

## PHYS 5794: Computational Physics HW 5

All program and output files can be found in: /home/k-class/rdcunha2/hw5

### **Method:**

A grid was chosen such that  $h=0.05$ , with 21 grid points in the x direction and 20001 grid points in the y direction, such that  $y$  varied  $\{0, 1000\}$  and  $x$  varied  $\{0, 1\}$ .

The grid was iterated over, using the finite difference formula to update the  $\varphi$ s, using the  $\varphi$ s calculated from before.

Formula:

$$\varphi^{\text{new}}(i, j) = (1-\omega)\varphi^{\text{old}}(i, j) - (\omega/4)*(\varphi(i+1, j) + \varphi(i, j+1) + \varphi(i-1, j) + \varphi(i, j-1))$$

The energy functional used to compute the final formula for phi was also calculated for each iteration.

Formula:

$$E = (h^2/2)*[(\{\varphi(i+1, j) - \varphi(i, j)\}/h)^2 + (\{\varphi(i, j+1) - \varphi(i, j)\}/h)^2]$$

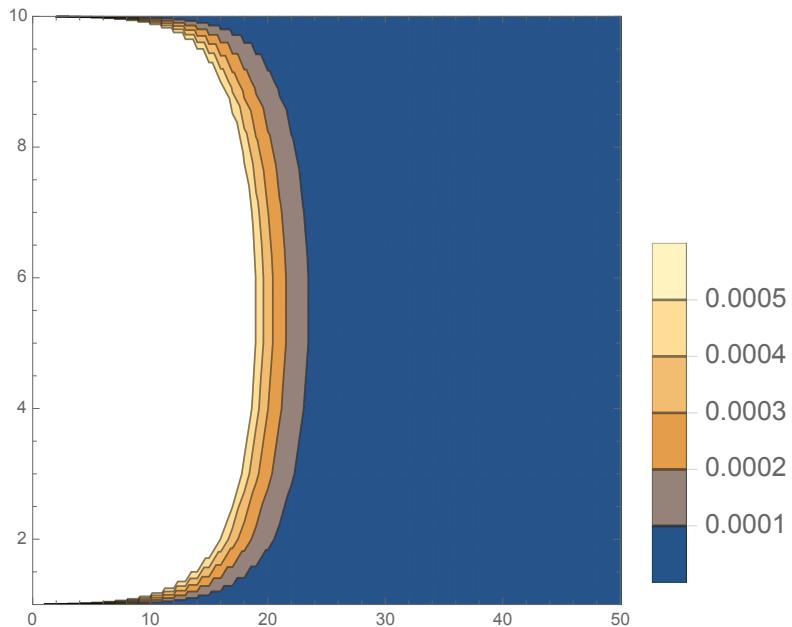
Convergence criterion was  $(\varphi^{\text{new}} - \varphi^{\text{old}})/n_i * n_j < 10^{-9}$

### **Verification of program:**

The matrix  $\varphi$  drops off exponentially from the boundary conditions and approaches zero. It has larger values towards  $x=0.5$  and drops down to 0 at both ends.

### **Data:**

**Figure 1. Contour plot of phi**



**Analysis:**

For h=0.05

$\omega$	E from program	E from analytical solution
0.5	0.0567881	0.03333
1.0	0.0567879	0.03333
1.5	0.0567879	0.03333

For  $\omega=0.5$ 

Grid spacing h	E from program	E analytical solution
0.01	0.068188*	0.03333
0.05	0.0567881	0.03333
0.1	0.0611994	0.03333

\*This value took too long to converge, so the criterion was relaxed to  $10^{-6}$ , which may have resulted in a higher value than with a smaller convergence criterion.

The analytical solution was calculated(attached).

**Interpretation:**

For the same grid spacing, changing the value of  $\omega$  from 0.5 to 1.0 and 1.5 does not change the value of the converged energy functional E(Table 2)

The size of the grid spacing relative to the size of  $\omega$  changes the value of the energy.(Table 3) A smaller grid spacing means a more converged energy, however, the time taken by the program increases, and the convergence criteria must be changed

**Log:**

8 hours

$$\frac{\delta^2 \phi}{\delta x^2} \neq \frac{\delta^2 \phi}{\delta y^2} = 0$$

$$\phi(x, y) = X(x) Y(y)$$

Separating the variables,

$$Y(y) \frac{\delta^2 X(x)}{\delta x^2} + X(x) \frac{\delta^2 Y(y)}{\delta y^2} = 0$$

$$\Rightarrow \frac{1}{X} \frac{\delta^2 X}{\delta x^2} = - \frac{1}{Y} \frac{\delta^2 Y}{\delta y^2}$$

These are dependent on different variables, so we can equate both sides to a constant,  $\lambda^2$ .

$$\frac{1}{X} \frac{\delta^2 X}{\delta x^2} = -\lambda^2 \Rightarrow \frac{\delta^2 X}{\delta x^2} = -\lambda^2 X$$

$$\frac{1}{Y} \frac{\delta^2 Y}{\delta y^2} = \lambda^2 \Rightarrow \frac{\delta^2 Y}{\delta y^2} = \lambda^2 Y$$

$$\text{with boundary conditions } \phi(0, y) = 0$$

$$\phi(1, y) = 0$$

$$X(x) = \sin n\pi x$$

$$\text{With boundary condition } \phi(x, 0) = 0$$

$$Y(y) = e^{-\lambda^2 y}$$

$$\text{But for the boundary condition } \phi(x, 0) = x(1-x)$$

we must have a linear combination of sin functions making up  $x(1-x)$

$$\text{So } \sum_n A_n \sin n\pi x = x(1-x)$$

$$\Rightarrow A_n = \int_0^1 x(1-x) \sin n\pi x \, dx$$

$$= \frac{2(1 - \cos n\pi)}{n^3 \pi^3}$$

$$\begin{aligned}\therefore \phi(x, y) &= \sum_n A_n X_n(x) Y_n(y) \\ &= \sum_n \frac{2(1 - \cos n\pi)}{n^3 \pi^3} \sin n\pi x e^{-n\pi y}\end{aligned}$$

$$\begin{aligned}E &= \int_0^1 dx \int_0^1 dy \frac{1}{2} [(\nabla \phi)^2 - \phi^2] \\ &= \int_0^1 dx \int_0^1 dy \frac{1}{2} [(\nabla \phi)^2] \\ &= \sum_n \frac{4(1 - \cos n\pi)}{n^4 \pi^4} \int_0^1 dy \left( \int_0^1 \cos n\pi x du - \int_0^1 \sin n\pi x du \right)^2 e^{-2n\pi y} \\ &= \sum_n \frac{2(1 - \cos n\pi)}{n^4 \pi^4} \int_0^1 dy \left( \frac{2}{n\pi} \right)^2 e^{-2n\pi y} \\ &= \sum_n \frac{8(1 - \cos n\pi)}{n^6 \pi^6} \cdot \frac{1}{n\pi} \\ &= \sum_n \frac{8(1 - \cos n\pi)}{n^7 \pi^7} \\ &\approx 0.03333\end{aligned}$$