Math 228B
Homework 2
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Introduction

In this problem set, we want to solve 3-D heat equation which is written as

$$u_t = \alpha \nabla^2 u$$

This equation describes heat (or temperature variation) in a region (S) over time. α is a positive constant and is called thermal diffusivity of the medium. Actually this constant physically imply that how fast the temperature is moving in the region.For solving heat equation we need boundary conditions on ∂S and one initial condition in S.

This equation is important since volumetric concentration, heat diffusion or even wave function of a single particle are all described with this equation. In this problem set, we will discuss about coordinate transformation to spherical coordinates and try to find numerically solve symmetric spherical problem. We will also discuss about different schemes to solve diffusion equation in 2 and 3 dimensions.

We will also discuss Crank Nicolson method and we will try to find its order of accuracy.

Problem

Crank Nicolson method for equation

$$\frac{\partial u}{\partial t} = F\left(x, t, u, u_x, u_{xx}\right) \tag{1}$$

is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha}{2\left(\Delta x\right)^2}\left(\left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right) + \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)\right) \tag{2}$$

For this scheme we will try to find the order and accuracy.

Another problem in this problem set is 3-D heat equation

$$u_t = \alpha \nabla^2 u$$

For this equation, we will find stability condition if we use forward Euler for time and D_+D_- for second derivatives on spatial coordinates. We will also discuss ADT method and its stability.

We will change coordinates to spherical coordinate and find form of heat equation in this coordinate which is

$$u_t = \alpha\nabla^2 u = \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)u \tag{3}$$

We will solve two different problems, one in spherical coordinate and one in cartesian coordinates.

Implementation

The scheme used for Crank-Nicholson is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2}\left[F_i^{n+1}\left(x, t, u, u_x, u_{xx}\right) + F_i^n\left(x, t, u, u_x, u_{xx}\right)\right] \tag{4}$$

which for 1-D heat equation ($u_t = \alpha u_{xx}$) could be written as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha}{2\left(\Delta x\right)^2}\left(\left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right) + \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)\right) \tag{5}$$

Scheme that we used for 3-d heat equation ($u_t = \alpha\nabla^2 u$) is

$$\begin{aligned}\frac{u_{i,j,k}^{n+1} - u_{i,j,k}^n}{\Delta t} = \alpha\Bigg(&\frac{u_{i+1,j,k}^n - 2u_{i,j,k}^n + u_{i-1,j,k}^n}{\Delta x^2} \\ &+\frac{u_{i,j+1,k}^n - 2u_{i,j,k}^n + u_{i,j-1,k}^n}{\Delta y^2} \\ &+\frac{u_{i,j,k+1}^n - 2u_{i,j,k}^n + u_{i,j,k-1}^n}{\Delta z^2}\Bigg)\end{aligned} \tag{6}$$

We also discussed alternating direction implicit(ADI) method, which is written as

$$\begin{aligned}u^{n+1/3} - u^n = \frac{\alpha\Delta t}{h^2}\Big[&\left(u_{i+1,j,k}^{n+1/3} - 2u_{i,j,k}^{n+1/3} + u_{i-1,j,k}^{n+1/3}\right) + \left(u_{i,j+1,k}^n - 2u_{i,j,k}^n + u_{i,j-1,k}^n\right) \\ &+ \left(u_{i,j,k+1}^n - 2u_{i,j,k}^n + u_{i,j,k-1}^n\right)\Big]\end{aligned} \tag{7}$$

and same two other steps as

$$\begin{aligned}u^{n+2/3} - u^{n+1/3} = \frac{\alpha\Delta t}{h^2}\Big[&\left(u_{i+1,j,k}^{n+1/3} - 2u_{i,j,k}^{n+1/3} + u_{i-1,j,k}^{n+1/3}\right) + \left(u_{i,j+1,k}^{n+2/3} - 2u_{i,j,k}^{n+2/3} + u_{i,j-1,k}^{n+2/3}\right) \\ &+ \left(u_{i,j,k+1}^{n+1/3} - 2u_{i,j,k}^{n+1/3} + u_{i,j,k-1}^{n+1/3}\right)\Big]\end{aligned} \tag{8}$$

and

$$\begin{aligned}u^{n+1} - u^{n+2/3} = \frac{\alpha\Delta t}{h^2}\Big[&\left(u_{i+1,j,k}^{n+1/3} - 2u_{i,j,k}^{n+2/3} + u_{i-1,j,k}^{n+2/3}\right) + \left(u_{i,j+1,k}^{n+2/3} - 2u_{i,j,k}^{n+2/3} + u_{i,j-1,k}^{n+2/3}\right) \\ &+ \left(u_{i,j,k+1}^{n+1} - 2u_{i,j,k}^{n+1} + u_{i,j,k-1}^{n+1}\right)\Big]\end{aligned} \tag{9}$$

Problems

1. Prove that the truncation error for Crank-Nicholson is second order in space and time.

   Crank-Nicolson method is a numerical scheme often applied to diffusion equation ($u_t = \alpha u_{xx}$). This method is based on central difference in space and trapezoidal rule in time. Consider partial differential equation

$$\frac{\partial u}{\partial t} = F\left(x, t, u, u_x, u_{xx}\right) \tag{10}$$

   let $u\left(i\Delta x, n\Delta t\right) = u_i^n$. The method of Crank Nicolson in a combination of forward Euler and backward Euler. However, this method is not simply an average. Because it contains both methods in an implicit way. Crank-Nocolson method could be written as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2}\left[F_i^{n+1}\left(x, t, u, u_x, u_{xx}\right) + F_i^n\left(x, t, u, u_x, u_{xx}\right)\right] \tag{11}$$

   where F must be discretized spatially with central difference. If we apply Crank-Nicolson to 1-D diffusion equation $u_t = \alpha u_{xx}$, we will have

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha}{2\left(\Delta x\right)^2}\left(\left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right) + \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)\right) \tag{12}$$

   We first expand one of the central difference in spatial coordinate to find it's error, we have

$$\begin{aligned} u_{i+1}^n - 2u_i^n + u_{i-1}^n &= u_i^n + u_x\Delta x + \frac{1}{2}u_{xx}\Delta x^2 + \frac{1}{3!}u_{xxx}\Delta x^3 + O\left(\Delta x^4\right) \\ &- 2u_i^n \\ &+ u_i^n - u_x\Delta x + \frac{1}{2}u_{xx}\Delta x^2 - \frac{1}{3!}u_{xxx}\Delta x^3 + O\left(\Delta x^4\right) \\ &= u_{xx}\Delta x^2 + O\left(\Delta x^4\right) \end{aligned}$$

   Expanding LHS over time and RHS over the space we will have

$$\frac{u_i^n + u_t\Delta t + \frac{1}{2}u_{tt}\left(\Delta t\right)^2 + O(\Delta t^3) - u_i^n}{\Delta t} = \frac{\alpha}{2\left(\Delta x\right)^2}\left(u_{xx}^{n+1}\Delta x^2 + O\left(\Delta x^4\right) + u_{xx}^n\Delta x^2 + O\left(\Delta x^4\right)\right) \tag{13}$$

   Henceforth,

$$u_t + \frac{1}{2}u_{tt}\Delta t + O\left(\Delta t^2\right) = \frac{\alpha}{2}\left(u_{xx}^n + u_{xxt}\Delta t + O\left(\Delta t^2\right) + u_{xx}^n\Delta x^2 + O\left(\Delta x^2\right)\right) \tag{14}$$

$$u_t + \frac{1}{2}u_{tt}\Delta t + O\left(\Delta t^2\right) = \alpha u_{xx} + \frac{\alpha}{2}u_{xxt}\Delta t + O\left(\Delta t^2\right) + O\left(\Delta x^2\right) \tag{15}$$

From the heat equation we know that $u_t = \alpha u_{xx}$, so we will have $u_{xxt} = u_{tt}$. This way both $\frac{1}{2}u_{tt}\Delta t$ on both sides cancel each other, so we get

$$u_t - \alpha u_{xx} = O\left(\Delta t^2\right) + O\left(\Delta x^2\right)$$

So, we started from the scheme , and we reached to the diffusion equation, with some order Δt^2 and Δx^2 on the other side. So, the scheme is heat equation up to order Δt^2 and Δx^2. So our scheme is order 2 in both space and time.

2. Consider the partial differential equation (*) given by $u_t = u_{xx} + u_{yy} + u_{zz}$

   (a) Derive a stability requirement on $\lambda = k/h^2$ (what is h?)
   In here, we will consider two different scheme, and then try to find stability condition for them.

      i. Forward Euler in time and centeral difference in space We consider same space interval of h, and time interval of k. the scheme suggests

$$\begin{aligned}\frac{u^{n+1}_{i,j,k} - u^n_{i,j,k}}{\Delta t} = \alpha \Bigg(& \frac{u^n_{i+1,j,k} - 2u^n_{i,j,k} + u^n_{i-1,j,k}}{\Delta x^2} \\ & + \frac{u^n_{i,j+1,k} - 2u^n_{i,j,k} + u^n_{i,j-1,k}}{\Delta y^2} \\ & + \frac{u^n_{i,j,k+1} - 2u^n_{i,j,k} + u^n_{i,j,k-1}}{\Delta z^2}\Bigg)\end{aligned} \tag{16}$$

If we do the Von-Neumann stability analysis for this method and trying to find the amplification factor, considering fourier transform on x,y and z we have

$$u^n_{i,j,k}\left(x,y,z\right) = \frac{1}{2\pi}\int \hat{u}^n_{i,j,k}\left(l,m,n\right)e^{ilx}e^{imy}e^{inz}dl\ dm\ dn \tag{17}$$

if we put this equation into our scheme and suppose that $\Delta x = \Delta y = \Delta z = h$ and $\Delta t = k$, we will have

$$\begin{aligned}&\frac{1}{2\pi}\int \hat{u}^{n+1}_{i,j,k}e^{i(lx+my+nz)}dl\ dm\ dn = \\ &\quad\left(\frac{\alpha k}{h^2}\right)\frac{1}{2\pi}\int \hat{u}^n_{i,j,k}e^{i(lx+my+nz)}\left(e^{ilh} + e^{-ilh} + e^{imh} + e^{-imh} + e^{inh} + e^{-inh} - 8\right)\end{aligned} \tag{18}$$

Since $e^{ilh} + e^{-ilh} - 2 = -2\sin(lh/2)$, It can be easily seen that

$$\hat{u}^{n+1} = \hat{u}^n\left(1 - \frac{4\alpha k}{h^2}\left(\sin^2\frac{lh}{2} + \sin^2\frac{mh}{2} + \sin^2\frac{nh}{2}\right)\right) \tag{19}$$

So the amplification factor $\hat{G}$ becomes

$$\hat{G}(l,m,n) = 1 - \frac{4\alpha k}{h^2}\left(\sin^2\frac{lh}{2} + \sin^2\frac{mh}{2} + \sin^2\frac{nh}{2}\right)$$

In the above equation we define $\lambda := \frac{k}{h^2}$. For stability, we demand that $|\hat{G}| \le 1$, so this would mean that

$$-1 \le 1 - 4\alpha\lambda(1+1+1) \le 1$$

This would easily imply that

$$\boxed{\alpha\lambda \le \frac{1}{6}}$$

So our method, is stable if $\lambda \le \frac{1}{6\alpha}$.

ii. Alternating direction implicit method (known as ADI) In this method, we take fractional steps in time, we first treat one row implicitly and solve backward euler, then we take other rows implicitly and solve implicitly and so forth. The method is as follows

$$u^{n+1/3} - u^n = \frac{\alpha\Delta t}{h^2}\Big[\Big(u^{n+1/3}_{i+1,j,k} - 2u^{n+1/3}_{i,j,k} + u^{n+1/3}_{i-1,j,k}\Big) + \big(u^n_{i,j+1,k} - 2u^n_{i,j,k} + u^n_{i,j-1,k}\big) + \big(u^n_{i,j,k+1} - 2u^n_{i,j,k} + u^n_{i,j,k-1}\big)\Big] \tag{20}$$

and same two other steps as

$$u^{n+2/3} - u^{n+1/3} = \frac{\alpha\Delta t}{h^2}\Big[\Big(u^{n+1/3}_{i+1,j,k} - 2u^{n+1/3}_{i,j,k} + u^{n+1/3}_{i-1,j,k}\Big) + \Big(u^{n+2/3}_{i,j+1,k} - 2u^{n+2/3}_{i,j,k} + u^{n+2/3}_{i,j-1,k}\Big) + \Big(u^{n+1/3}_{i,j,k+1} - 2u^{n+1/3}_{i,j,k} + u^{n+1/3}_{i,j,k-1}\Big)\Big] \tag{21}$$

and

$$u^{n+1} - u^{n+2/3} = \frac{\alpha\Delta t}{h^2}\Big[\Big(u^{n+1/3}_{i+1,j,k} - 2u^{n+2/3}_{i,j,k} + u^{n+2/3}_{i-1,j,k}\Big) + \Big(u^{n+2/3}_{i,j+1,k} - 2u^{n+2/3}_{i,j,k} + u^{n+2/3}_{i,j-1,k}\Big) + \big(u^{n+1}_{i,j,k+1} - 2u^{n+1}_{i,j,k} + u^{n+1}_{i,j,k-1}\big)\Big] \tag{22}$$

Again, these equations are written as $\Delta x = \Delta y = \Delta z = h$, which means same interval of space for 3 dimensions. We here again, do the Von-Neumann stability analysis. This time since equations are same type (central difference) we use the results of previous parts. Here we have

$$\frac{\hat{u}^{n+1/3}}{\hat{u}^n} = \frac{1 - 2\frac{\alpha k}{h^2}\sin^2\frac{lh}{2}}{1 + 2\frac{\alpha k}{h^2}\sin^2\frac{mh}{2}} \tag{23}$$

Similarly

$$\frac{\hat{u}^{n+2/3}}{\hat{u}^{n+1/3}} = \frac{1 - 2\frac{\alpha k}{h^2}\sin^2\frac{mh}{2}}{1 + 2\frac{\alpha k}{h^2}\sin^2\frac{nh}{2}} \tag{24}$$

and

$$\frac{\hat{u}^{n+1}}{\hat{u}^{n+2/3}} = \frac{1 - 2\frac{\alpha k}{h^2}\sin^2\frac{nh}{2}}{1 + 2\frac{\alpha k}{h^2}\sin^2\frac{lh}{2}} \tag{25}$$

multiplying these terms, we will have

$$\frac{\hat{u}^{n+1}}{\hat{u}^n} = \frac{1-2\frac{\alpha k}{h^2}\sin^2\frac{lh}{2}}{1+2\frac{\alpha k}{h^2}\sin^2\frac{mh}{2}}.\frac{1-2\frac{\alpha k}{h^2}\sin^2\frac{mh}{2}}{1+2\frac{\alpha k}{h^2}\sin^2\frac{nh}{2}}.\frac{1-2\frac{\alpha k}{h^2}\sin^2\frac{nh}{2}}{1+2\frac{\alpha k}{h^2}\sin^2\frac{lh}{2}} \tag{26}$$

putting simmilar terms on a same fraction we see

$$\frac{\hat{u}^{n+1}}{\hat{u}^n} = \frac{1-2\frac{\alpha k}{h^2}\sin^2\frac{lh}{2}}{1+2\frac{\alpha k}{h^2}\sin^2\frac{lh}{2}}.\frac{1-2\frac{\alpha k}{h^2}\sin^2\frac{mh}{2}}{1+2\frac{\alpha k}{h^2}\sin^2\frac{mh}{2}}.\frac{1-2\frac{\alpha k}{h^2}\sin^2\frac{nh}{2}}{1+2\frac{\alpha k}{h^2}\sin^2\frac{nh}{2}} \tag{27}$$

no each term is less than one. So this scheme is $\boxed{\textbf{unconditionally stable}}$.

(b) Transform (*) to spherical coordinates (ρ, θ, ϕ).
In spherical coordinate we have

$$x = r\sin\theta\cos\phi \tag{28}$$
$$y = r\sin\theta\sin\phi \tag{29}$$
$$z = r\cos\theta \tag{30}$$

From cartesian to spherical coordinate, the inverse of above equation is

$$r = \sqrt{x^2+y^2+z^2} \tag{31}$$
$$\cos\theta = \frac{z}{\sqrt{x^2+y^2+z^2}} \qquad \cos\phi = \frac{x}{\sqrt{x^2+y^2}} \tag{32}$$
$$\sin\theta = \frac{\sqrt{x^2+y^2}}{\sqrt{x^2+y^2+z^2}} \qquad \sin\phi = \frac{y}{\sqrt{x^2+y^2}} \tag{33}$$

Now we should find derivatives of r, θ and ϕ with respect to x, y and z. We start with r. we have

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin\theta\cos\phi \tag{34}$$
$$\frac{\partial r}{\partial y} = \frac{y}{r} = \sin\theta\sin\phi \tag{35}$$
$$\frac{\partial r}{\partial z} = \frac{z}{r} = \cos\theta \tag{36}$$

Now we try to find derivatives of θ w.r.t. cartesian coordinates, using equation 32 and taking deruvatives of this equation we will have

$$-\sin\theta d\theta = \frac{z(-x)}{r^3}dx \Rightarrow \frac{\partial\theta}{\partial x} = \frac{\cos\theta\cos\phi}{r} \tag{37}$$
$$-\sin\theta d\theta = \frac{z(-y)}{r^3}dx \Rightarrow \frac{\partial\theta}{\partial x} = \frac{\cos\theta\sin\phi}{r} \tag{38}$$

for the z derivative we use equation 33, we have

$$\cos\theta d\theta = \frac{\sqrt{x^2+y^2}(-z)}{r^3}dz \Rightarrow \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r} \tag{39}$$

for ϕ direction, using 32 and 33 we have

$$\begin{aligned} -\sin\phi d\phi &= \left(\frac{1}{\sqrt{x^2+y^2}} - \frac{x^2}{\sqrt{(x^2+y^2)^3}}\right)dx \\ &= \frac{\sin^2\phi}{r\sin\theta}dx \end{aligned} \tag{40}$$

so we will have

$$\frac{\partial\phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta} \tag{41}$$

Similary for dervative with respect to y, we will have

$$\begin{aligned} \cos\phi d\phi &= \left(\frac{1}{\sqrt{x^2+y^2}} - \frac{y^2}{\sqrt{(x^2+y^2)^3}}\right)dx \\ &= \frac{\cos^2\phi}{r\sin\theta}dx \qquad (42) \\ \frac{\partial\phi}{\partial y} &= \frac{\cos\phi}{r\sin\theta} \qquad (43) \end{aligned}$$

Now we use the chain rule to compute the laplacian terms.

$$\frac{\partial^2}{\partial z^2} = \left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right)\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right) \tag{44}$$

and for two other terms as well, we have

$$\begin{aligned} \frac{\partial^2}{\partial x^2} &= \left(\sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right) \\ &\times\left(\sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right) \qquad (45) \\ \frac{\partial^2}{\partial y^2} &= \left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\theta}{r\sin\theta}\frac{\partial}{\partial\phi}\right) \\ &\times\left(\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\theta}{r\sin\theta}\frac{\partial}{\partial\phi}\right) \qquad (46) \end{aligned}$$

Sadly there are 22 terms to compute!! starting from the terms that have second derivative in r we have

$$\left[\cos^2\theta + \sin^2\theta\left(\cos^2\phi + \sin^2\phi\right)\right]\frac{\partial^2}{\partial r^2} = \frac{\partial^2}{\partial r^2} \tag{47}$$

checking terms for second derivative of ϕ, we will have

$$\frac{\sin^2\phi - \sin\phi\cos\phi + \cos^2\phi + \cos\phi\sin\phi}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi^2} = \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{48}$$

Similarly, for θ derivative we will have the following conclusion that, this becomes

$$\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} \tag{49}$$

Now still 14 terms remain. We first collect all terms that have product of r and θ derivative, we have (This way, there won't remain any terms from z derivatives)

$$\frac{\sin^2\theta + \cos^2\theta}{r}\frac{\partial}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r} \tag{50}$$

Now consider $4 - \theta - \phi$ terms, we have

$$\frac{\left(\sin^2\phi + \cos^2\phi\right)\cos\theta}{r^2\sin\theta} = \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} \tag{51}$$

writing $r - \phi$ terms that does not cancel each other, we will have

$$\frac{\sin^2\phi\sin\theta + \cos^2\phi\sin\theta}{r\sin\theta}\frac{\partial}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r} \tag{52}$$

Adding all the terms that we found, we no can write the Laplacian, which is

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{53}$$

(c) Solve the problem $u_t = \nabla^2 u$ (in spherical coordinates) with initial condition $u(R, t = 0) = 1$ for $0 < R < 1$ and boundary condition $u(1, t) = 0$. Solve this up to time $T = 1$.

Since we have θ and ϕ symmetry in both initial conditions and diffusivity constant, we can just write r terms in the diffusion equation. So our differential equation will look like as

$$\frac{\partial u}{\partial t} = \nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} \tag{54}$$

$$\begin{cases} u(r, t = 0) = 1 & \text{I.C.} \\ u(1, t) = 0 & \text{B.C.} \\ \frac{\partial u}{\partial r}(0, t) = 0 & \text{B.C.} \end{cases} \tag{55}$$

The last boundary condition comes from the symmetry that we have in our system. So the problem that we are solving is clearly stated above. It's actually 1-D diffusion equation with an extra term of $\frac{2}{r}\frac{\partial u}{\partial r}$. We define an extra node at negative r before the origin, so we can this way impose our boundary condition of

$\frac{\partial u}{\partial r}(0,t) = 0$. We use, forward Euler for time, central difference for second radial differentiation and second order central difference. So the method will look like

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta r^2} + \frac{2}{r_j}\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta r} \tag{56}$$

So, the domain on which we are integrating is as

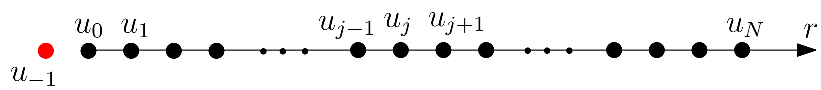

Figure 1: Schematic of 1-D domain on radius with imaginary node in red

We should remind that initial value of all nodes are 1 (as initial condition suggests) and value of u_N (last node) is always kept 0, since one of boundary conditon is $u(1,t) = 0$. Other boundary condition is implemented with the imaginary node. the value of this imaginary node is chosen such that $\frac{\partial u}{\partial r}(0,t) = 0$. This means

$$D_c u_0 = 0 \Rightarrow \frac{u_1 - u_{-1}}{2\Delta x} = 0 \Rightarrow u_{-1} = u_1 \tag{57}$$

This way, we assure that, second order (spatially) of first derivative at $r = 0$ is always zero. The next issue is that the differential equation has $\frac{1}{r}$ in the denominator and it is singular at $r = 0$. So the differential equation becomes invalid at $r = 0$. We take the limit as r goes to zero, using L'hopital's rule, we get

$$u_t = u_{rr} + \lim_{x\to 0}\frac{2}{r}\frac{\partial u}{\partial r} = u_{rr} + \lim_{x\to 0}\frac{2}{1}\frac{\partial^2 u}{\partial r^2} = 3u_{rr} \tag{58}$$

So at $r = 0$, we use this scheme

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = 3\,\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta r^2} \tag{59}$$

We have implemented this method using the routine that we wrote in the first assignment. In the following are some figures of the results that we got.

We also checked the convergence of the method by decreasing values of h and λ. In the following are some figures for different values of h and l at different times.

As the above figures suggest, our method is converging and solutions are getting close together.

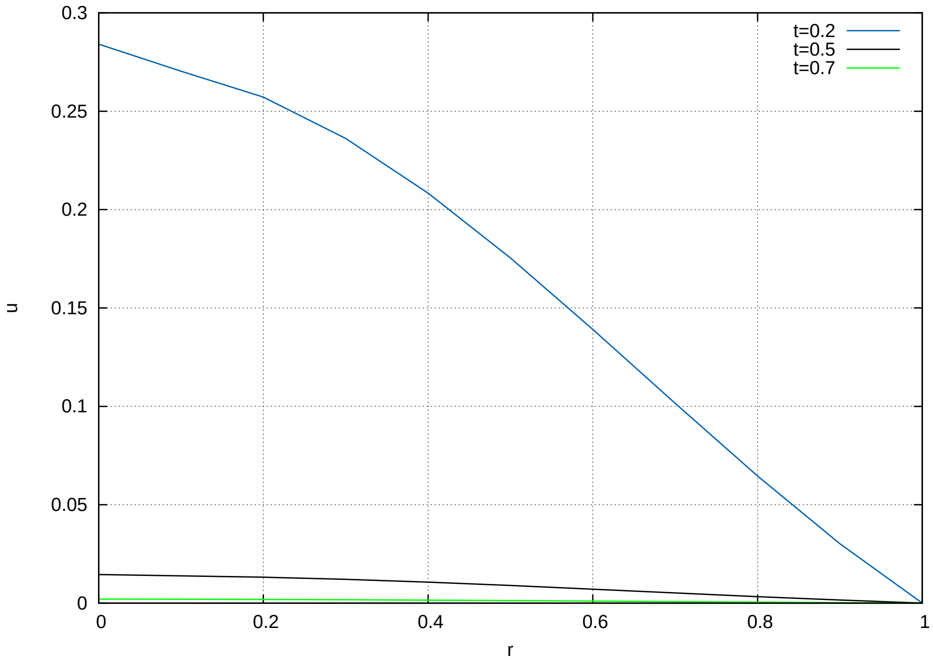

Figure 2: Time evolution of Tempreture vs Radius for different times, for $h = 0.1$ and $\lambda = 1/6$

(d) Solve the problem $u_t = \nabla^2 u$ (in spherical coordinates) with initial condition $u(R, t = 0) = 1$ for $0 < R < 1$ and boundary condition $u(0, t) = 1, u(1, t) = 0$. Solve this up to time $T = 1$. Caution–this is messy, not necessarily clear, etc. You figure it out.

Again for this part, I used the same procedure as in previous part. In this part again the problem is as

$$\frac{\partial u}{\partial t} = \nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} \tag{60}$$

$$\begin{cases} u(r, t = 0) = 1 & \text{I.C.} \\ u(1, t) = 0 & \text{B.C.} \\ u(0, t) = 1 & \text{B.C.} \end{cases} \tag{61}$$

and the numerical scheme would be

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta r^2} + \frac{2}{r_j}\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta r} \tag{62}$$

Here comes the interesting part! As we plotted the result, we saw a strange behavior as can be seen in Figure 5. The solution should be smoosh or flatten. However we see a sharp change at very first node!! This is because, we set $u = 1$

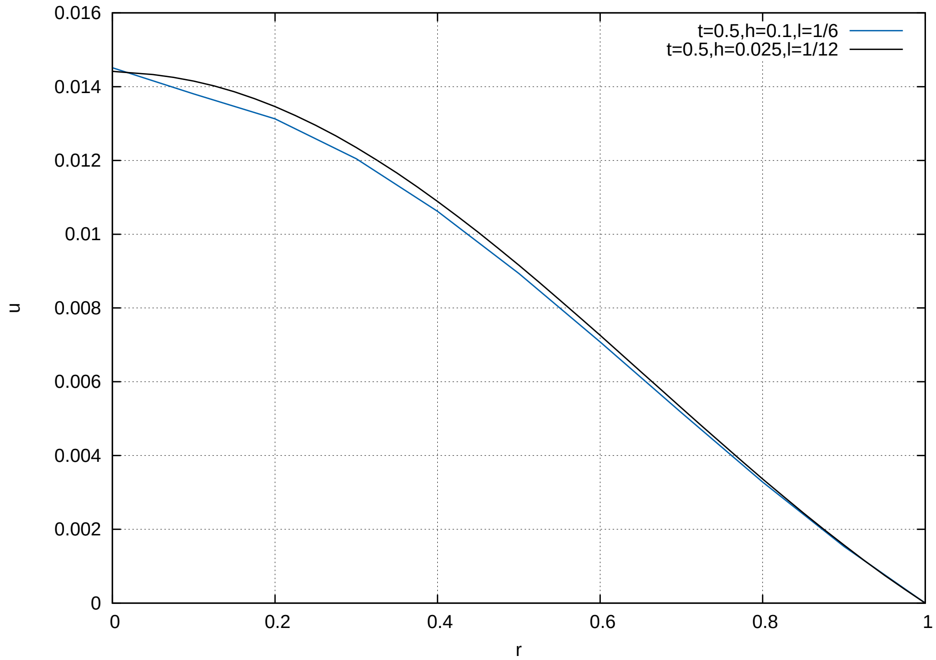

Figure 3: Solution at t=0.5, for different h and λ

at he origin and as we go to first node after the origin the singularity of $\frac{2}{r}$ catches us and makes trouble. If we write the equation that we are solving for different nodes, it is as follows

$$u_j^{n+1} = (\lambda + \frac{\lambda}{j})u_{j+1}^n + (1 - 2\lambda)u_j^n + (\lambda - \frac{\lambda}{j})u_{j-1}^n \tag{63}$$

As it is seen in the equation 80, for node 1, the value of u^{n+1} is just depending on value of u_{j+1}. So this means that at very first node, the node does not talk with its left neighbor node. So node 1 is apart from whole domain. This is the source of the problem in our solution.

The j in the denominator is actually the source. This j comes from the r in $\frac{2}{r}$. I proposed change of variable of $s = \frac{1}{r}$. This way, we are mapping our radius from $0 \leq r \leq 1$ to $1 \leq s < \infty$. Actually we are transferring the singularity to infinity and this may help. We have

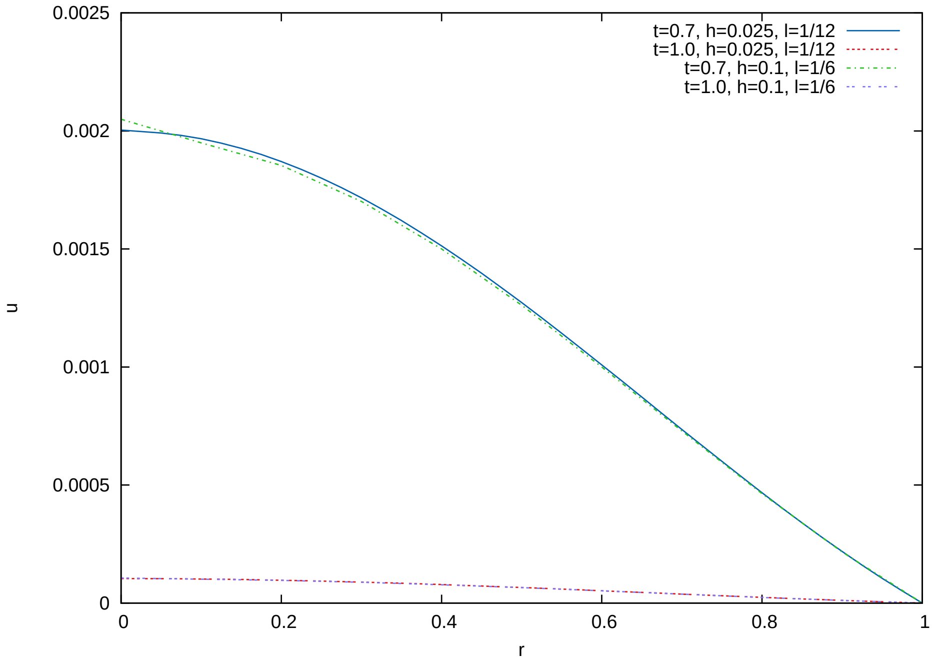

Figure 4: Solution at $t = 0.7$ and $t = 1.0$ for different values of h and λ

$$s = \frac{1}{r} \tag{64}$$

$$\frac{\partial}{\partial r} = \frac{\partial s}{\partial r}.\frac{\partial}{\partial s} = -s^2\frac{\partial}{\partial s} \tag{65}$$

$$\frac{\partial^2}{\partial r^2} = \frac{\partial s}{\partial r}.\frac{\partial}{\partial s}\left(-s^2\frac{\partial}{\partial s}\right) \tag{66}$$

$$\frac{\partial^2}{\partial r^2} = -s^2\left(-2s\frac{\partial}{\partial s} - s^2\frac{\partial^2}{\partial s^2}\right) \tag{67}$$

$$\frac{\partial^2}{\partial r^2} = 2s^3\frac{\partial}{\partial s} + s^4\frac{\partial^2}{\partial s^2} \tag{68}$$

So our equation becomes

$$u_t = u_{rr} + \frac{2}{r}u_r \tag{69}$$

$$u_t = 2s^3u_s + s^4u_{ss} + 2s\left(-s^2u_s\right) \tag{70}$$

So the main equation that we are solving now is

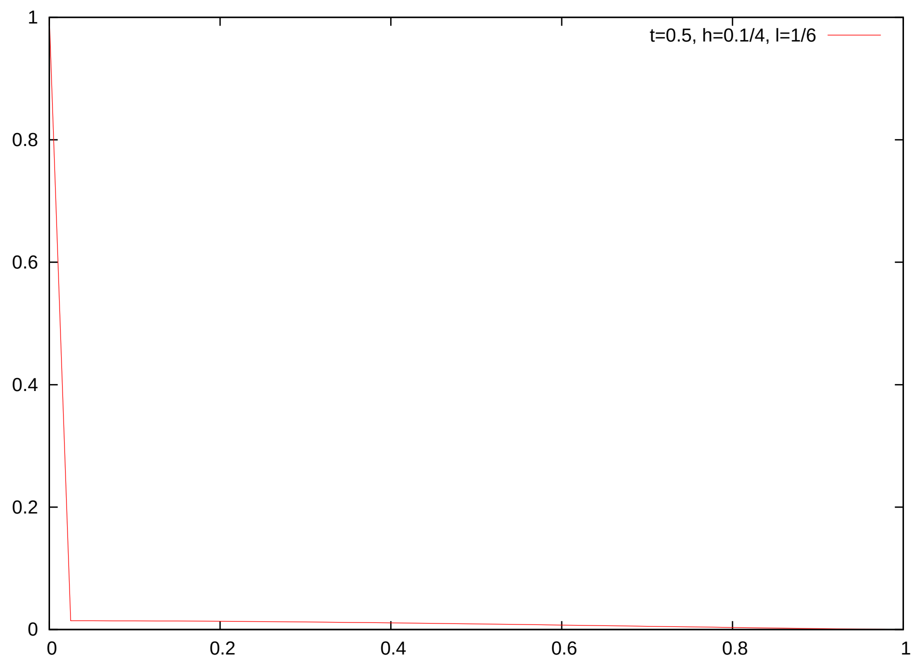

Figure 5: Strange behaviour of solution, $t = 0.5$, for $h = 0.025$ and $\lambda = 1/6$

$$\frac{\partial u}{\partial t} = s^4 \frac{\partial^2 u}{\partial s^2} \tag{71}$$

$$\begin{cases} u(r, t = 0) = 1 & \text{I.C.} \\ u(1, t) = 0 & \text{B.C.} \\ u(\infty, t) = 1 & \text{B.C.} \end{cases} \tag{72}$$

We chose 5 to be our ∞. Bigger values for infinity, will give better results for values near the zero. Scheme is still the same. Just for completeness, Here will be the scheme

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = s_j^4 \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta s^2} \tag{73}$$

Simplifying, the above equation we will have

$$u_j^{n+1} = u_j^n + (j\Delta s)^4 \Delta t \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta s^2} \tag{74}$$

$$u_j^{n+1} = j^4 \lambda' u_{j+1}^n + (1 - 2j^4\lambda') u_j^n + j^4 \lambda' u_{j-1}^n \qquad \lambda' = \Delta s^2 \Delta t \tag{75}$$

This exactly looks like as numerical scheme that we had for heat equation $u_t = u_{xx}$. We should just redefine $\lambda = j\lambda'$. In problem set one we found that for stability we should have

$$\lambda < \frac{1}{2} \tag{76}$$

Hence forth, in here, we should have

$$j\lambda' < \frac{1}{2} \quad \Rightarrow \quad \Delta t\ \Delta s^2 < \frac{1}{2j} \tag{77}$$

Worst case happens at $j = 1$. So for stability we should have

$$\Delta t\ \Delta s^2 < \frac{1}{2} \tag{78}$$

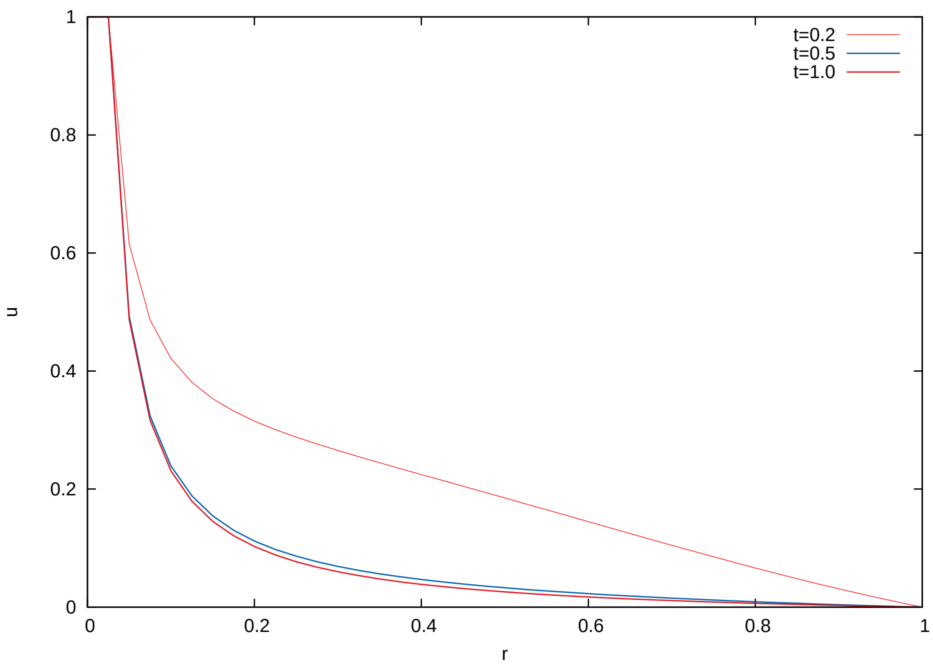

Figure 6: Solution at different times for $h = 0.025$ and $\lambda = 1/6$

When we map back the method to physical space, we see that, this assumption that infinity is some finite number, simply means that, to start solving diffusion equation form some node other than $j = 1$, all through all the other nodes. So, we started the scheme from $j = 2$ and plotted the solution. Solution for different times can be seen in figure 6 and also convergence is seen in figure 7.

(e) Has your stability requirement been altered (what is it in spherical coordinates?)

For stability analysis, we should check the maximum of eigenvalues of the matrix that we have for the solution. Solution is as

$$u^{n+1} = \mathbf{A}u^n \tag{79}$$

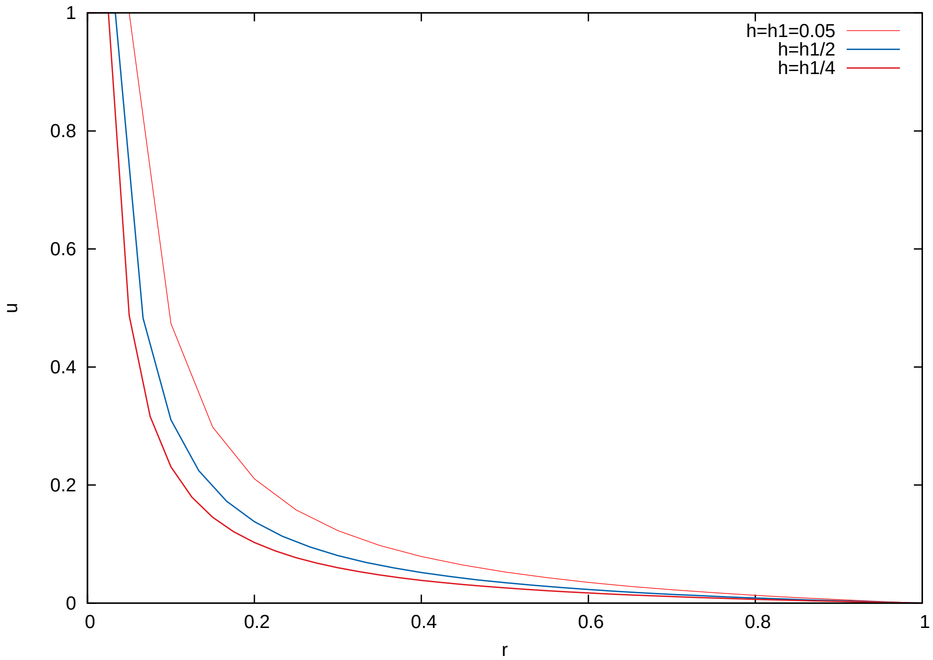

Figure 7: Solution at $t = 1.0$ for different values of h

Maximum eigenvalue of $\mathbf{A}$ should be less or equal to 1 for our method to be stable. Our method is as

$$u_j^{n+1} = (\lambda + \frac{\lambda}{j})u_{j+1}^n + (1 - 2\lambda)u_j^n + (\lambda - \frac{\lambda}{j})u_{j-1}^n \tag{80}$$

Using Von-Neumann stability analysis, we insert $e^{ikx}U$ into the scheme, we have

$$U^{n+1} = \left(1 + \lambda(e^{ik} + e^{-ik} - 2) + \lambda\frac{1}{j}(e^{ik} - e^{-ik})\right)U^n \tag{81}$$

Henceforth the growth factor becomes

$$\rho(\hat{k}) = 1 - 4\lambda\sin^2\frac{k}{2} + \frac{2i\lambda}{j}\sin k \tag{82}$$

The absolute value of this factor will be

$$|\rho(\hat{k})|^2 = (1 - 4\lambda\sin^2\frac{k}{2})^2 + (\frac{2\lambda}{j}\sin k)^2 \tag{83}$$

Worst case will happen, when $j = 1$. So we will have

$$|\rho(\hat{k})|^2 = (1 - 4\lambda\sin^2\frac{k}{2})^2 + (2\lambda\sin k)^2 \tag{84}$$

So

$$|\rho(\hat{k})|^2 = (1 - 8\lambda \sin^2 \frac{k}{2} + 16\lambda^2 \sin^4 \frac{k}{2}) + (16\lambda^2 \sin^2 \frac{k}{2} \cos^2 \frac{k}{2}) \tag{85}$$

$$|\rho(\hat{k})|^2 = 1 + 8\lambda \sin^2 \frac{k}{2}(-1 + 2\lambda) \tag{86}$$

So we should have

$$\lambda(-1 + 2\lambda) \leq 0 \qquad \Rightarrow \qquad \lambda \leq \frac{1}{2} \tag{87}$$

So the stability condition is $\boxed{\lambda \leq \frac{1}{2}}$

3. How hot can a swimming pool get? Consider a unit square cube and use the differential equation $u_t = \nabla^2 u$. On all walls except the top, assume insulating boundary conditions (i.e. $du/dn = 0$ where n is the normal vector). On the top surface, we have the boundary condition $u = 1$ during the day and $u = 0$ at night. Find, as a function of the ratio of day length/night length, the maximum temperature reached at the bottom of the pool after 5 cycles of day/night. Assume initial condition u=0. Use a variable time cycle.

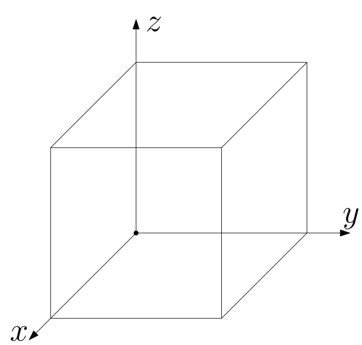

Figure 8: Definition of coordinate system for water pool

We put the coordinate system in one of down coordinate.(As in figure 8) This way boundaries will become $x = 0, 1$, $y = 0, 1$ and $z = 0, 1$. The equation that we are solving with boundary conditions and initial condition is

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \tag{88}$$

$$\begin{cases} \frac{\partial u(x,t)}{\partial n} = 0 \quad x = 0, 1 \\ \frac{\partial u(x,t)}{\partial n} = 0 \quad y = 0, 1 \\ \frac{\partial u(x,t)}{\partial n} = 0 \quad z = 0 \\ u|_{z=1} = 1 \\ u|_{t=0} = 0 \end{cases} \tag{89}$$

We will use forwad Euler for time and central difference with same spatial spacing for space coordinates. The scheme will become

$$\begin{aligned}\frac{u_{i,j,k}^{n+1}-u_{i,j,k}^{n}}{\Delta t}=&\frac{u_{i+1,j,k}^{n}-2u_{i,j,k}^{n}+u_{i-1,j,k}^{n}}{\Delta x^2}\\&+\frac{u_{i,j+1,k}^{n}-2u_{i,j,k}^{n}+u_{i,j-1,k}^{n}}{\Delta y^2}\\&+\frac{u_{i,j,k+1}^{n}-2u_{i,j,k}^{n}+u_{i,j,k-1}^{n}}{\Delta z^2}\end{aligned}\tag{90}$$

Assuming same spatial spacing (i.e. $\Delta x = \Delta y = \Delta z = h$), defining $\lambda := k/h^2$, we will have

$$\begin{aligned}u_{i,j,k}^{n+1}=u_{i,j,k}^{n}+\lambda(&u_{i+1,j,k}^{n}-2u_{i,j,k}^{n}+u_{i-1,j,k}^{n}\\&+u_{i,j+1,k}^{n}-2u_{i,j,k}^{n}+u_{i,j-1,k}^{n}\\&+u_{i,j,k+1}^{n}-2u_{i,j,k}^{n}+u_{i,j,k-1}^{n})\end{aligned}\tag{91}$$

Simplifying the above equation, it will become

$$u_{i,j,k}^{n+1}=(1-6\lambda)u_{i,j,k}^{n}+\lambda(u_{i+1,j,k}^{n}+u_{i-1,j,k}^{n}+u_{i,j+1,k}^{n}+u_{i,j-1,k}^{n}+u_{i,j,k+1}^{n}+u_{i,j,k-1}^{n})\tag{92}$$

Stability analysis of the above equation has been done in Problem 2. In this problem we found that, for stability, we should have

$$\lambda \le \frac{1}{6}\tag{93}$$

For the boundary conditions, on the top surface we now the temperature is fixed so, u is constant. For insulation on the other surfaces of the water pool, same as question 2, we define virtual nodes on surfaces after outer surface of the pool. Values of these nodes are computed such that first derivative of temperature on the boundary surfaces becomes zero. Considering N nodes for each direction of x, y and z we will have

$$u_{0,j,k}=u_{2,j,k} \qquad j,k=\{1,2,...,N\}\tag{94}$$

$$u_{N+1,j,k}=u_{N-1,j,k} \qquad j,k=\{1,2,...,N\}\tag{95}$$

$$u_{i,0,k}=u_{i,2,k} \qquad i,k=\{1,2,...,N\}\tag{96}$$

$$u_{i,N+1,k}=u_{i,N-1,k} \qquad i,k=\{1,2,...,N\}\tag{97}$$

$$u_{i,,j,0}=u_{i,j,2} \qquad i,j=\{1,2,...,N\}\tag{98}$$

$$u_{i,j,N+1}=u_{i,j,N-1} \qquad i,j=\{1,2,...,N\}\tag{99}$$

These 5 equations define insulating boundary conditions. On the top surface, the boundary condition is as

$$u_{i,j,N} = \begin{cases} 1 & \text{t} = \text{Day time} \\ 0 & \text{t} = \text{Night time} \end{cases} \tag{100}$$

for $i, j = \{1, 2, ..., N\}$ This virtual nodes will make sure that first derivative of temperature w.r.t. normal direction (i.e. u_n) is zero, since at $x = 0$ for instance we have

$$\frac{\partial u}{\partial n} = \frac{\partial u_{1,j,k}}{\partial x} = \frac{u_{2,j,k} - u_{0,j,k}}{2h} = 0 \tag{101}$$

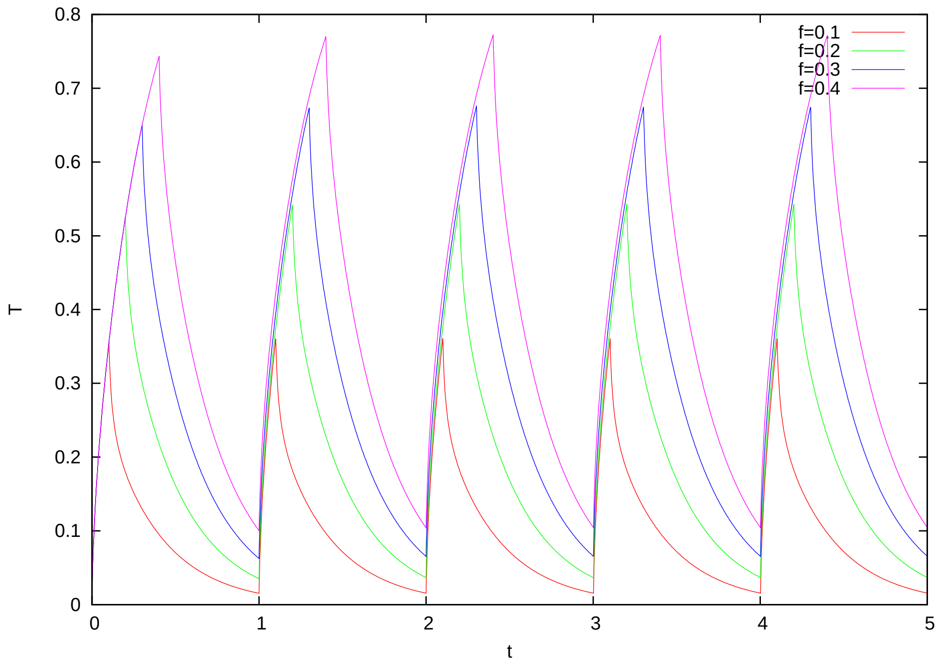

Figure 9: Temperature Variation for different fractions of $f := \frac{Day}{Day+Night}$

We implemented the method. For different values of $f := \frac{\text{Day Time}}{\text{Total Day time}}$, we computed average values of u. f could normally vary between 0.1 and 0.5. For different values of f we plotted the average of water temperature. The results are in figure **??**

4. Extra: Deal with the angle of the sun on the pool.

   In this part, we changed the variation of u in day to night, from discontinuous step function to a continuous function as

$$u_{i,j,N} = \begin{cases} sin(\pi t/f) & \text{t} = \text{Day time} \\ 0 & \text{t} = \text{Night time} \end{cases} \tag{102}$$

   where f is fraction of daytime. Whole day is 1 unit of time. This way, u will continuously change from 0 to 1 and then reach back to zero. This way for instance, from

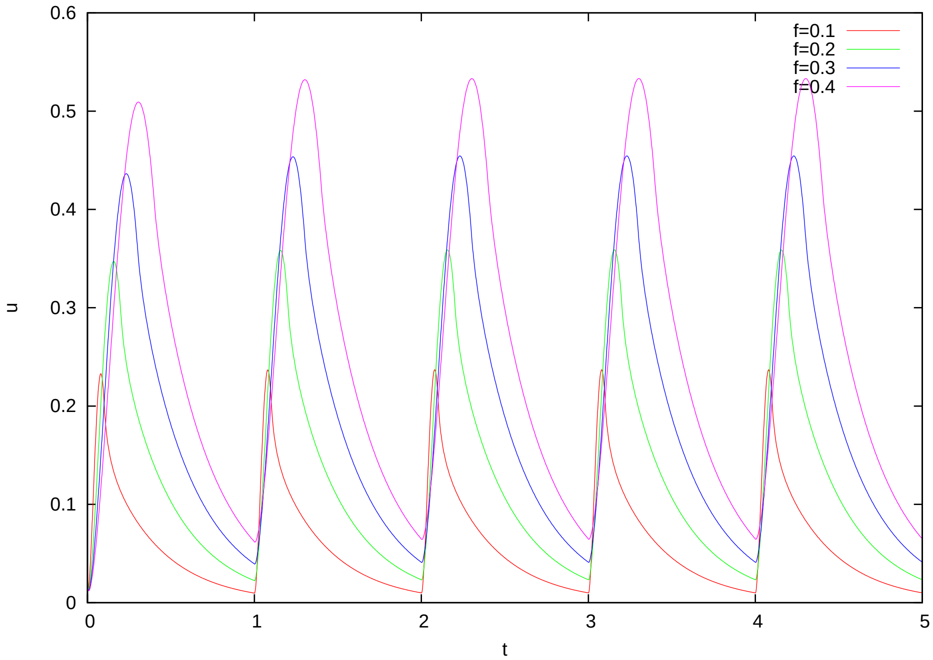

Figure 10: Temperature Variation for different fractions of $f := \frac{Day}{Day+Night}$

morning to noon, temperature of surface will gradually increase to final value of 1 and then reach back to zero. The result for this part is in figure 10. As it can be seen the tips will get smoothed. Still since the derivatives are not continuous the result is not completely smooth.

5. Extra: Use real physical constants in your problem.

   diffusion equation that we are solving is

$$u_t = \alpha \nabla^2 u \tag{103}$$

where $\alpha = \frac{k}{\rho c_P}$. k is conductivity, ρ is density, and c_p is constant pressure heat capacity. Values for water is as

$$k = 0.58 \qquad w/mK \tag{104}$$
$$\rho = 998 \qquad g/m^3 \tag{105}$$
$$c_p = 4185 \qquad J/kgK \tag{106}$$

So

$$\alpha = 1.43 \times 10^{-7} m^2 s \tag{107}$$

We take size of the pool to be $2 \times 2 \times 2$. Variation of energy of sun perpendicular to area is shown in figure 11. Our estimation to this figure is plotted in figure 12. We

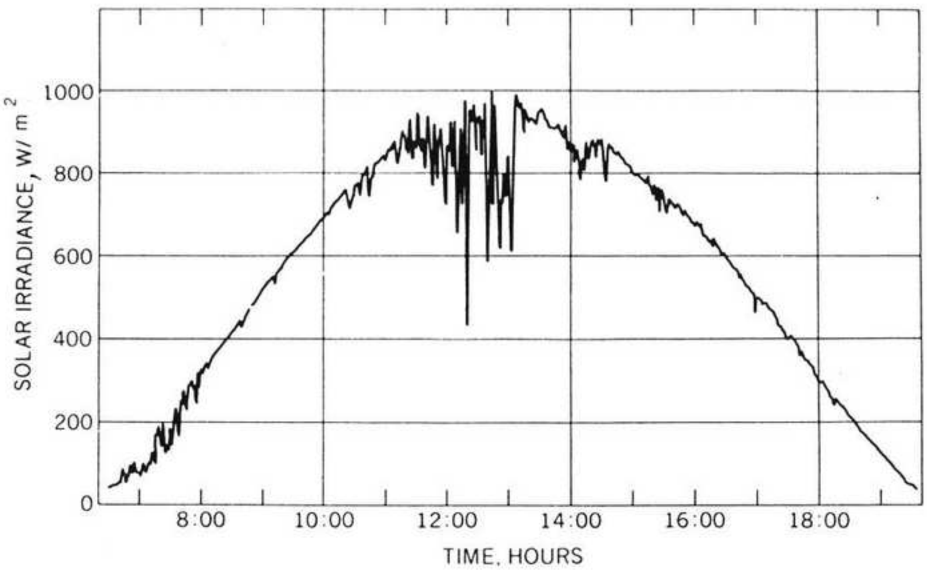

Figure 11: Total irradiation on a horizontal surface for a mostly clear day

estimate this value by $E_{sun} = 1000 \sin\left(\pi \frac{t}{8}\right)\ w/day$. We have scaled time to hours of a day. each day is considered as 1 unit of time. This way we have

$$\alpha = 0.0123552 m^2/day \tag{108}$$

and u on the surface becomes

$$u_{i,j,N} = \begin{cases} sin(\pi t/f) & \text{t = Day time} \\ 0 & \text{t = Night time} \end{cases} \tag{109}$$

where $f = \frac{8}{24} = \frac{1}{3}$. For the boundary condition of the top surface we have

$$k_{water} * \left(\frac{u_{N,j,k} - u_{N-1,j,k}}{h}\right) = E_{sun} * \Delta t \tag{110}$$

For our problem we see that in each time step, Sun will cause the temperature of the surface to rise as

$$\Delta u = \frac{hkE_{sun}}{k} = 0.287 \sin\left(\pi \frac{t}{8}\right) \tag{111}$$

For the outside temperature in night, we set the value to be $6\,C$. The figure in 5 days will become as in figure 13.

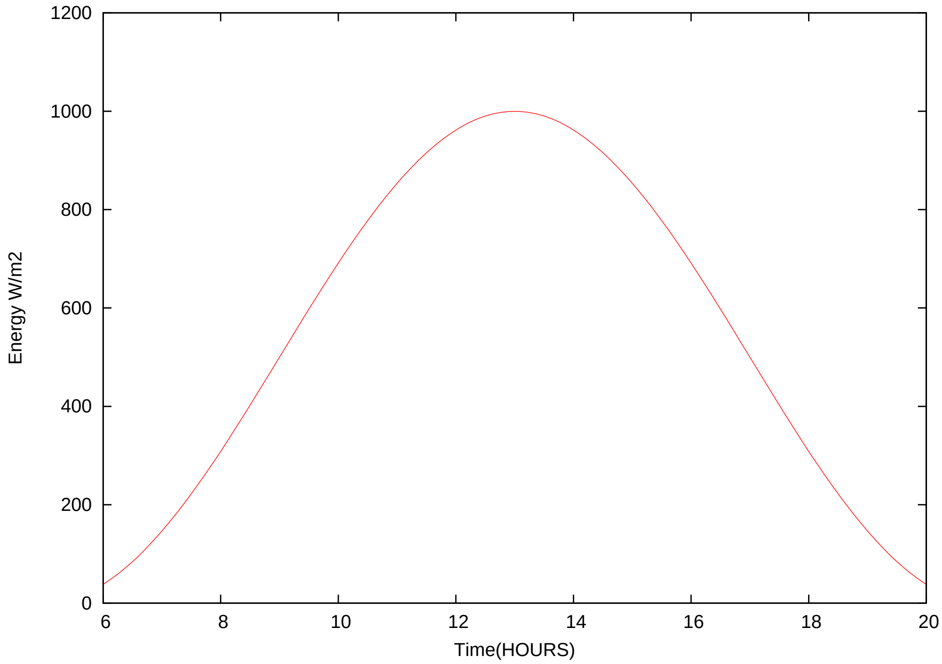

Figure 12: Estimation of total irradiation on a horizontal surface for a mostly clear day

As it can be seen from the figures, temperature will reach to a steady state solution and begin to oscillate around $17C$. This temperature sounds reasonable, considering day time fraction and maximum of energy absorbed. The bottom tempreture is also shown in the figure 15.

Conclusion

We saw that Crank-Nicolson method is order 2 on both spatial and temporal coordinates. This method is implicit and unconditionally stable.

We also found that transformed laplacian in spherical coordinates with θ and ϕ symmetries is like 1-D equation with an extra term which has singularity. We saw how to handle this instability (either by changing coordinates or using L'Hopital for origin and cautiously writing finite difference equations for near zero nodes).

We discussed ADI method, and saw it is unconditionally stable, however its implicit and hard to solve. We saw that if we use same finite difference method as what we used for 1-D, for stability condition, $\alpha\lambda$ should take smaller and smaller values. Its maximum value change as $\frac{1}{d}$, where d is number of dimension of space.(e.g. for $d = 3$, stability condition becomes $\alpha\lambda \leq \frac{1}{6}$, considering same spatial intervals of h and temporal intervals of k and λ is defined as $\frac{k}{h^2}$). So as number of dimension gets bigger, for our solution to be stable, we should either use smaller values of λ or change our scheme.

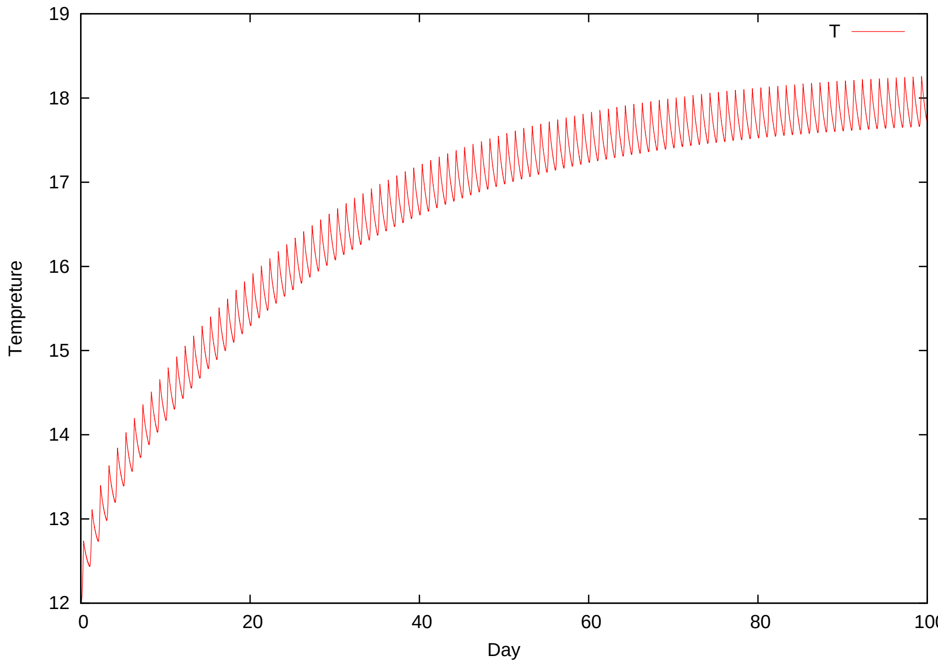

Figure 13: Temperature change in 100 days

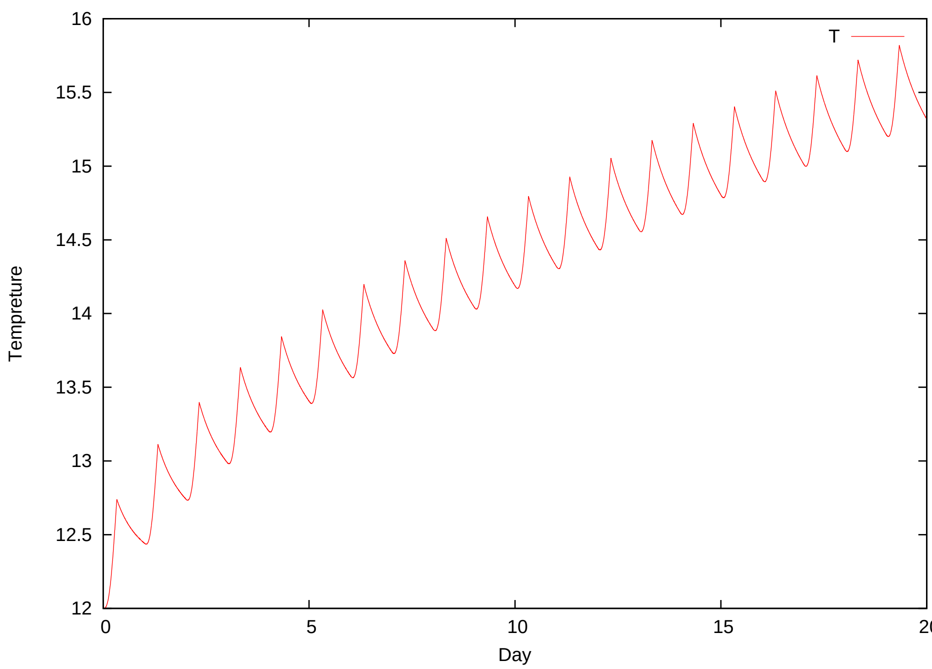

Figure 14: Temperature change in 20 days

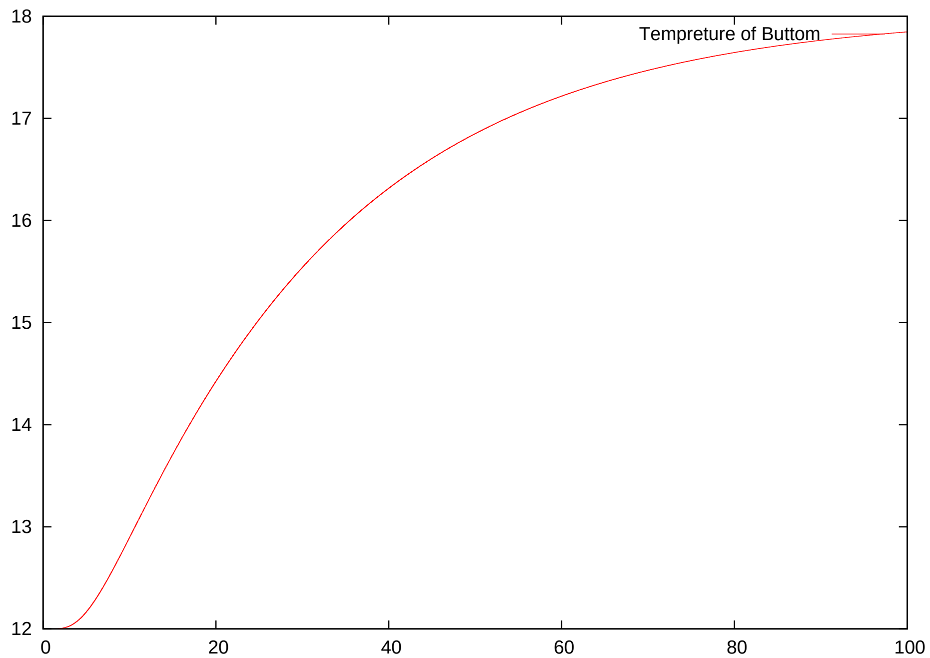

Figure 15: Average temperature of bottom face in 100 days