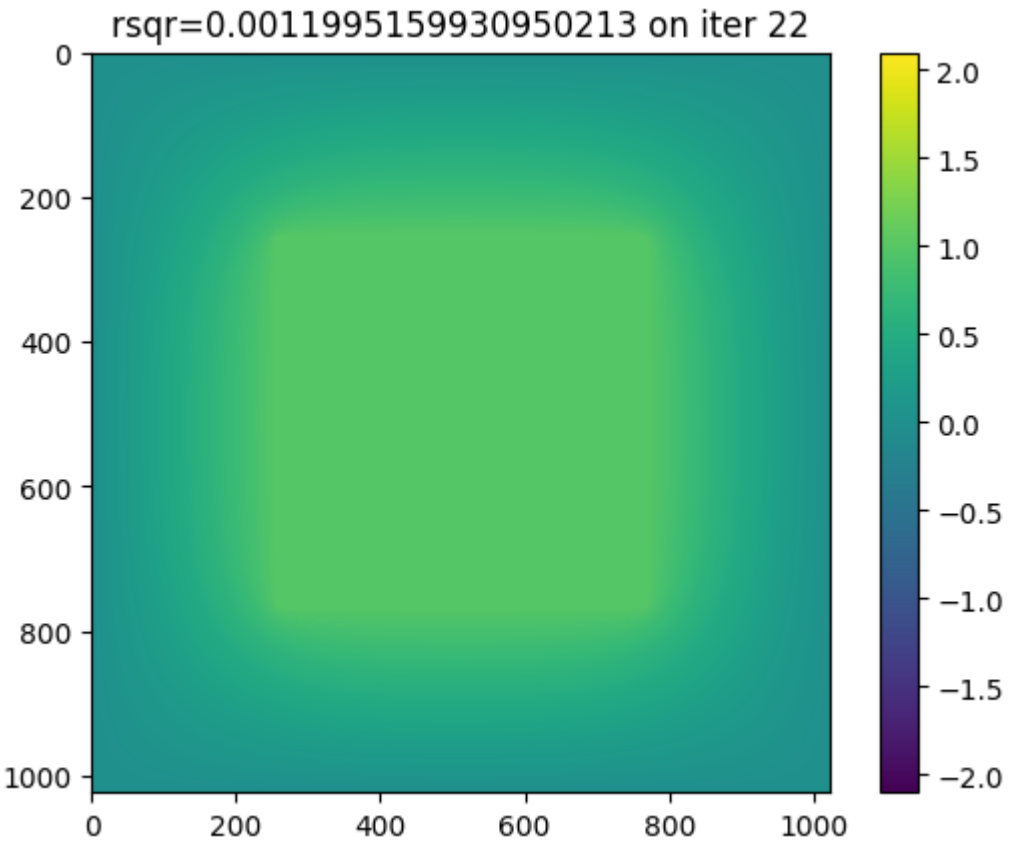

rsqr=0.2452710848069477 on iter 17
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

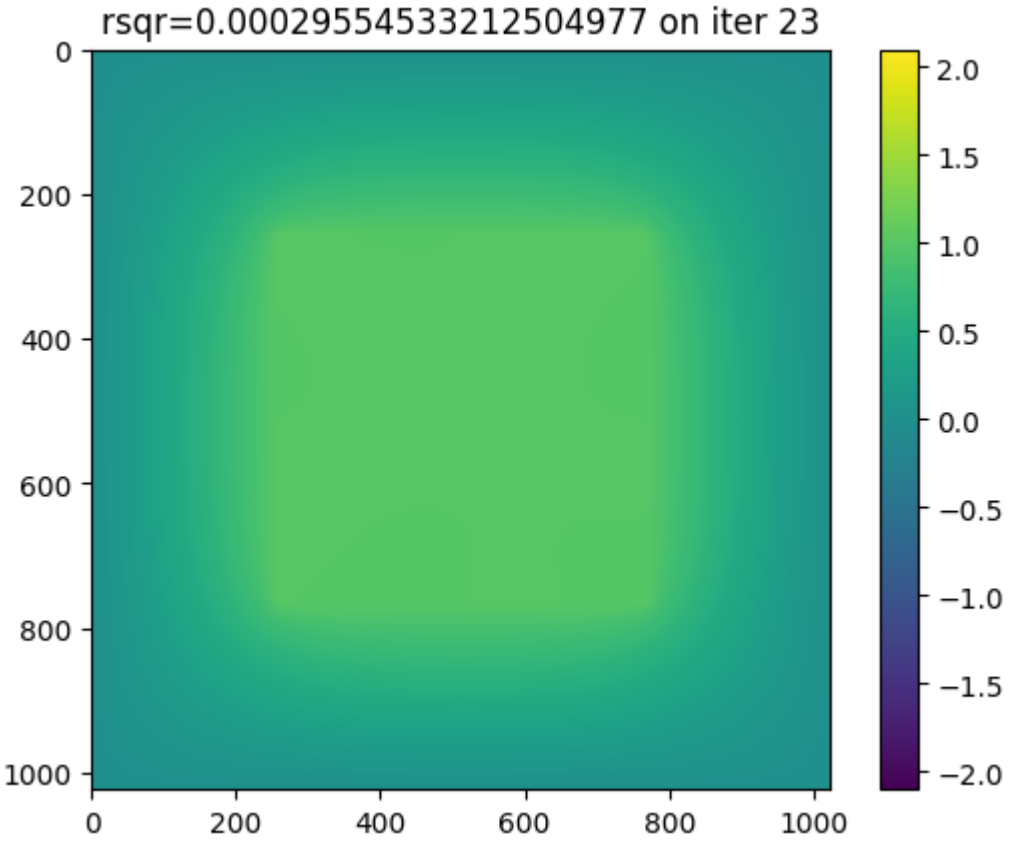

rsqr=0.002522575151021448 on iter 18
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

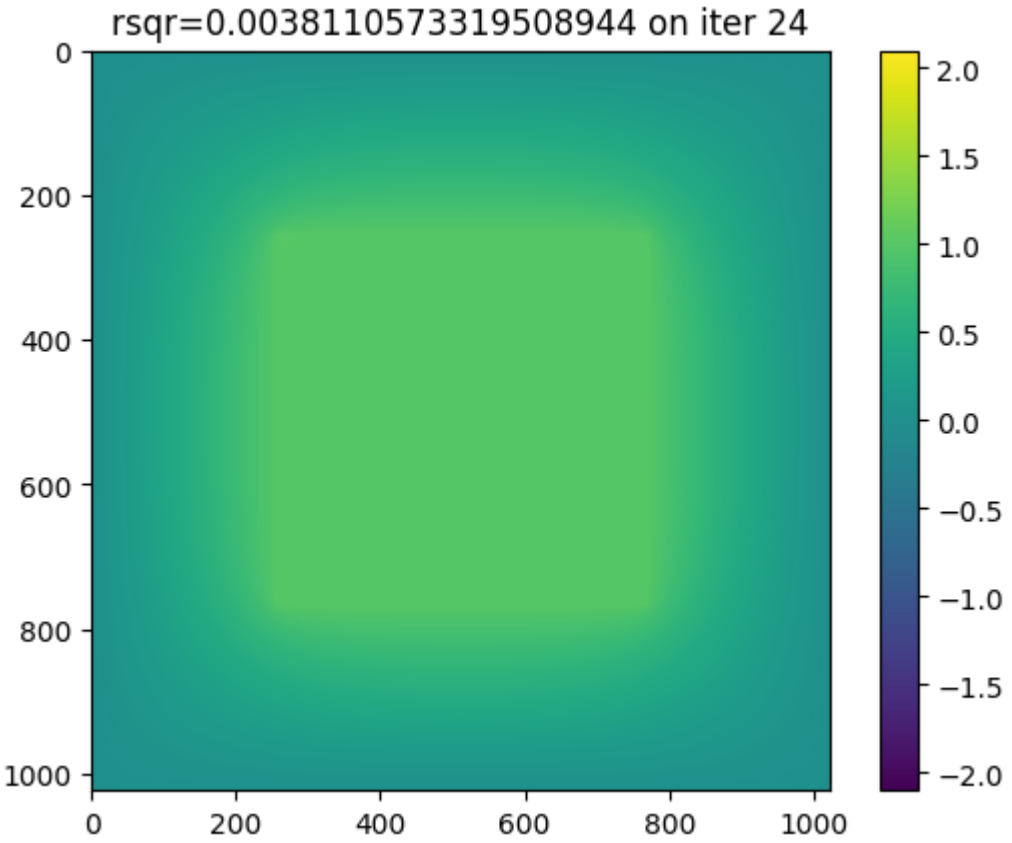

rsqr=0.0015730819992760352 on iter 19
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

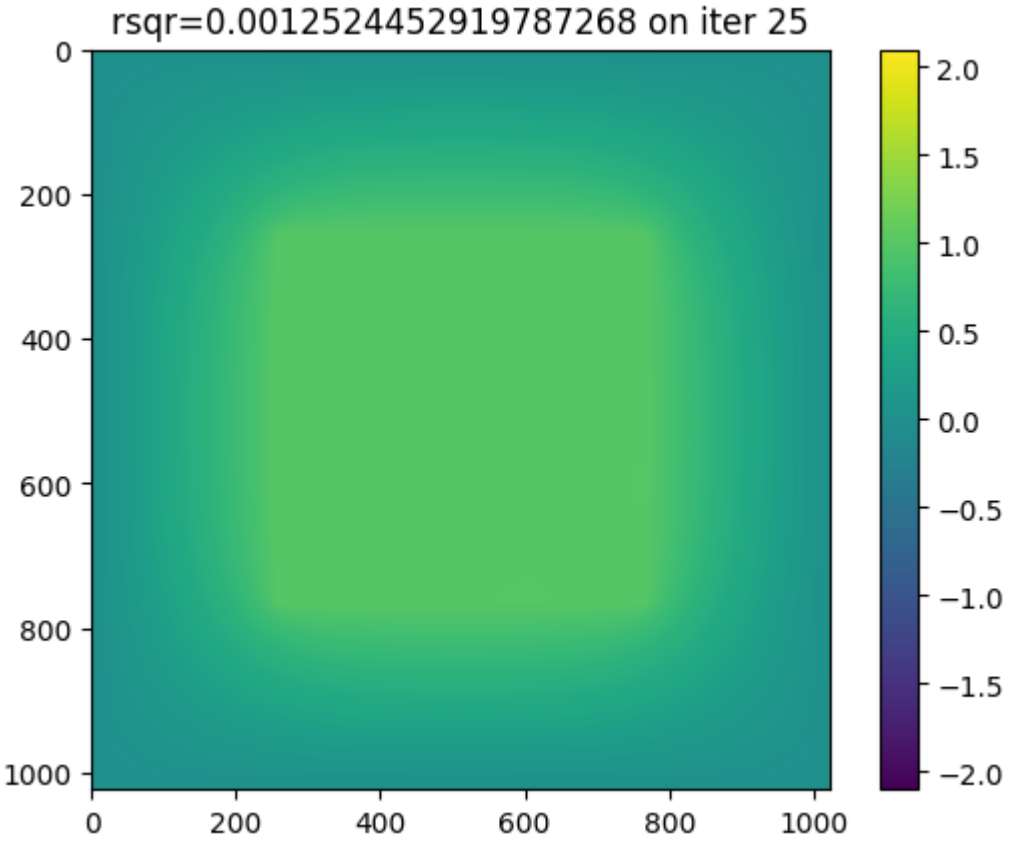

rsqr=0.0007458267319196592 on iter 20
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

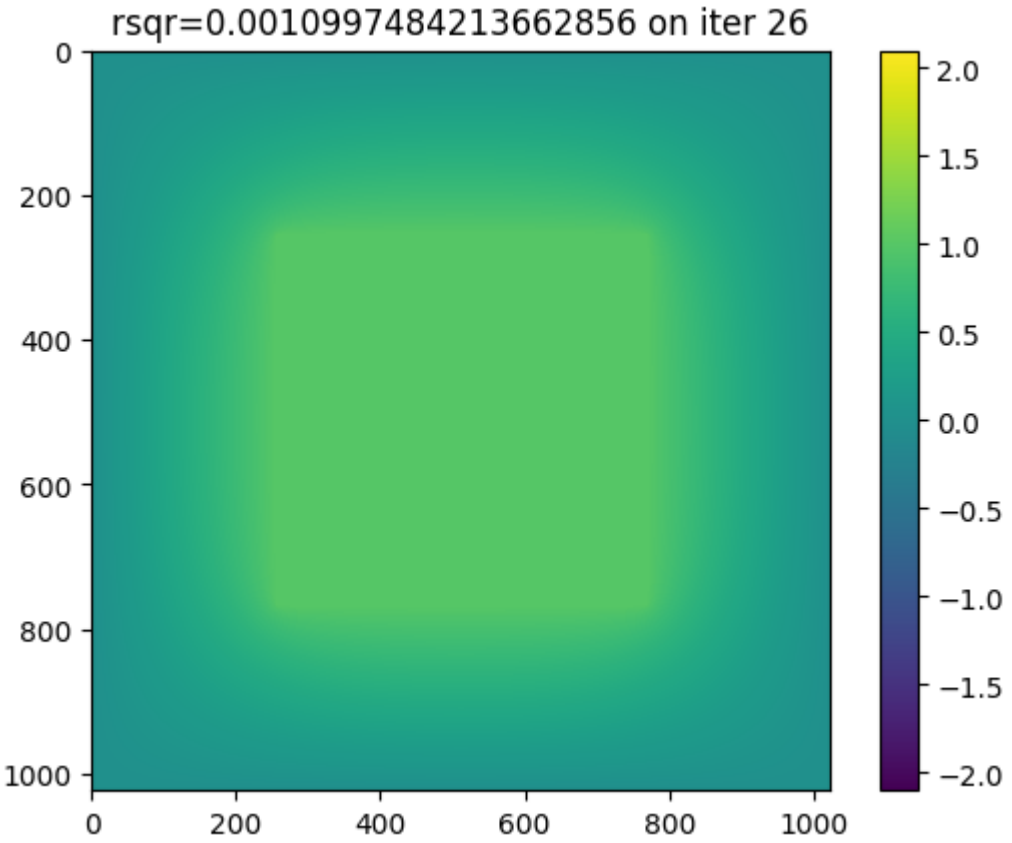

rsqr=0.0040607421336871 51 on iter 21
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

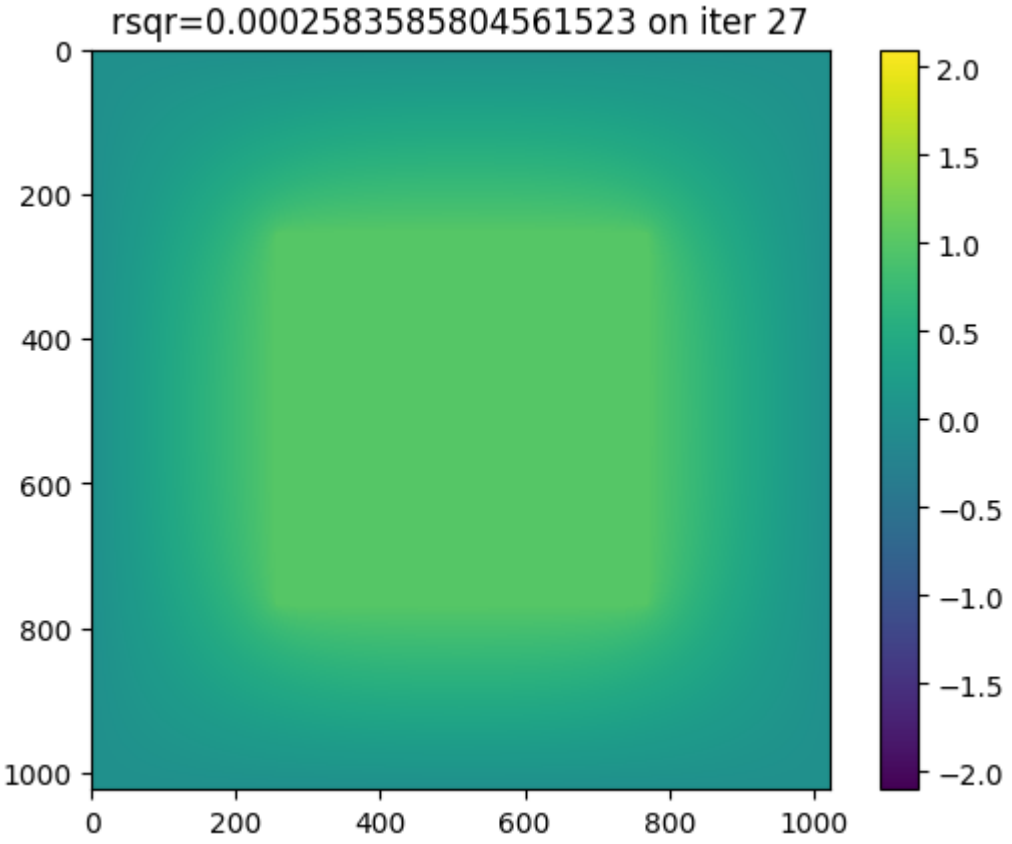

rsqr=0.0011995159930950213 on iter 22
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

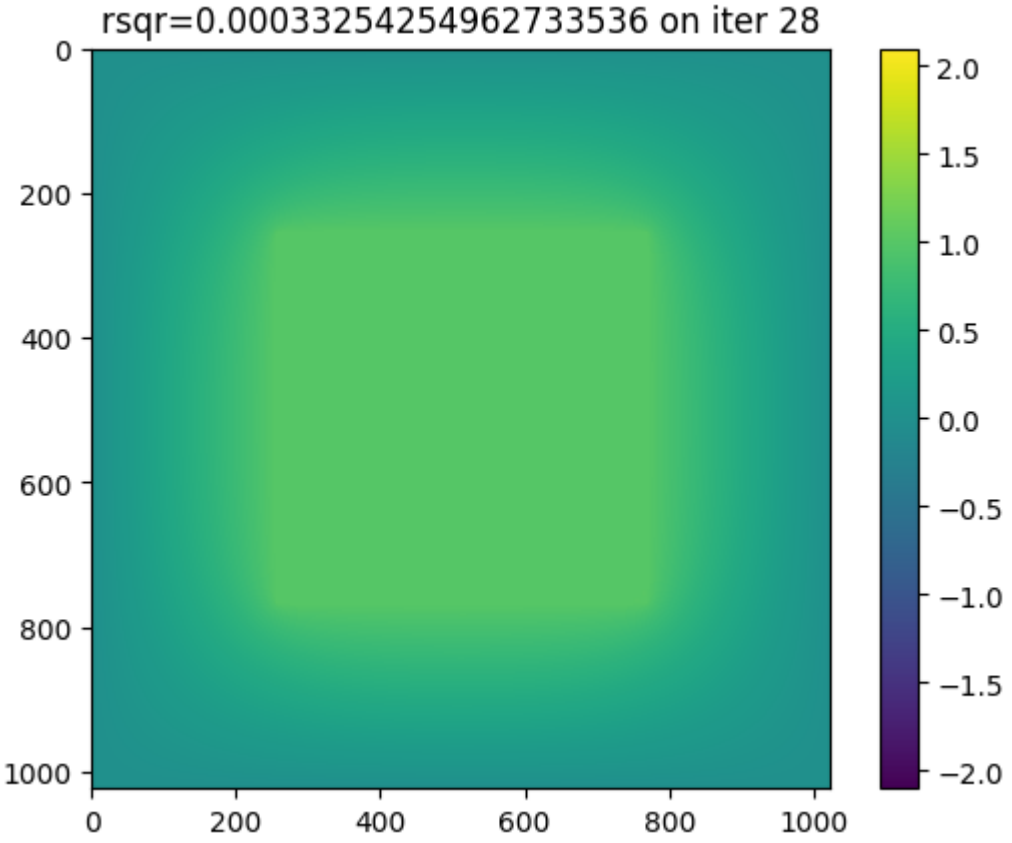

rsqr=0.00029554533212504977 on iter 23
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

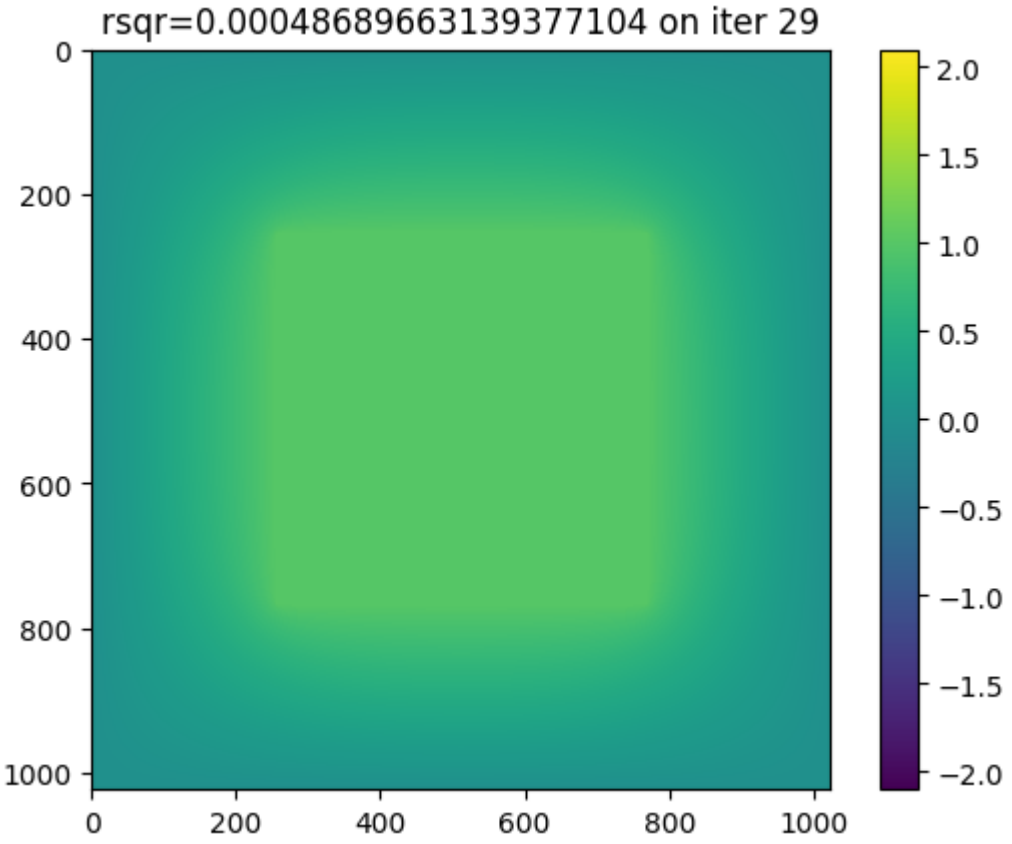

rsqr=0.0038110573319508944 on iter 24
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

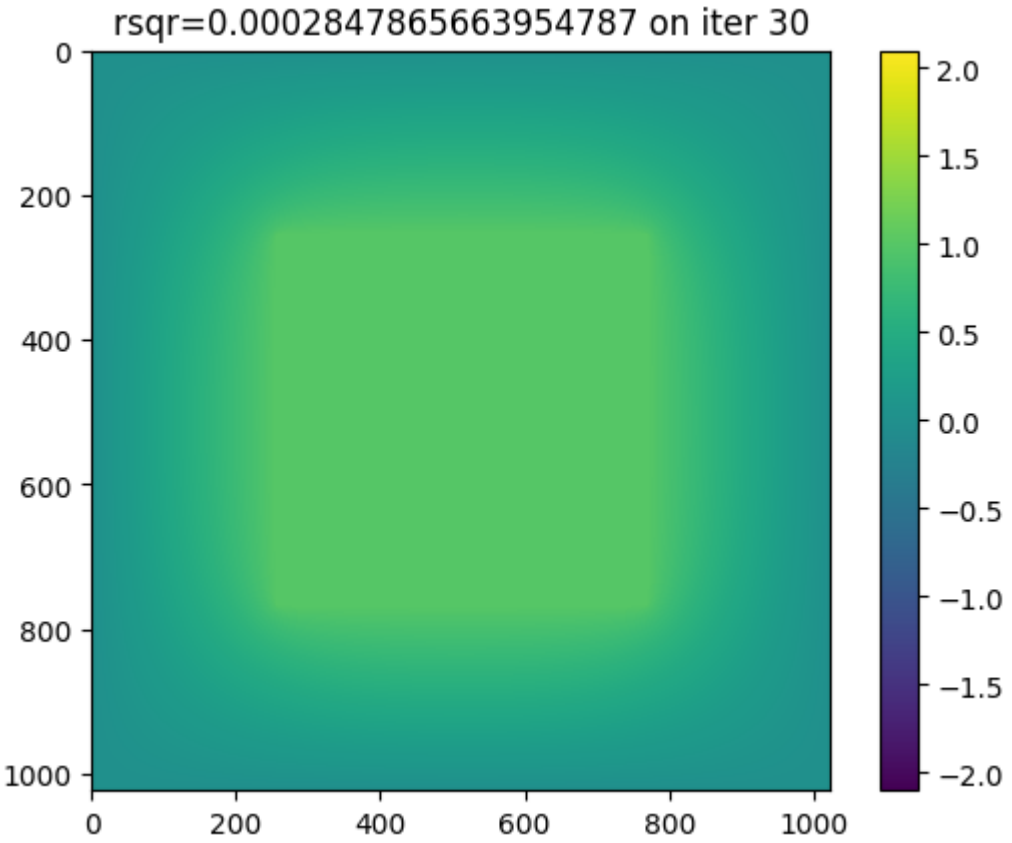

rsqr=0.0012524452919787268 on iter 25
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

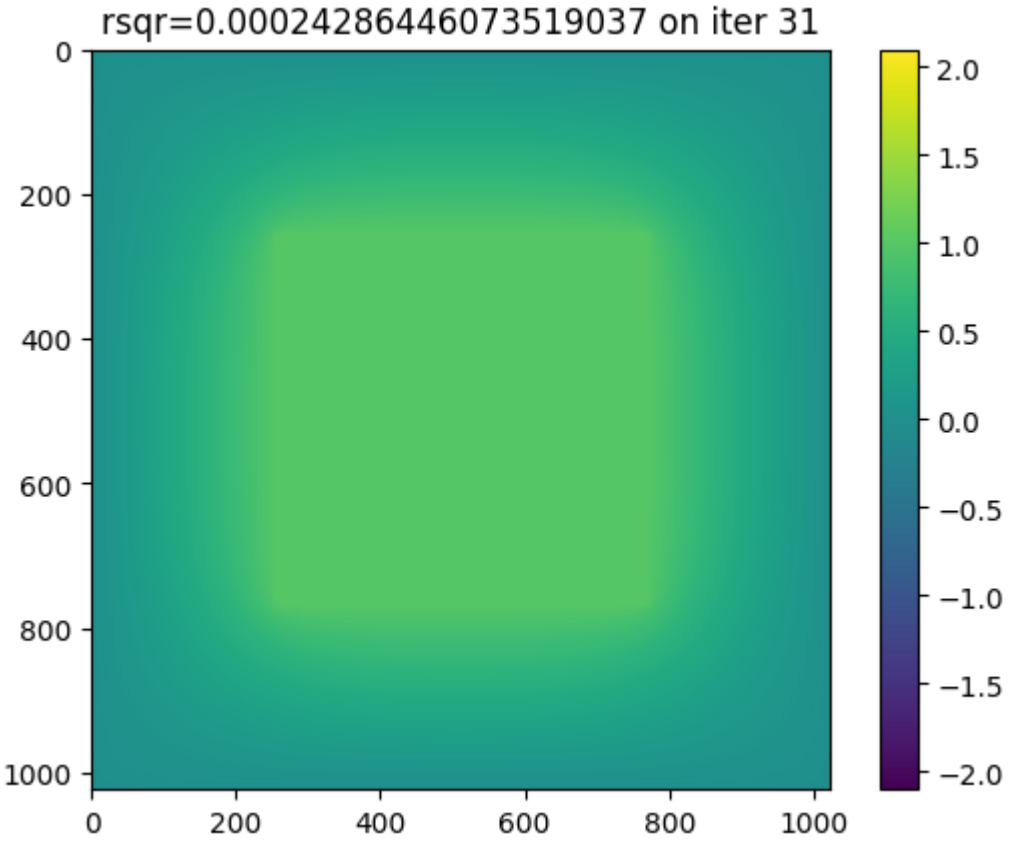

rsqr=0.0010997484213662856 on iter 26
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

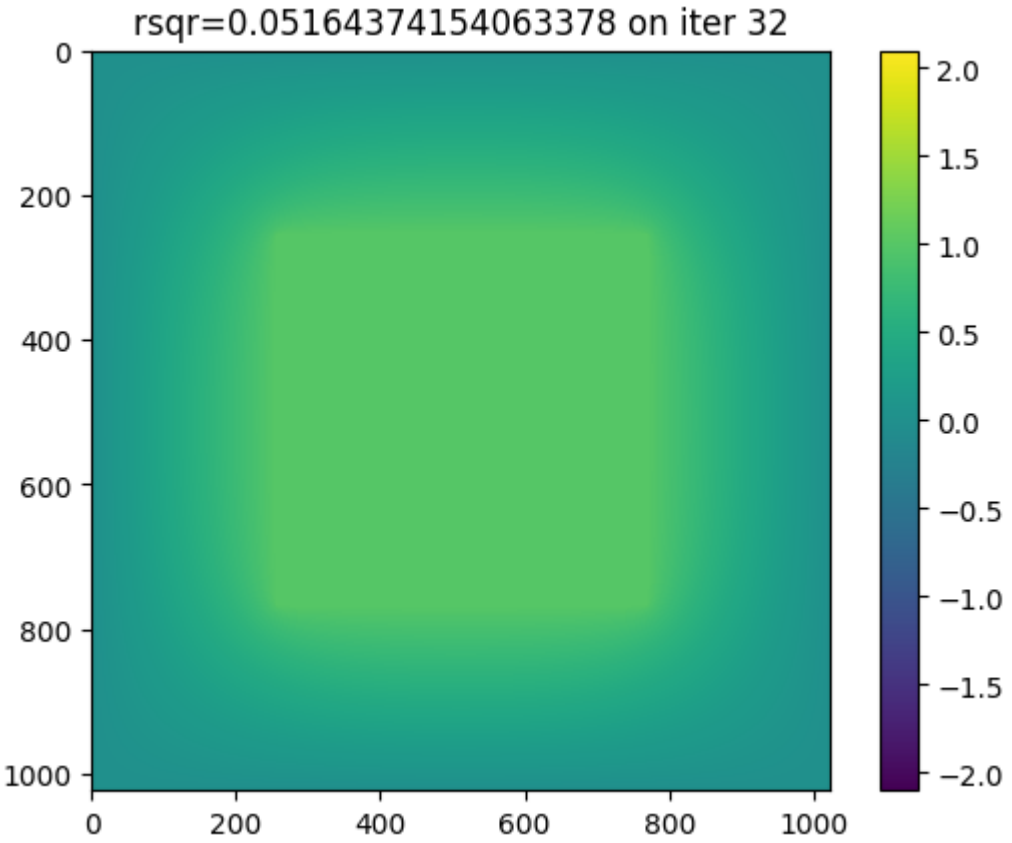

rsqr=0.0002583585804561523 on iter 27
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

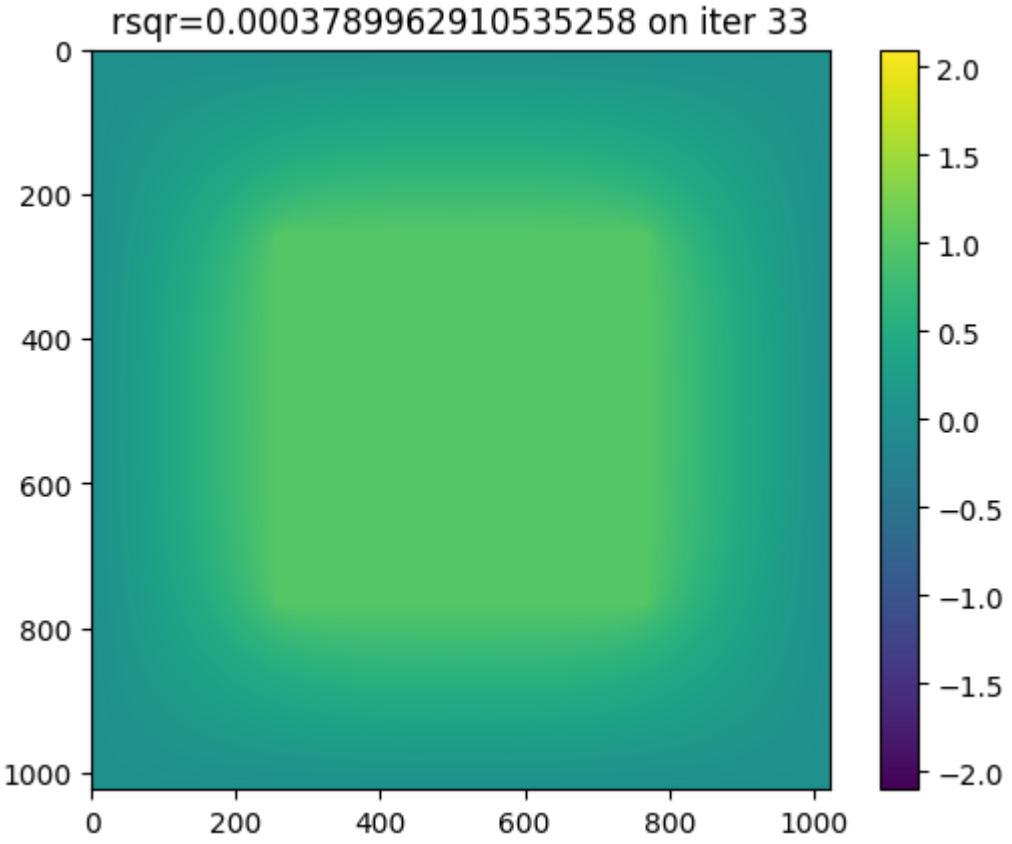

rsqr=0.0003325425496273536 on iter 28
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

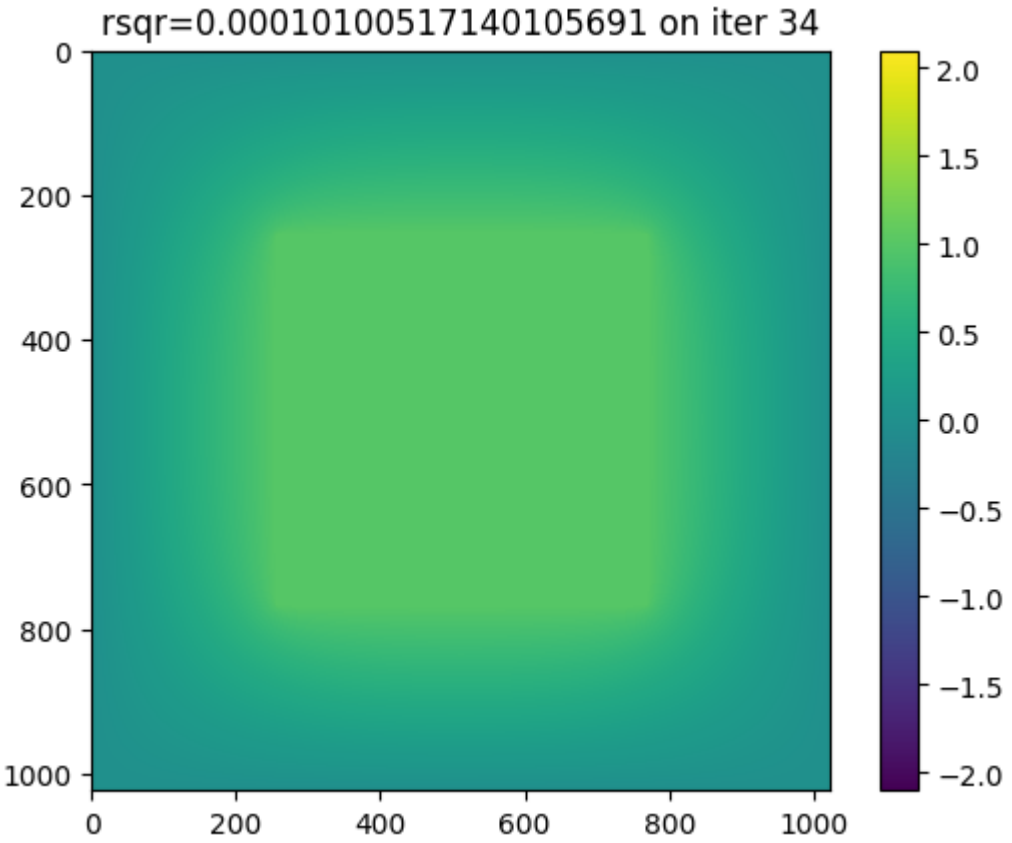

rsqr=0.00048689663139377104 on iter 29
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

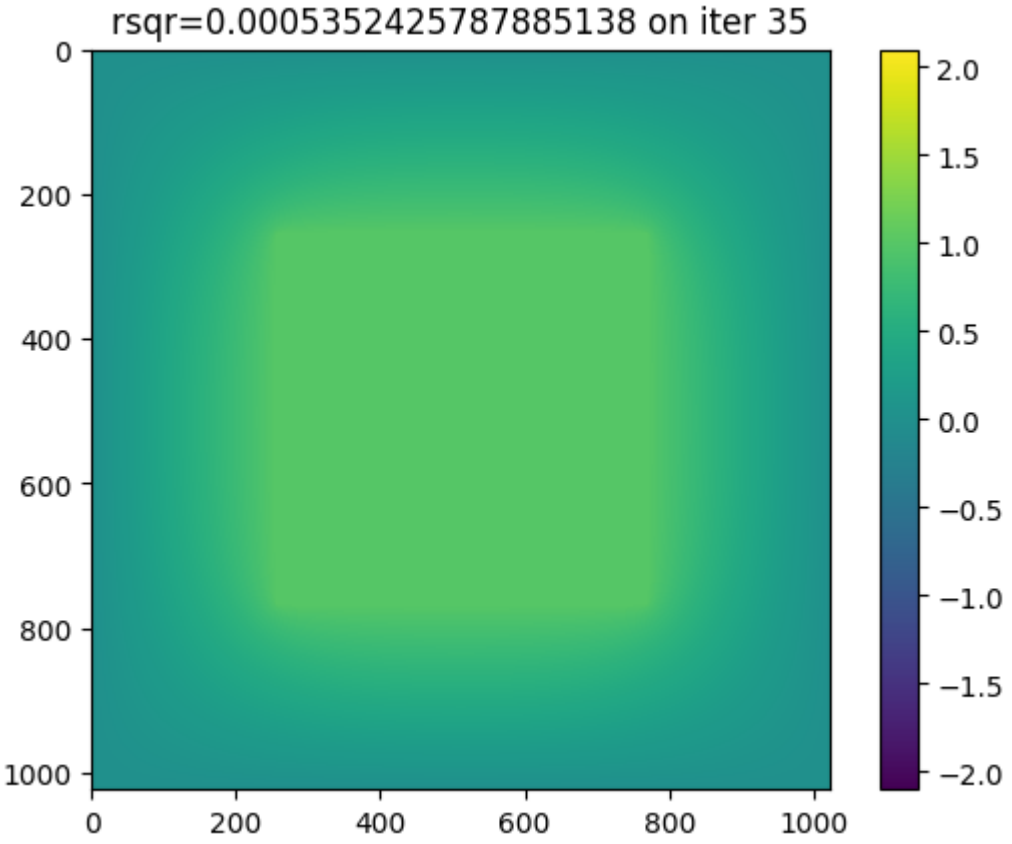

rsqr=0.0002847865663954787 on iter 30
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

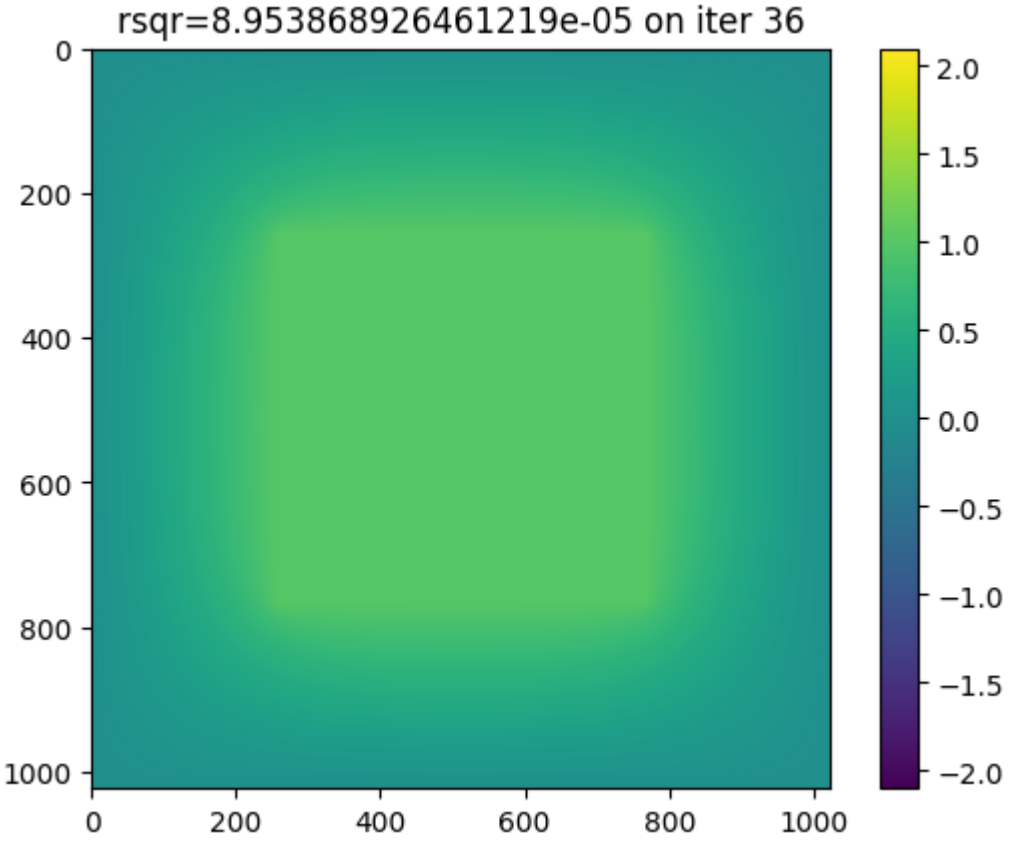

rsqr=0.00024286446073519037 on iter 31
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

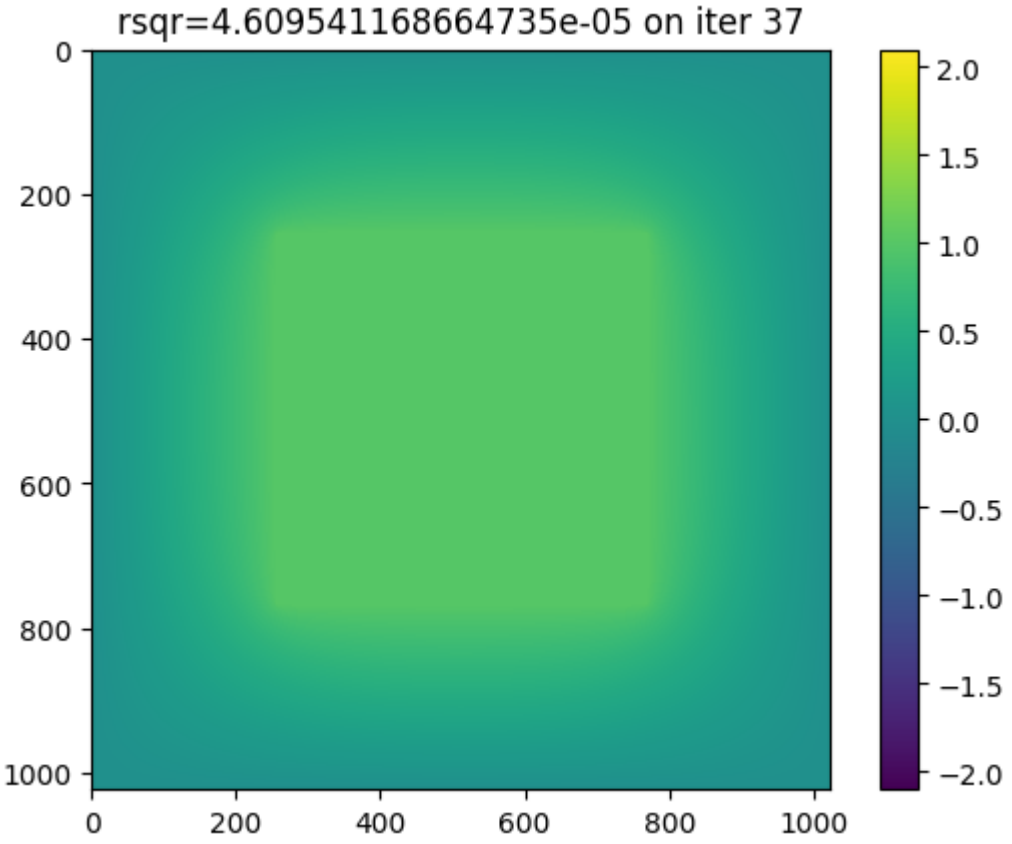

rsqr=0.05164374154063378 on iter 32
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

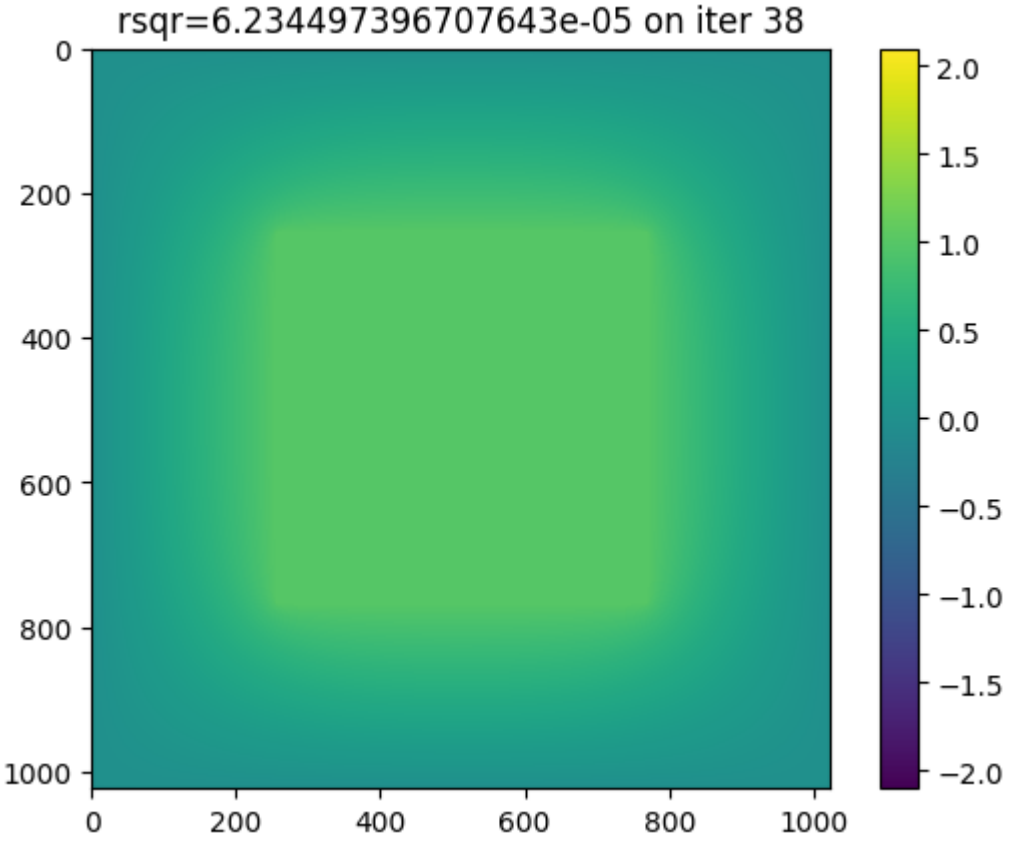

rsqr=0.0003789962910535258 on iter 33
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

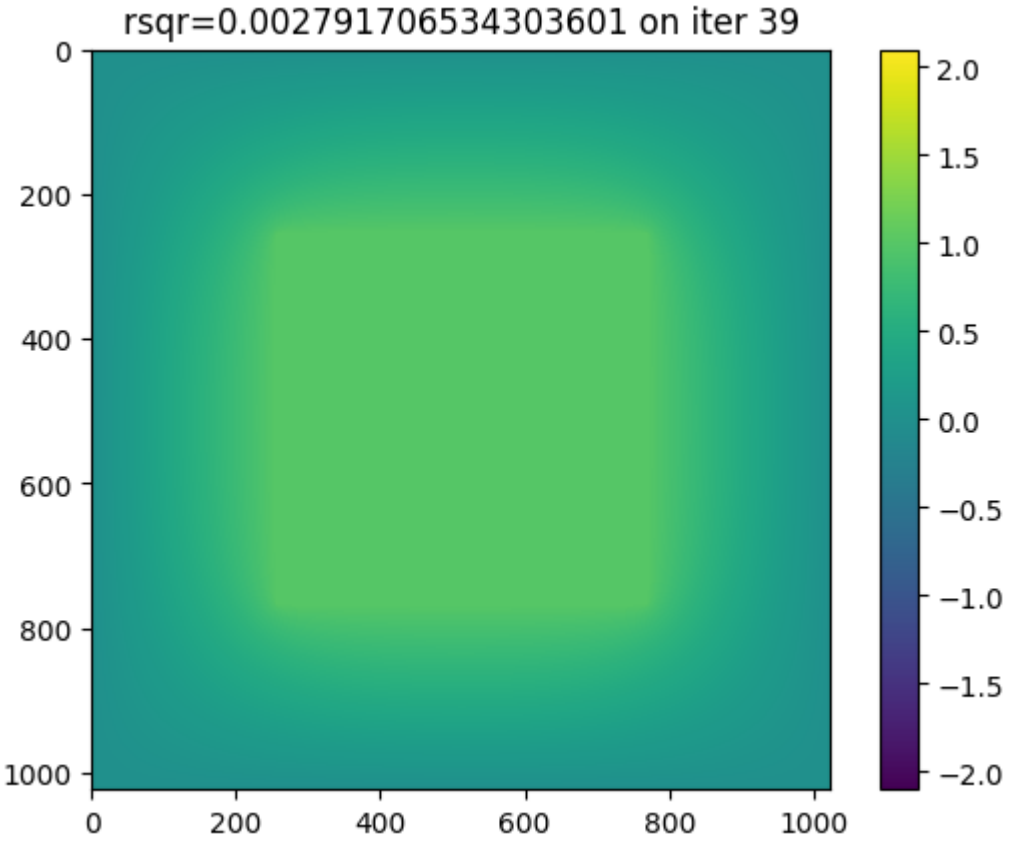

rsqr=0.00010100517140105691 on iter 34
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0

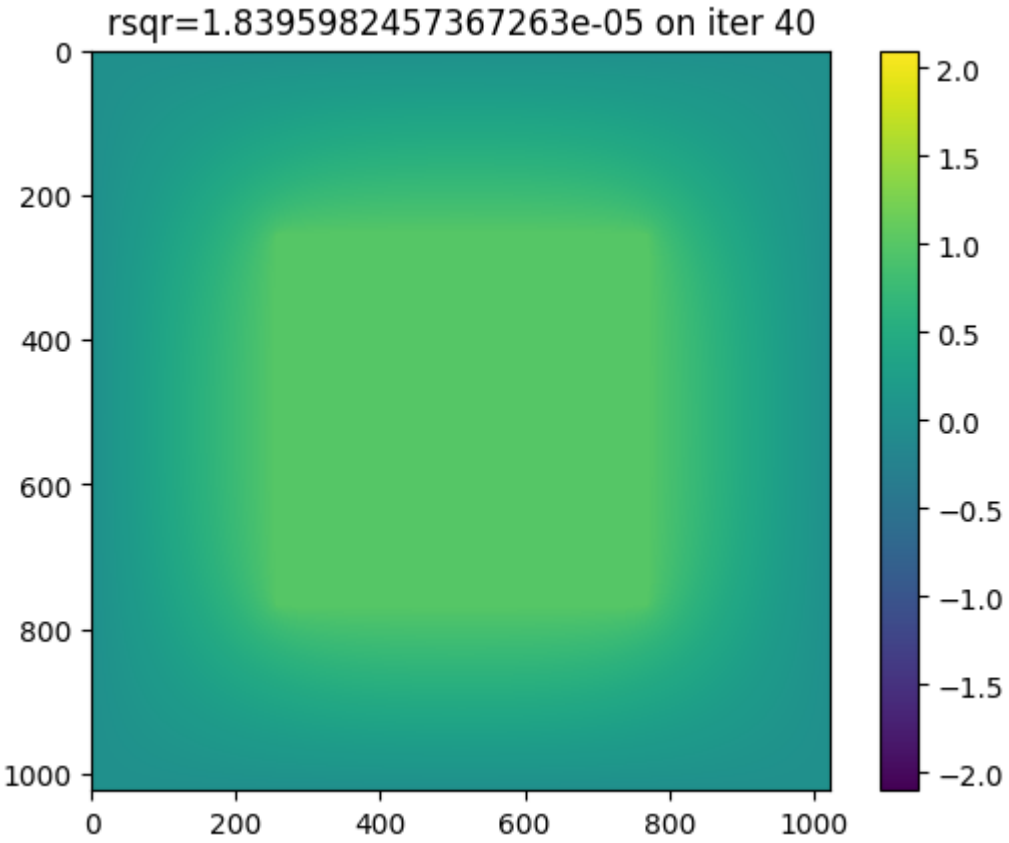

rsqr=0.0005352425787885138 on iter 35
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0


rsqr=8.953868926461219e-05 on iter 36
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0


rsqr=4.609541168664735e-05 on iter 37
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0


rsqr=6.234497396707643e-05 on iter 38
0
200
400
600
800
1000
0
200
400
600
800
1000
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0



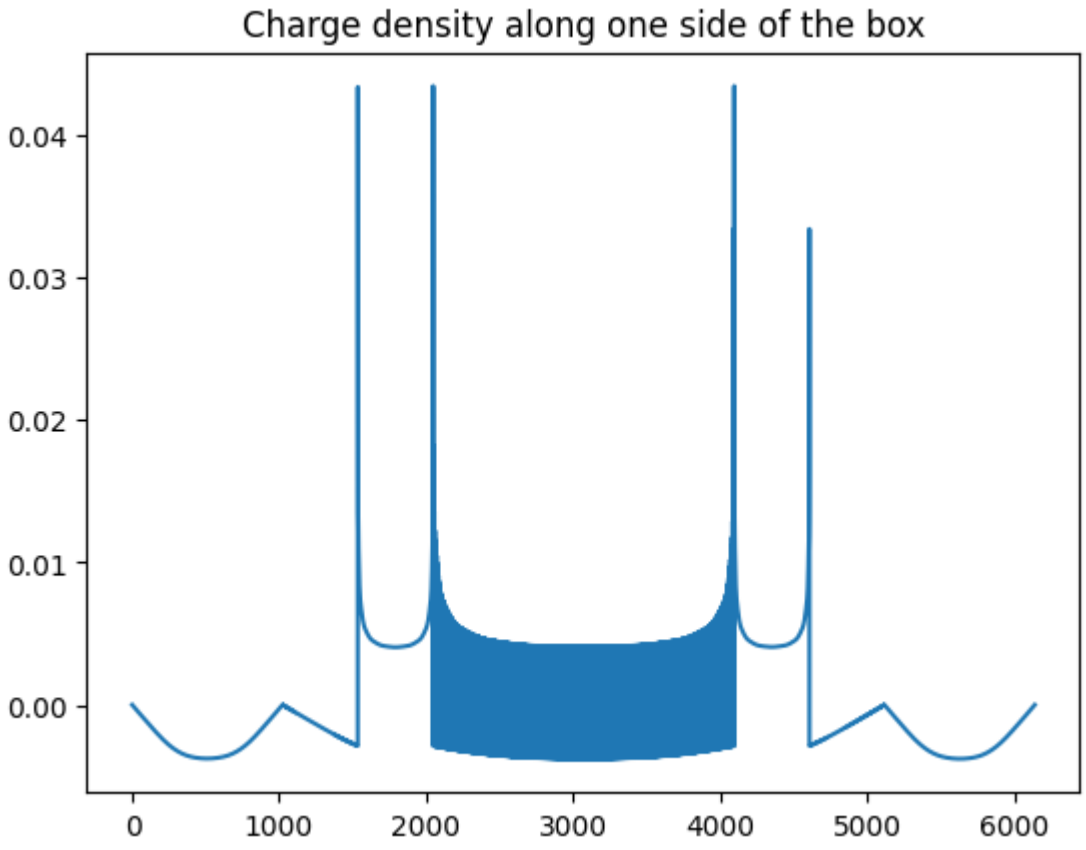



```
final rsqr is  0.00010513260959439755
```

In [281…

```
plt.plot(rho_out)
plt.title("Charge density along one side of the box")
```

Out[281]: Text(0.5, 1.0, 'Charge density along one side of the box')

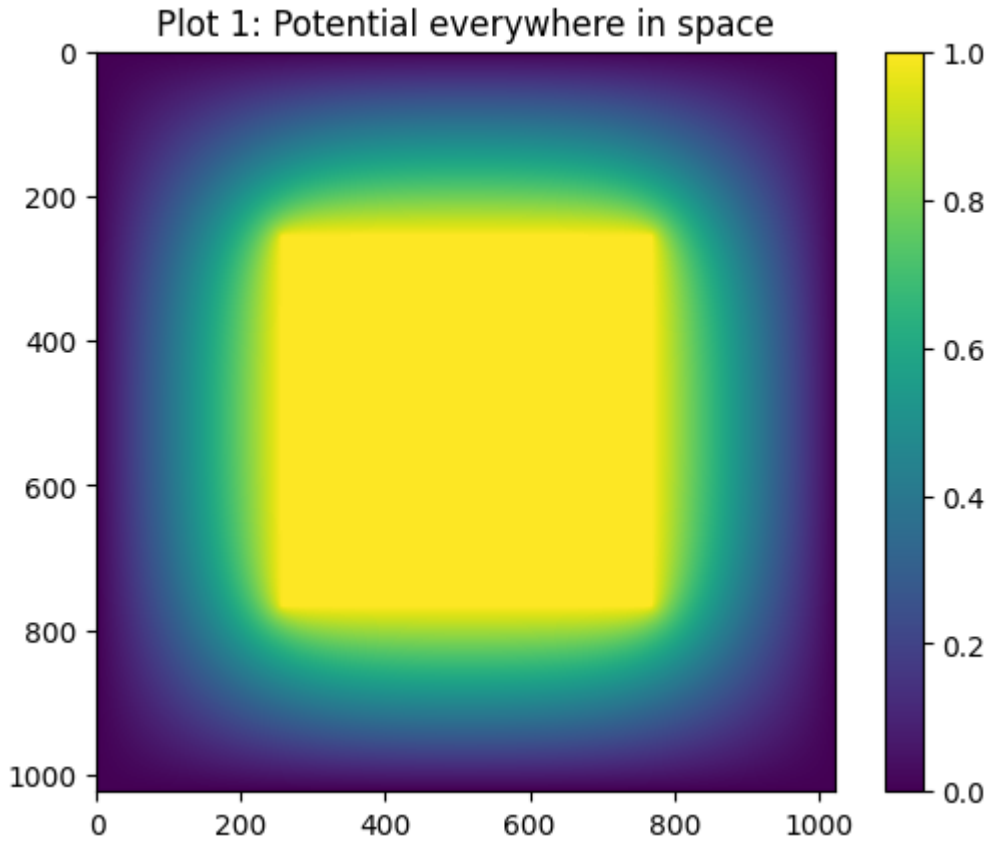


c)

Using this charge to find the potential everywhere in space:

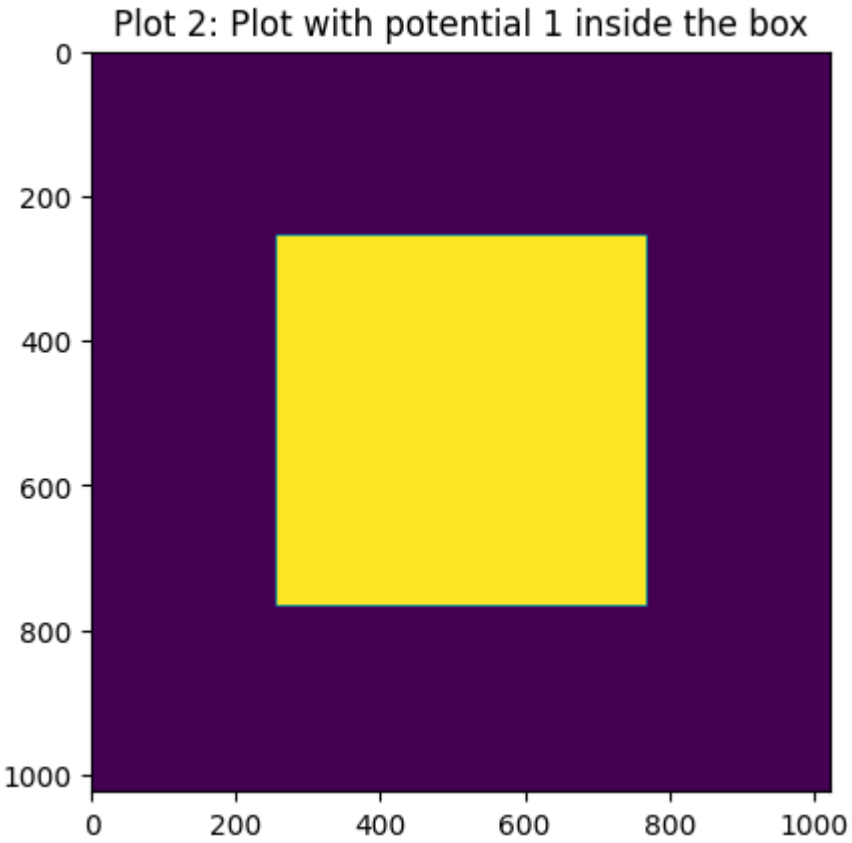
In [282…
```
pot=rho2pot_masked(rho_out,mask,kernelft,True)
plt.imshow(pot)
plt.colorbar()
plt.title("Plot 1: Potential everywhere in space")
```

Out[282]: Text(0.5, 1.0, 'Plot 1: Potential everywhere in space')



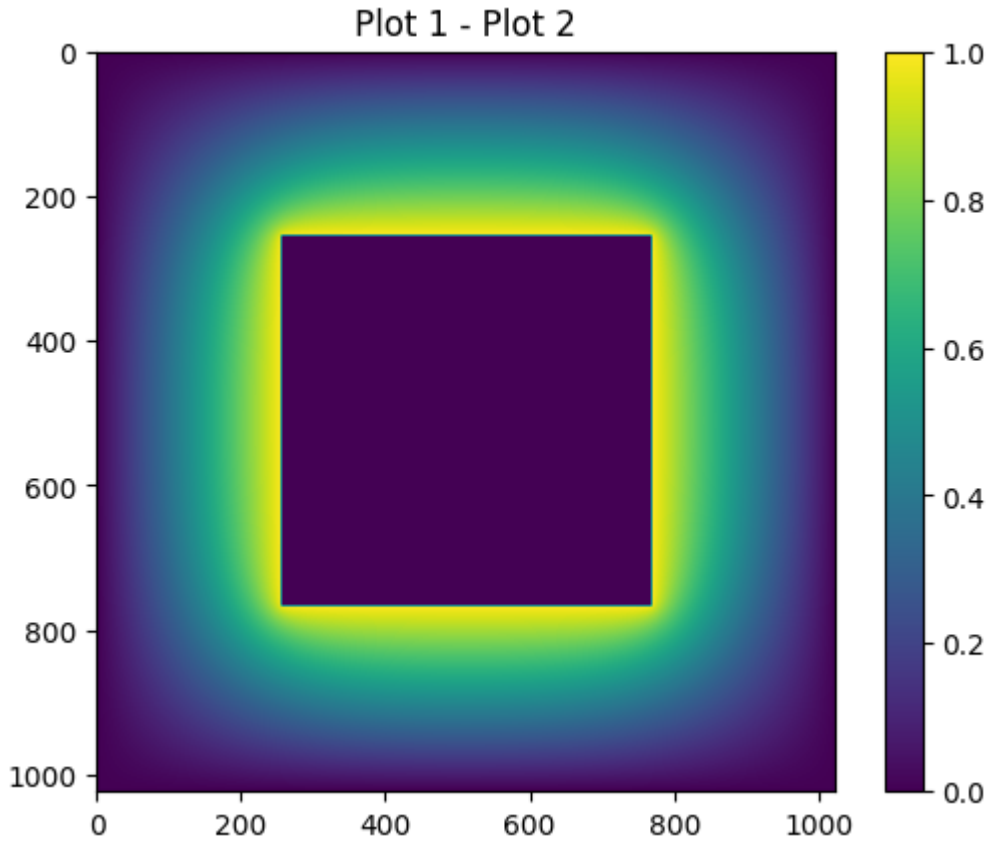
In [283…
```
pot_tmp = np.zeros([n,n])
pot_tmp[n//4:3*n//4,n//4:3*n//4] = 1
plt.imshow(pot_tmp)
plt.title("Plot 2: Plot with potential 1 inside the box")
```

Out[283]: Text(0.5, 1.0, 'Plot 2: Plot with potential 1 inside the box')



In [284…
```
diff = pot - pot_tmp
plt.imshow(diff)
plt.colorbar()
plt.title("Plot 1 - Plot 2")
```

Out[284]:
```
Text(0.5, 1.0, 'Plot 1 - Plot 2')
```

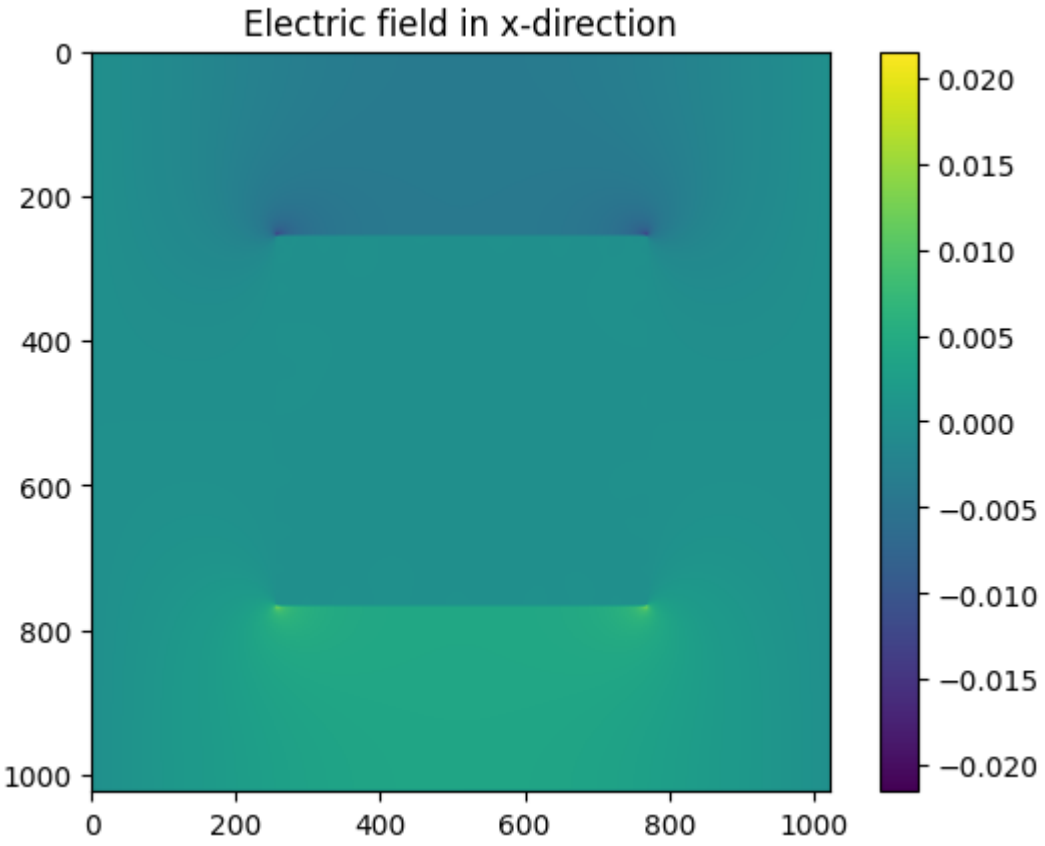


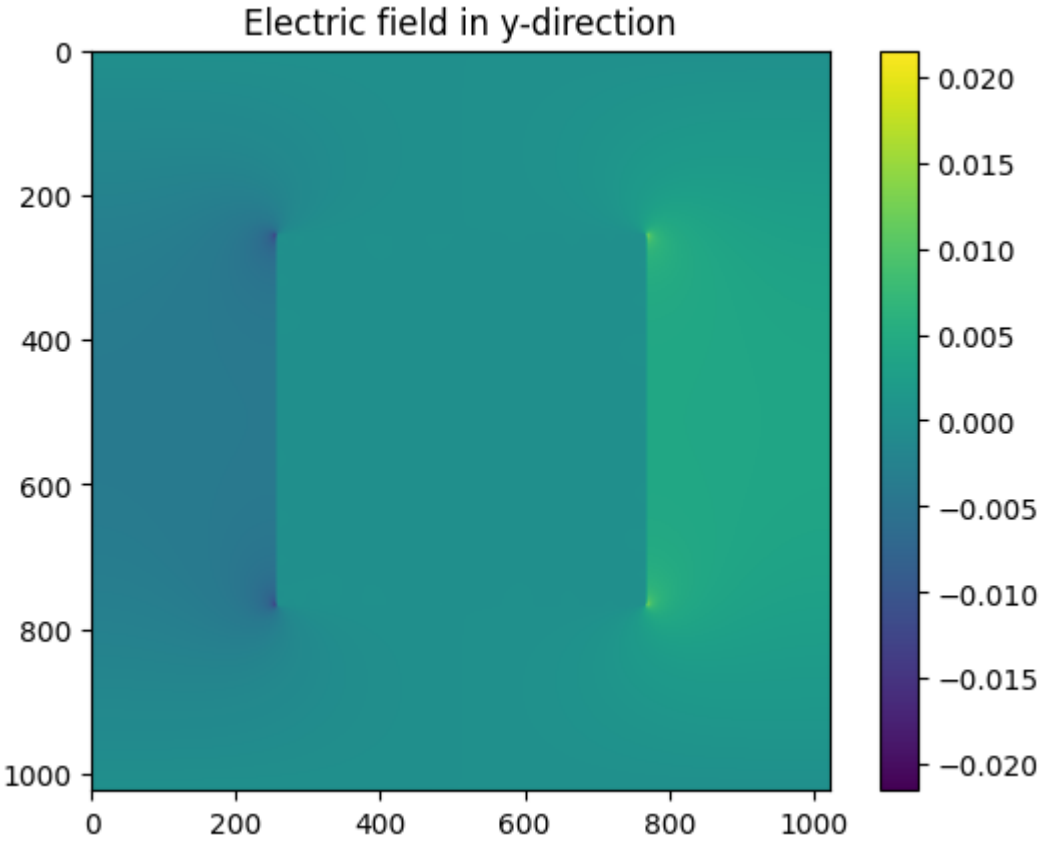
As can be seen from the above graphs, the potential inside the box is 1.

Since the electric field is the gradient of V, Ex = (V(x+1) - V(x))/dx and Ey = (V(y+1) - V(y))/dy:

In [285…
```
Ex = pot - np.roll(pot,-1,0)
Ey = pot - np.roll(pot, -1, -1)
plt.imshow(Ex)
plt.colorbar()
plt.title("Electric field in x-direction")
plt.figure()
plt.imshow(Ey)
plt.colorbar()
plt.title("Electric field in y-direction")
```

Out[285]: `Text(0.5, 1.0, 'Electric field in y-direction')`





As can be seen, the field is perpendicular to the equipotential surface of the square box and is thus as expected