Science in the Kitchen

THE UNIVERSITY OF ARIZONA®

Numerical Modeling of Diffusion and Phase Transitions in Heterogeneous Media

By: Jonathan Arellano, Katherine Borg, Victor Godoy Cortes, Karina Rodriguez, & Denise Villanueva

Mentor: Jeffrey Hyman

Introduction

- Studying thermal diffusion of an egg being boiled in water
- Goal: Develop a model of the thermal diffusion inside the egg.

Scientific Definitions

Thermal Diffusion – motion of all particles through a temperature gradient

Convection – Heat transfer from fluid to surroundings

Specific heat – material property of a substance that determines the amount of heat required to raise the temperature of 1 kg of the substance by 1°C.

Thermal Conductivity –material property that measures the material's ability to conduct heat (a perfect thermal conductor transmits heat instantaneously)

Egg Composition

- Inside the shell of an egg there is the egg white and the yolk made up of different substances.

- Prior to boiling the egg, the white is in a liquid state, while the yolk is between a liquid and solid state.

Governing Equation

THE UNIVERSITY OF ARIZONA®

$$\frac{\delta u}{\delta t} = \frac{dD}{dx}\frac{\delta u}{\delta x} + D\frac{\delta^2 u}{\delta x^2}$$

- x – position inside egg
- t – time elapsed of egg inside the water
- u(x,t) – temperature function dependent on the position and time
- D(x) – diffusion coefficient at position x

*By the end of this presentation, we will have derived this equation.

Two Immediate Problems

1. An egg is not an easily defined shape (i.e cube, sphere, cylinder, etc)

2. The yolk and egg white have different diffusion constants (i.e. the rate of temperature increase in yolk and white will differ when placed in the boiling water)

Initial Assumptions

1. Egg is perfectly spherical

   → Radial symmetry permits 1D analysis

2. The diffusion coefficient is constant (D)

   → $D_y = D_w$

3. Surrounding temperature is constant (u_w)

4. Width of shell is infinitesimally small

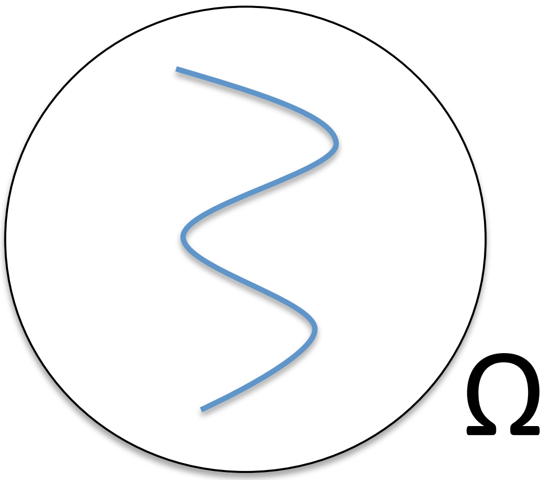
5. Perfect thermal conductivity egg shell

Intermediate Goal

Intermediate goal: Use previously stated assumptions to develop a simplified mathematical model.

Once we have developed the simplest mathematical model from the intermediate goal, we will consider varying D.

Stokes' Theorem & Fick's First Law



Stokes' Theorem:

$$\int_{s\Omega} \vec{f} \bullet n \, ds\Omega = \int_{\Omega} \nabla f \, d\Omega = \frac{du}{dt}$$

Fick's First Law:

$$f = D \nabla u$$

Governing Equation

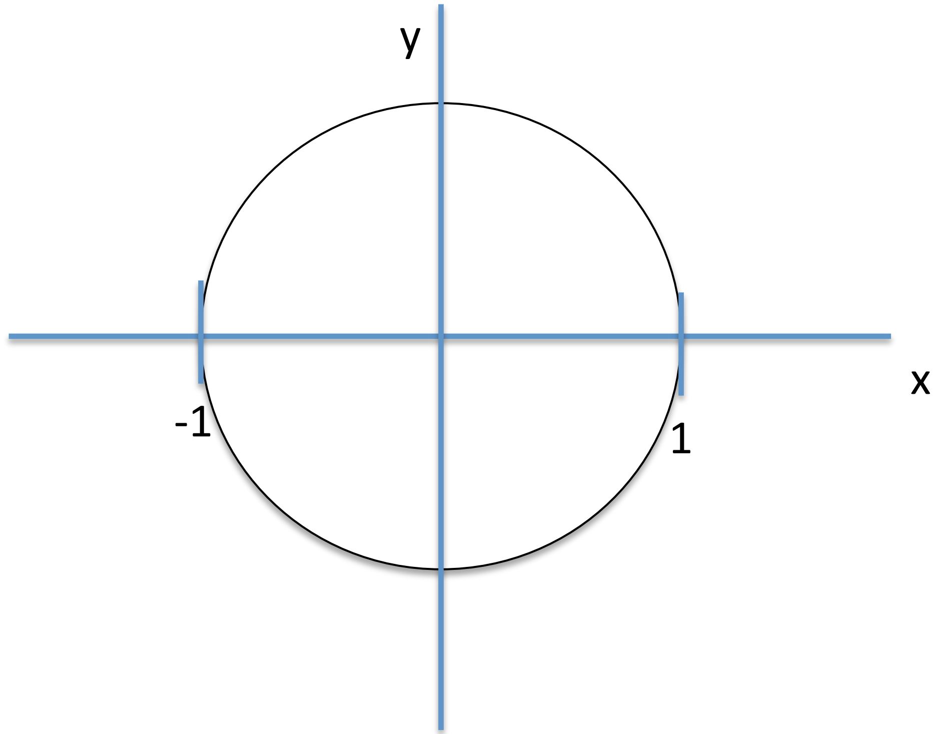
Combining the results from Stokes' Theorem and Fick's First Law we obtain:

$$\frac{\delta u}{\delta t} = \nabla \cdot [D grad(u)]$$

This equation holds for every point in the egg! It can be rewritten as:

$$\frac{\delta u}{\delta t} = \frac{dD}{dx}\frac{\delta u}{\delta x} + D\frac{\delta^2 u}{\delta x^2}$$

Defining Domain & Axes of Egg



We assume the egg is centered on our axes and the outer bounds are x=-1 and x=1. Moreover, due to radial symmetry we can just consider the x axis in our analysis.

Boundary Conditions & Initial Condition

- Boundary Conditions:

$$u(-1,t)=u_w$$

$$u(1,t)=u_w$$

i.e. the temperature at the outer boundaries of the egg is the same as the water temperature

- Initial Condition:

$$u(x,0)=f(x)$$

where f(x) is the profile of initial heat distribution throughout the egg

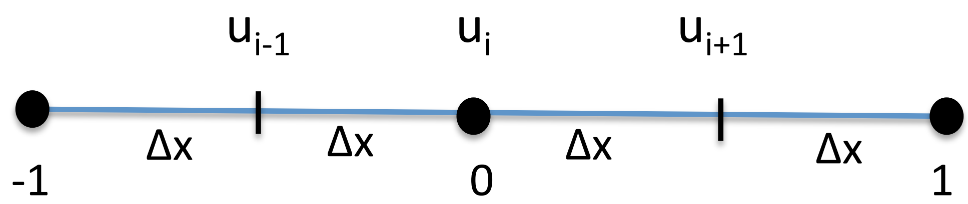
Assuming D is Constant

Since we are assuming D is constant, our original governing equation simplifies to:

$$\frac{\delta u}{\delta t} = D\frac{\delta^2 u}{\delta x^2}$$

Notice that this is the common heat equation studied in introductory courses to PDEs. Although we have solutions to this equation from PDE analysis, we will use the finite difference approximations to build up to the non-constant D model.

Finite Difference



$$\frac{\delta u}{\delta x} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

*Use Method of Undetermined Coefficients

To check the accuracy of finite difference approximation, we can use Taylor Series Expansion of u_{i+1} and u_{i-1}, which yields

$$u_{i+1} = u_i + \Delta x u_x + \frac{\Delta x^2}{2} u_{xx} + \frac{\Delta x^3}{6} u_{xxx} + \cdots$$

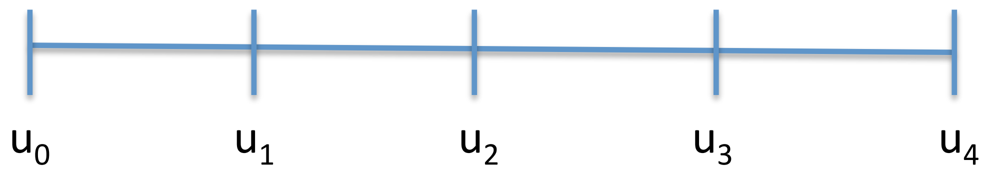
$$u_{i-1} = u_i - \Delta x u_x + \frac{\Delta x^2}{2} u_{xx} - \frac{\Delta x^3}{6} u_{xxx} + \cdots$$

Comparing Taylor Series and Finite Difference Approximations

$$u_{xx} + \frac{\Delta x^2}{4!} u_{xxxx} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

- From this equation, notice that their will be a small error associated with the finite difference approximation method.

Method of Lines



- At u_0 and u_4, they are equal to u_w (boundary conditions)

- You use the following formula for u_1, u_2, and u_3.

$$\frac{\delta u}{\delta t} = D\,\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

Physical Meaning

Imagine a pot of boiling water on the stove at a constant temperature of 100°C. You put an egg in the water and want to know how long it takes to heat the center of the egg to 60°C.

Remember that based on our assumptions we have an ideal egg, meaning

- The shell is very small and a perfect thermal conductor
- The egg is perfectly spherical
- Most importantly, the diffusion constant is uniform throughout the egg

Here are two videos demonstrating the diffusion rate at different D values.

- High Diffusion Constant:
  https://www.youtube.com/watch?v=W76NGGDOtto

- Low Diffusion Constant:
  https://www.youtube.com/watch?v=unrxGUjfvGo

Summary of Videos

Diffusion Coefficients	Time
$1x10^{-1}$	4.6
$1x\ 10^{-2}$	44.8

- Equation is in dimensionless form
- Higher diffusion constant → shorter time
- Lower diffusion constant → longer time
- Results match derived equation (rate of change of temperature directly proportional to diffusion constant)

Removing an Assumption

We derived an equation for an ideal model with these assumptions:

1. Egg is perfectly spherical
   → Radial symmetry permits 1D analysis
2. The diffusion coefficient is constant (D)
   → $D_y = D_w$
3. Surrounding temperature is constant (u_w)
4. Width of shell is infinitesimally small
5. Perfect thermal conductivity egg shell

Now we will derive a more complex equation by removing assumption number 2.

Original Governing Equation

Originally, we had this equation:

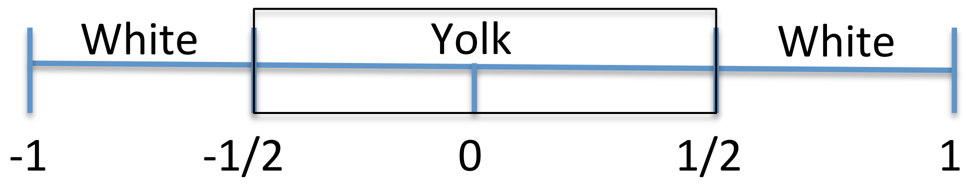
$$\frac{\delta u}{\delta t} = \frac{dD}{dx}\frac{\delta u}{\delta x} + D\frac{\delta^2 u}{\delta x^2}$$

By assuming constant D, the term below went to 0. We will now develop a model that includes this term.

$$\frac{dD}{dx}\frac{\delta u}{\delta x}$$

Model with Varying D

One Dimension Model of Egg:



- Diffusion Function

$$D(x) = D_w \qquad |x| \geq \frac{1}{2}$$

$$D(x) = D_y \qquad |x| < \frac{1}{2}$$

*Note: the diffusion function is discontinuous which presents problems in analysis

- Boundary Conditions:

u(-1,t)=u(1,t)

- Initial Condition:

u(x,0)=f(x)

*We have the same boundary conditions and initial conditions as before.

Two Steps

1. Compute Flux, $D\frac{\delta u}{\delta x}$

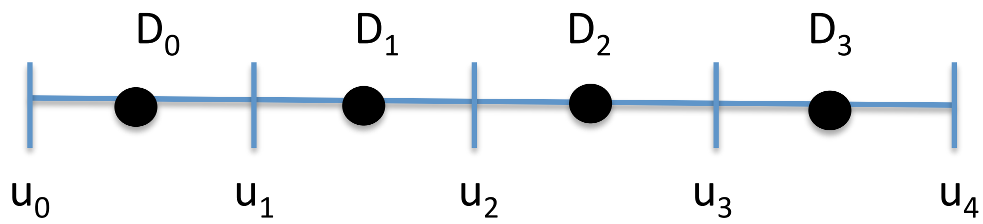
2. Compute Derivative of Flux, $\frac{df}{dx}$ or $\frac{f_{i+1} - f_i}{\Delta x}$

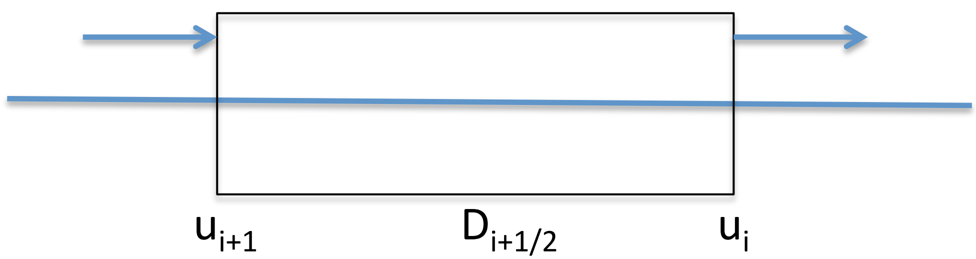
We need to create a finite volume approximation to obtain the previously ignored term.

Notice that we are using finite volume and not finite difference approximations like before.

Finite Volume Approximation

THE UNIVERSITY OF ARIZONA®





Step 1: Finding the flux.

$$f_{i+1/2} = D_{i+1/2} \frac{u_{i+1} - u_i}{\Delta x}$$

Varying D Derivation

Step 2: Derivative of the flux from the definition of a derivative.

$$\frac{\delta}{\delta x} f_{i+1} = \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x}$$

Putting together our results, we obtain the following end result:

$$\frac{\delta u}{\delta t} = \frac{D_{i+\frac{1}{2}}(u_{i+1} - u_i) - D_{i-\frac{1}{2}}(u_i - u_{i-1})}{\Delta x^2}$$

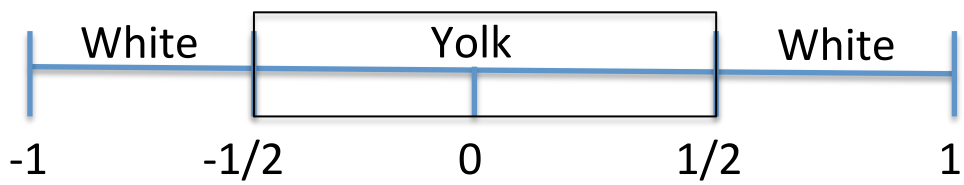
Notice that if $D_{i+1/2}=D_{i-1/2}$, then we get the constant D equation, which is

$$\frac{\delta u}{\delta t} = D\,\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

Scheme for Non-Uniform Diffusion

$$\frac{\delta u}{\delta t} = \frac{D_{i+\frac{1}{2}}(u_{i+1} - u_i) - D_{i-\frac{1}{2}}(u_i - u_{i-1})}{\Delta x^2}$$

The above equation is relevant to this model.



It is also equivalent to this:

$$\frac{\delta u}{\delta t} = \frac{dD}{dx}\frac{\delta u}{\delta x} + D\frac{\delta^2 u}{\delta x^2}$$

So we were able to successfully develop our original governing equation. However, keep in mind that this governing equation is constrained by numerous assumptions still.

Summary

- An egg is composed of 2 materials, the yolk and egg white, which results in a non-constant thermal diffusion coefficient, D(x).

- Using finite difference approximations, a simple governing equation is obtained.

$$\frac{\delta u}{\delta t} = D\frac{\delta^2 u}{\delta x^2} \quad \text{or} \quad \frac{\delta u}{\delta t} = D\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

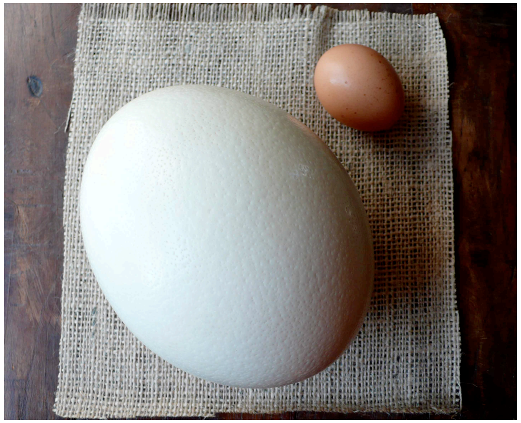
- Using finite volume approximations, a governing equation for non-constant D was found.

$$\frac{\delta u}{\delta t} = \frac{dD}{dx}\frac{\delta u}{\delta x} + D\frac{\delta^2 u}{\delta x^2} \quad \text{or} \quad \frac{\delta u}{\delta t} = \frac{D_{i+\frac{1}{2}}(u_{i+1} - u_i) - D_{i-\frac{1}{2}}(u_i - u_{i-1})}{\Delta x^2}$$

- The changing diffusion coefficient is what makes this problem interesting.

Next Steps

- Use applied analysis lab to test our equation
- Try to determine the actual values of D_y and D_w
- Study the effects of changing parameters, i.e. width and egg type
- Attempt to develop a 3D diffusion model



Essentially, we want to test our current model for varying D and then attempt to develop a more exact model via the elimination of our assumptions.

Questions/References

Any questions?

References:

Aslamazov, L. G., A. A. Varlamov, and A. A. Abrikosov. *The Wonders of Physics*. Singapore: World Scientific, 2001. 37-52. Print.

Hoffmann, Franz. *The Finite Volume Method for Solving Partial Differential Equations*. Tech. New Orleans: Tulane University, 2012. Print.