2-D Cylindrical Finite Difference Time Dependent Heat Equation for Non-Constant Thermal Conductivity with Constant Spacing

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1 Introduction

Solving the heat equation in cylindrical coordinates is of great interest to applications where heat energy is deposited normal to a surface via a laser exposure. With Dr. Clark's work in solving the heat equation with thermal conductivity, κ as a function of z allowed for better simulating the weakly homogenous media of tissue. The following derivation aims to take this work a step further, solving with $\kappa = \kappa(r, z)$, in order to extend our weak homogeny to the radial direction, especially valuable in situations with irregularities such as a hair follicle in the center of the beam path.

2 The Problem

The problem is first expanding the differential equation to reflect the radial dependence of thermal conductivity. We implement a finite difference method in order to substitute our derivatives for the values of T and κ that are easily implemented in a computational setting. In the derivation, our result is discontinuous at $r = 0$ and so we utilize L'Hospital's rule and create a solution valid for the case where $r \to 0$.

3 Derivation

We begin with the heat transfer equation

$$\rho c \frac{d\mathrm{T}}{dt} = \vec{\nabla} \cdot \kappa \vec{\nabla} \mathrm{T} + A \tag{1}$$

We ignore the source term, A for now and proceed by expanding the gradient, considering no phi dependence, so $\frac{\partial \mathrm{T}}{\partial \phi} = 0$. Using the cylindrical gradient gives

$$\rho c \frac{d\mathrm{T}}{dt} = \vec{\nabla} \cdot \kappa \left[\frac{\partial \mathrm{T}}{\partial r} \hat{r} + \frac{\partial \mathrm{T}}{\partial z} \hat{z} \right] \tag{2}$$

We rewrite κ to state it's radial and z dependence

$$\rho c \frac{d\mathrm{T}}{dt} = \vec{\nabla} \cdot \left[\frac{\partial \mathrm{T}}{\partial r} \kappa(r,z) \hat{r} + \frac{\partial \mathrm{T}}{\partial z} \kappa(r,z) \hat{z} \right] \tag{3}$$

Expanding the divergence (again in cylindrical coordinates)

$$\rho c \frac{d\mathrm{T}}{dt} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial \mathrm{T}}{\partial r} \kappa(r,z) \right] + \frac{\partial}{\partial z} \left[\frac{\partial \mathrm{T}}{\partial z} \kappa(r,z) \right] \tag{4}$$

We use the product rule to expand each of these derivatives, giving

$$\rho c \frac{d\mathrm{T}}{dt} = \frac{1}{r} \left[\frac{\partial \mathrm{T}}{\partial r} \kappa(r,z) + r \frac{\partial^2 \mathrm{T}}{\partial r^2} \kappa(r,z) + r \frac{\partial \mathrm{T}}{\partial r} \frac{\partial \kappa}{\partial r} \right] + \frac{\partial^2 \mathrm{T}}{\partial z^2} \kappa(r,z) + \frac{\partial \mathrm{T}}{\partial z} \frac{\partial \kappa}{\partial z} \tag{5}$$

distributing out the $\frac{1}{r}$ gives our final purely analytical term, which we pause on before continuing

$$\rho c \frac{d\mathrm{T}}{dt} = \frac{1}{r} \frac{\partial \mathrm{T}}{\partial r} \kappa(r,z) + \frac{\partial^2 \mathrm{T}}{\partial r^2} \kappa(r,z) + \frac{\partial \mathrm{T}}{\partial r} \frac{\partial \kappa}{\partial r} + \frac{\partial^2 \mathrm{T}}{\partial z^2} \kappa(r,z) + \frac{\partial \mathrm{T}}{\partial z} \frac{\partial \kappa}{\partial z} \tag{6}$$

3.1 Finite Difference Expansion of Derivatives

For all spacial derivatives we expanded using a central difference method, as aside from at boundaries this information is available to us. We aim to reduce this to an easily calculable form in order to implement into our code. Our time derivative is a forward difference, so we can solve for the temperature at the next 'time step'

$$\begin{aligned} \rho c \frac{d\mathrm{T}}{dt} = \frac{1}{r} \left[\frac{\mathrm{T}^n_{r+1,z} - \mathrm{T}^n_{r-1,z}}{2\Delta r} \right] \kappa^n_{r,z} + \left[\frac{\mathrm{T}^n_{r+1,z} - 2\mathrm{T}^n_{r,z} + \mathrm{T}^n_{r-1,z}}{(\Delta r)^2} \right] \kappa^n_{r,z} + (\frac{\mathrm{T}^n_{r+1,z} - \mathrm{T}^n_{r-1,z}}{2\Delta r})(\frac{\kappa^n_{r+1,z} - \kappa^n_{r-1,z}}{2\Delta r}) \\ + \left[\frac{\mathrm{T}^n_{r,z+1} - 2\mathrm{T}^n_{r,z} + \mathrm{T}^n_{r,z-1}}{(\Delta z)^2} \right] \kappa^n_{r,z} + (\frac{\mathrm{T}^n_{r,z+1} - \mathrm{T}^n_{r,z-1}}{2\Delta z})(\frac{\kappa^n_{r,z+1} - \kappa^n_{r,z-1}}{2\Delta z}) \end{aligned} \tag{7}$$

From here on we designate the first central difference derivative of κ to be $(\frac{\Delta\kappa}{\Delta z})^n_{r,z}$, since we can calculate it seperately before the bulk of the rest of calculations

$$\begin{aligned} \rho c \frac{d\mathrm{T}}{dt} = \frac{1}{r} \left[\frac{\mathrm{T}^n_{r+1,z} - \mathrm{T}^n_{r-1,z}}{2\Delta r} \right] \kappa^n_{r,z} + \left[\frac{\mathrm{T}^n_{r+1,z} - 2\mathrm{T}^n_{r,z} + \mathrm{T}^n_{r-1,z}}{(\Delta r)^2} \right] \kappa^n_{r,z} + (\frac{\mathrm{T}^n_{r+1,z} - \mathrm{T}^n_{r-1,z}}{2\Delta r})(\frac{\Delta\kappa}{\Delta r})^n_{r,z} \\ + \left[\frac{\mathrm{T}^n_{r,z+1} - 2\mathrm{T}^n_{r,z} + \mathrm{T}^n_{r,z-1}}{(\Delta z)^2} \right] \kappa^n_{r,z} + (\frac{\mathrm{T}^n_{r,z+1} - \mathrm{T}^n_{r,z-1}}{2\Delta r})(\frac{\Delta\kappa}{\Delta z})^n_{r,z} \end{aligned} \tag{8}$$

Now we expand the time derivative to a forward difference, since it is the physical parameters at the current $\mathrm{T}^n_{r,z}$ that causes the temperature change to $\mathrm{T}^{n+1}_{r,z}$

$$\begin{aligned} \rho c \frac{\mathrm{T}^{n+1}_{r,z} - \mathrm{T}^n_{r,z}}{\Delta t} = \frac{1}{r} \left[\frac{\mathrm{T}^n_{r+1,z} - \mathrm{T}^n_{r-1,z}}{2\Delta r} \right] \kappa^n_{r,z} + \left[\frac{\mathrm{T}^n_{r+1,z} - 2\mathrm{T}^n_{r,z} + \mathrm{T}^n_{r-1,z}}{(\Delta r)^2} \right] \kappa^n_{r,z} \\ + (\frac{\mathrm{T}^n_{r+1,z} - \mathrm{T}^n_{r-1,z}}{2\Delta r})(\frac{\Delta\kappa}{\Delta r})^n_{r,z} + \left[\frac{\mathrm{T}^n_{r,z+1} - 2\mathrm{T}^n_{r,z} + \mathrm{T}^n_{r,z-1}}{(\Delta z)^2} \right] \kappa^n_{r,z} + (\frac{\mathrm{T}^n_{r,z+1} - \mathrm{T}^n_{r,z-1}}{2\Delta r})(\frac{\Delta\kappa}{\Delta z})^n_{r,z} \end{aligned} \tag{9}$$

We regroup terms to be calculable as coefficient to our various T values

$$
\begin{aligned}
\mathrm{T}^{n+1}_{r,z} - \mathrm{T}^{n}_{r,z} = \mathrm{T}^{n}_{r,z} &\left[\frac{\Delta t}{\rho c}\left(\frac{-2\kappa^n_{r,z}}{(\Delta r)^2} - \frac{2\kappa^n_{r,z}}{(\Delta z)^2}\right)\right] \\
&+ \mathrm{T}^{n}_{r-1,z}\left[\frac{\Delta t}{\rho c}\left(\frac{-\kappa^n_{r,z}}{2r\Delta r} + \frac{\kappa^n_{r,z}}{(\Delta r)^2} - \frac{1}{2\Delta r}\left(\frac{\Delta \kappa}{\Delta r}\right)^n_{r,z}\right)\right] \\
&+ \mathrm{T}^{n}_{r+1,z}\left[\frac{\Delta t}{\rho c}\left(\frac{\kappa^n_{r,z}}{2r\Delta r} + \frac{\kappa^n_{r,z}}{(\Delta r)^2} + \frac{1}{2\Delta r}\left(\frac{\Delta \kappa}{\Delta r}\right)^n_{r,z}\right)\right] \\
&+ \mathrm{T}^{n}_{r,z-1}\left[\frac{\Delta t}{\rho c}\left(\frac{\kappa^n_{r,z}}{(\Delta z)^2} - \frac{1}{2\Delta z}\left(\frac{\Delta \kappa}{\Delta z}\right)^n_{r,z}\right)\right] \\
&+ \mathrm{T}^{n}_{r,z+1}\left[\frac{\Delta t}{\rho c}\left(\frac{\kappa^n_{r,z}}{(\Delta z)^2} + \frac{1}{2\Delta z}\left(\frac{\Delta \kappa}{\Delta z}\right)^n_{r,z}\right)\right]
\end{aligned} \tag{10}
$$

We create the following calculable variables to simplifly our equations

$$A^n_{r,z} = \left[\frac{\Delta t}{\rho c}\left(\frac{-2\kappa^n_{r,z}}{(\Delta r)^2} - \frac{2\kappa^n_{r,z}}{(\Delta z)^2}\right)\right] \tag{11}$$

$$B^n_{r,z} = \left[\frac{\Delta t}{\rho c}\left(\frac{-\kappa^n_{r,z}}{2r\Delta r} + \frac{\kappa^n_{r,z}}{(\Delta r)^2} - \frac{1}{2\Delta r}\left(\frac{\Delta \kappa}{\Delta r}\right)^n_{r,z}\right)\right] \tag{12}$$

$$C^n_{r,z} = \left[\frac{\Delta t}{\rho c}\left(\frac{\kappa^n_{r,z}}{2r\Delta r} + \frac{\kappa^n_{r,z}}{(\Delta r)^2} + \frac{1}{2\Delta r}\left(\frac{\Delta \kappa}{\Delta r}\right)^n_{r,z}\right)\right] \tag{13}$$

$$D^n_{r,z} = \left[\frac{\Delta t}{\rho c}\left(\frac{\kappa^n_{r,z}}{(\Delta z)^2} - \frac{1}{2\Delta z}\left(\frac{\Delta \kappa}{\Delta z}\right)^n_{r,z}\right)\right] \tag{14}$$

$$E^n_{r,z} = \left[\frac{\Delta t}{\rho c}\left(\frac{\kappa^n_{r,z}}{(\Delta z)^2} + \frac{1}{2\Delta z}\left(\frac{\Delta \kappa}{\Delta z}\right)^n_{r,z}\right)\right] \tag{15}$$

resulting in the final form

$$\mathrm{T}^{n+1}_{r,z} = \mathrm{T}^{n}_{r,z} + A^n_{r,z}\mathrm{T}^{n}_{r,z} + B^n_{r,z}\mathrm{T}^{n}_{r-1,z} + C^n_{r,z}\mathrm{T}^{n}_{r+1,z} + D^n_{r,z}\mathrm{T}^{n}_{r,z-1} + E^n_{r,z}\mathrm{T}^{n}_{r,z+1} \tag{16}$$

3.2 Case for $r = 0$

Looking back at Eq.6, we can see it is discontinuous at $r = 0$. In order to remedy this, we take the limit as $r \to 0$ of Eq.6, where we can focus on the first term

$$\rho c\frac{d\mathrm{T}}{dt} = \frac{1}{r}\frac{\partial \mathrm{T}}{\partial r}\kappa(r,z) + \frac{\partial^2 \mathrm{T}}{\partial r^2}\kappa(r,z) + \frac{\partial \mathrm{T}}{\partial r}\frac{\partial \kappa}{\partial r} + \frac{\partial^2 \mathrm{T}}{\partial z^2}\kappa(r,z) + \frac{\partial \mathrm{T}}{\partial z}\frac{\partial \kappa}{\partial z} \tag{17}$$

The limit results in an indeterminate form, which we can preform L'Hospital's rule on in order to obtain a meaningful value of our limit

$$\begin{aligned}
\lim_{r\to 0}\left[\frac{\frac{\partial \mathrm{T}}{\partial r}\kappa(r,z)}{r}\right] &= \frac{0}{0} \\
\lim_{r\to 0}\left[\frac{\frac{\partial \mathrm{T}}{\partial r}\kappa(r,z)}{r}\right] &\overset{\text{L}}{=} \lim_{r\to 0}\left[\frac{\frac{\partial}{\partial r}\left[\frac{\partial \mathrm{T}}{\partial r}\kappa(r,z)\right]}{\frac{\partial}{\partial r}\left[r\right]}\right] \\
&= \lim_{r\to 0}\left[\frac{\partial^2 \mathrm{T}}{\partial r^2}\kappa(r,z) + \frac{\partial \mathrm{T}}{\partial r}\frac{\partial \kappa(r,z)}{\partial r}\right]
\end{aligned} \tag{18}$$

Inspecting the second term, we can see that since we have symmetry about the origin due to out lack of phi dependence. $\frac{\partial T}{\partial r} \to 0$ due to this symmetry as $r \to 0$

$$\lim_{r\to 0}\left[\frac{\partial \mathrm{T}}{\partial r}\frac{\partial \kappa(r,z)}{\partial r}\right] = \lim_{r\to 0}\left[\frac{\partial \mathrm{T}}{\partial r}\right]\lim_{r\to 0}\left[\frac{\partial \kappa(r,z)}{\partial r}\right] = 0 \tag{19}$$

Our remaining term is continuous at $r = 0$ so for the limit we can simply evaluate it at the limiting value.

$$\begin{aligned}
\frac{\partial^2 \mathrm{T}}{\partial r^2}\kappa(r,z)|_{r=0} &= \left[\frac{\mathrm{T}^n_{1,z} - 2\mathrm{T}^n_{0,z} + \mathrm{T}^n_{-1,z}}{(\Delta r)^2}\right]\kappa^n_{0,z} \\
&= \frac{\mathrm{T}^n_{1,z}\kappa^n_{0,z}}{(\Delta r)^2} - \frac{2\mathrm{T}^n_{0,z}\kappa^n_{0,z}}{(\Delta r)^2} + \frac{\mathrm{T}^n_{-1,z}\kappa^n_{0,z}}{(\Delta r)^2}
\end{aligned} \tag{20}$$

By removing the original contribution of our first term of Eq. 6 from the coefficients it contributed to, and adding the contributions from the limiting value of the first term we have just calculated for, we are able to generate a new set of coefficients, corresponding to the same T terms from before

$$A^n_{r=0,z} = \left[\frac{-4\kappa^n_{0,z}}{(\Delta r)^2} - \frac{2\kappa^n_{0,z}}{(\Delta z)^2}\right] \tag{21}$$

$$B^n_{r=0,z} = \left[\frac{2\kappa^n_{0,z}}{(\Delta r)^2} - \frac{1}{2\Delta r}(\frac{\Delta \kappa}{\Delta r})^n_{0,z}\right] \tag{22}$$

$$C^n_{r=0,z} = \left[\frac{2\kappa^n_{0,z}}{(\Delta r)^2} + \frac{1}{2\Delta r}(\frac{\Delta \kappa}{\Delta r})^n_{0,z}\right] \tag{23}$$

$$D^n_{r=0,z} = \left[\frac{\kappa^n_{0,z}}{(\Delta z)^2} - \frac{1}{2\Delta z}(\frac{\Delta \kappa}{\Delta z})^n_{0,z}\right] \tag{24}$$

$$E^n_{r=0,z} = \left[\frac{\kappa^n_{0,z}}{(\Delta z)^2} + \frac{1}{2\Delta z}(\frac{\Delta \kappa}{\Delta z})^n_{0,z}\right] \tag{25}$$