Science in the Kitchen:

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Numerical Modeling of Diffusion and Phase Transitions in Heterogeneous Media

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Project Description:

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Develop a mathematical model of thermal diffusion within an egg being boiled

- ❖ Apply model to predict phase transitions from liquid to a solid state in the yolk and egg white
- ❖ Apply model to predict phase transitions from liquid to solid in the yolk and no phase transition in the egg white

Scientific Challenges:

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Why is studying the thermal diffusion in an egg important?

- Understand behavior of boiling eggs at various times and temperatures
- Increases the range of foods we can eat
- Reduces the risk of food poisoning

Scientific Definitions:

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Heat: energy flow from a hot body to a cold one

Temperature: measure of which way heat will flow

Specific Heat: the amount of heat required to raise the temperature of 1 kg of the substance by 1 Degree Celsius

Latent Heat: heat added to change the state of a substance that does not change the temperature of the substance

Thermal Diffusion: measure of thermal inertia. In a substance with high thermal diffusivity, heat moves rapidly through it because the substance conducts heat quickly relative to its volumetric heat capacity

Convection: the transfer of heat by the circulation of the heated parts of a liquid or gas

Cooking Theory:

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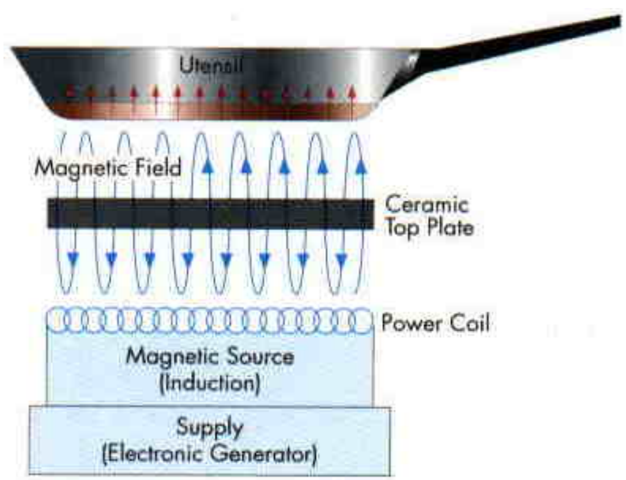
- Temperature gradient forms when two objects at different temperatures are placed close together

- The heat flow causes the temperature to rise in the colder body and since the boiling water is constantly being supplied thermal energy from the stove, it will remain constant.

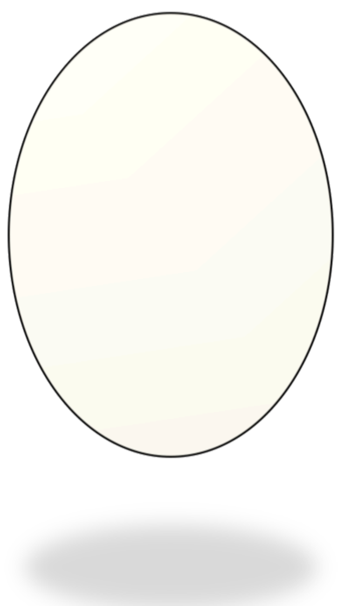
- Thermal equilibrium is reached and no more heat flows



Heat Flow:

The flow of heat in a physical situation depends on the following:

- How well 2 objects are in contact
- How fast heat can flow through the objects
- The specific heat of each object (material property)
- The temperature gradient that exists between the two objects
    - The rate of heat flow decreases as thermal equilibrium is reached



Boiling An Egg:

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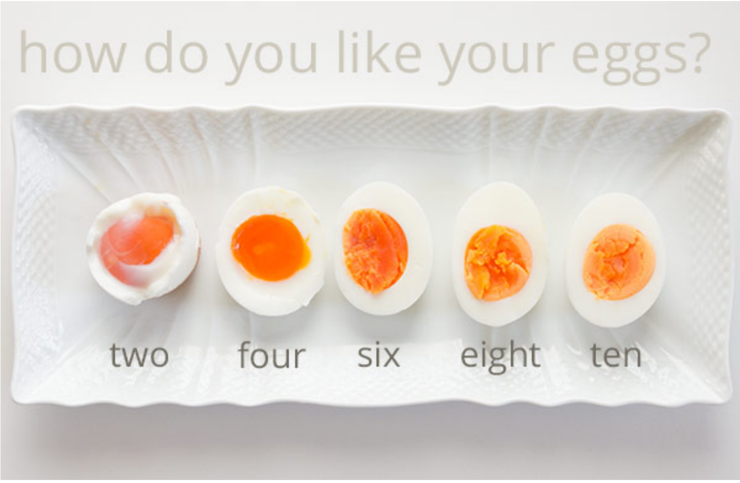
Perfect Boiled Egg Dilemma:

1. Everyone wants it differently
2. Every egg is different and cooks differently
3. The equipment used is not always the same



Although all of the factors are not possible for one model to take into account, understanding of what actually happens to an egg in general when it boils permits a reasonable prediction.

Project Fundamentals:

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Foundation of Our Project:

❖ By understanding the basics of the manner in which heat flows into a body, we can calculate the cooking times for any situation.

Expectations for Our Model:

❖ Calculated cooking times reasonably match literature and experimental values

❖ Cooking time depends on the square of the radius of the dish we are cooking

$$t \propto \frac{r^2}{D^2 c^2 [log(T - T_c)]^2}$$

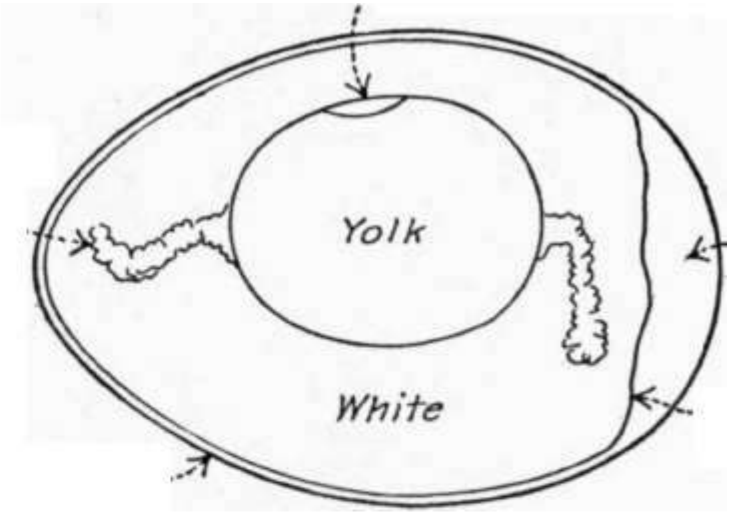
t : cooking time (min)
r : mean radius of egg (mm)
D : thermal diffusivity
c : specific heat
T : egg temperature (C)
Tc : cooking temperature (C)

*Peter Barham The Science of Cooking, Springer, 2001 ISBN-10: 3540674667, ISBN-13: 978-3540674665

Egg Composition:

Egg is composed of 2 primary regions inside the shell:

1. Albumen (egg white)
2. Yolk



The Science of Cooking an Egg:

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As eggs cook, the proteins first denature and then coagulate

- ❖ Egg White → Coagulation occurs at ~63°C
- ❖ Egg Yolk → Coagulation occurs at 70°C (controls runniness)

Temperature	Effects on Egg-White	Effects on Yolk
Below 55°C	Risk of Salmonella	
Up to 63°C	Soft and gelatinous similar texture to partially set jellies or non-drip paints	'runny' liquid with similar "thickness" to washing up liquid
65°C - 70°C	Set as a soft gel-similar texture to well set jelly	Still runny, but liquid starting to thicken-viscosity increasing to that of treacle
73°C	Hardening of white, texture of soft fruit, strawberries, etc.	Soft gel like texture rather like a thick shampoo
77°C	White continues to harden	Hard boiled still soft, but solid texture of set yoghurt
80°C		Onset of green discoloration around edge of yolk
90°C	Overcooked tough white, texture of damp sponge	Yolk completely dry, crumbly solid

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Derivation of the Heat Equation:

Variables:

- u(x,y,z,t) → temperature of the material at location (x,y,z) at time t
- D → thermal diffusivity

$$u_t = \nabla \cdot (Dgrad(u))$$

This is the general non-uniform conservative form of the heat equation.

Governing Equation:

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Transformation equations are: $x = \rho sin(\theta)cos(\phi)$

$$y = \rho sin(\theta)sin(\phi)$$

$$z = \rho cos(\theta)$$

$$\frac{\partial u}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}(Dr^2\frac{\partial u}{\partial r}) + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial \theta}(Dsin\theta\frac{\partial u}{\partial \theta}) + \frac{1}{r^2 sin^2\theta}\frac{\partial}{\partial \phi}(D\frac{\partial u}{\partial \phi})$$

By assuming radial symmetry, the above 3D spherical model simplifies to:

$$\frac{\partial u}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}(Dr^2\frac{\partial u}{\partial r})$$

- U(r, θ , ϕ ,t) – temperature function dependent on the position and time
- D(r) – diffusion coefficient at radius r in egg

Finite Volume Approximation:

The governing PDE is numerically integrated using code we developed in MATLAB.

$$\frac{\partial u}{\partial t}\Big|_{r_i} = D\left(\frac{2}{r_i}\frac{u_{i+1} - u_{i-1}}{2\Delta r} + \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta r)^2}\right)$$

Diffusivity Defined:

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Since the egg is composed of different materials, the diffusion coefficient will vary with position.

$$D = \begin{cases} D_y & r < 0.5r_{egg} \\ \frac{2D_yD_w}{D_w+D_y} & r = 0.5r_{egg} \\ D_w & r > 0.5r_{egg} \end{cases}$$

At the interface between the yolk and white, the diffusion constant is given by the Harmonic mean. We found this by analyzing the flux at the interface and employing The Fundamental Theorem of Calculus.

Numerical Model in Non-Uniform Media

Theory of Code:

1. Break the domain of the egg up into many infinitesimally small segments
2. At a specified time, calculate the temperature at each point in the egg (D changes based on position in egg).
3. Repeat calculations at small time steps until the temperature at the center of the yolk is a specified temperature

Water Temp (°C)	Large Egg 'd' (cm)	Xlarge Egg 'd' (cm)	Yolk Diffusion Coefficient (cm^2/1e-5 s)	Albumen Diffusion Coefficient (cm^2/1e-5 s)
100	4.584	4.902	1.66*10^(-5)	0.37*10^(-5)

LARGE EGG

Temperature (°C)	Time (min)
58	8.4
64	9.3
66	10.1
70	10.9
80	13.5

XLARGE EGG

Temperature (°C)	Time (min)
58	9.7
64	10.6
66	11.6
70	12.6
80	15.4

Changing Parameters:

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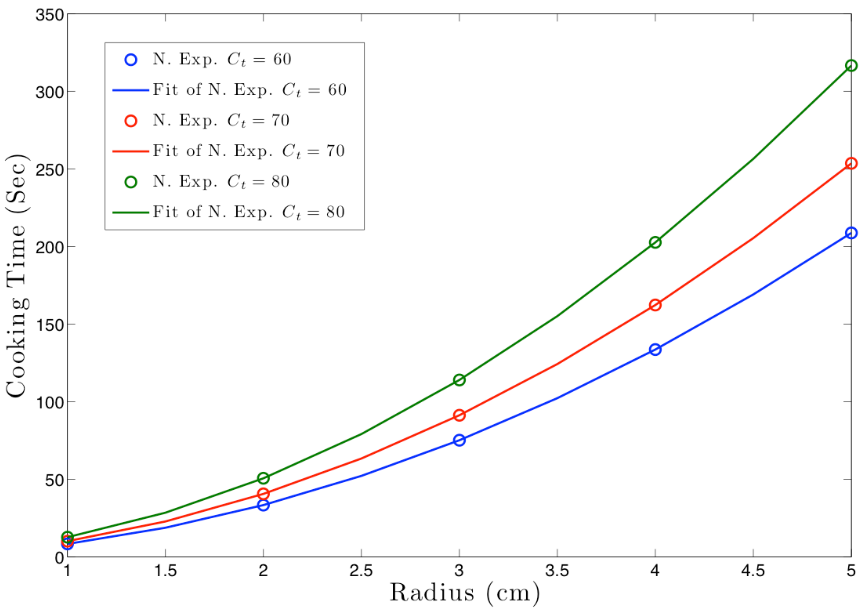
Once the code was developed, we were able to vary one parameter at a time to determine how it affected the cooking time and behavior of the system.

From this analysis, we found the following:

- Cooking time depends on the square of the radius of the egg.
- By cooking the egg at a lower temperature, we are able to cook the yolk so that it is solid without solidifying the egg white.



Literature Approach:

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$$t = 0.0015 d^2 log_e\left[\frac{2(T_{water} - T_0)}{T_{water} - T_{yolk}}\right]$$

d: diameter of the egg (mm)
T_0: temperature of the egg before it was put into the water (C)

LARGE EGG

Temperature (°C)	Time (min)
58	4.9
64	5.3
66	5.5
70	5.9
80	7.2

XLARGE EGG

Temperature (°C)	Time (min)
58	5.5
64	6.1
66	6.3
70	6.7
80	8.1

*Peter Barham The Science of Cooking, Springer, 2001 ISBN-10: 3540674667, ISBN-13: 978-3540674665

Experimental Results:

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LARGE EGG

Time (Min)	Temperature (°C)
8.4	59
9.3	62
10.1	65
10.9	67
13.5	77

XLARGE EGG

Time (Min)	Temperature (°C)
9.7	57
10.6	62
11.6	65
12.6	69
15.4	75

Summary of Results:

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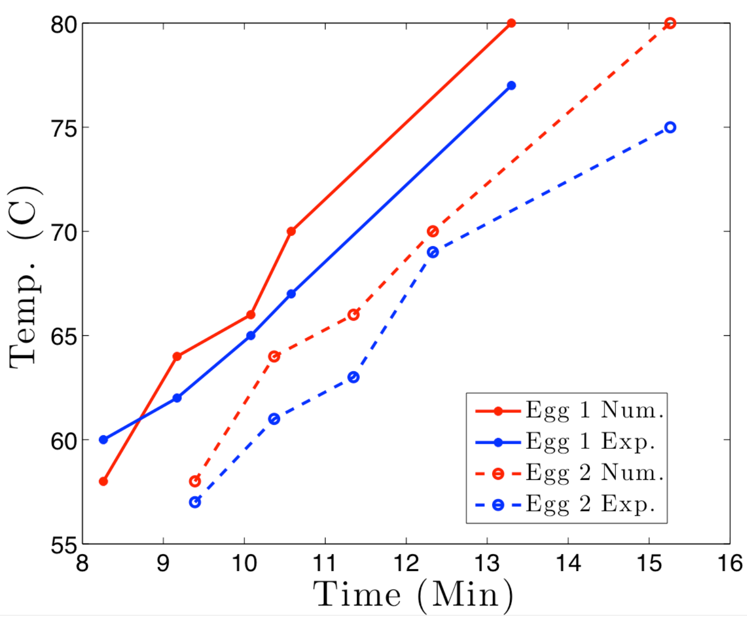

LARGE EGG

Time (min)	Predicted Temp (°C)	Experimental Temp (°C)
8.4	58	59
9.3	64	62
10.1	66	65
10.9	70	67
13.5	80	77

XLARGE EGG

Time(min)	Predicted Temp (°C)	Experimental Temp (°C)
9.7	58	57
10.6	64	62
11.6	66	65
12.6	70	69
15.4	80	75

Summary of Results:

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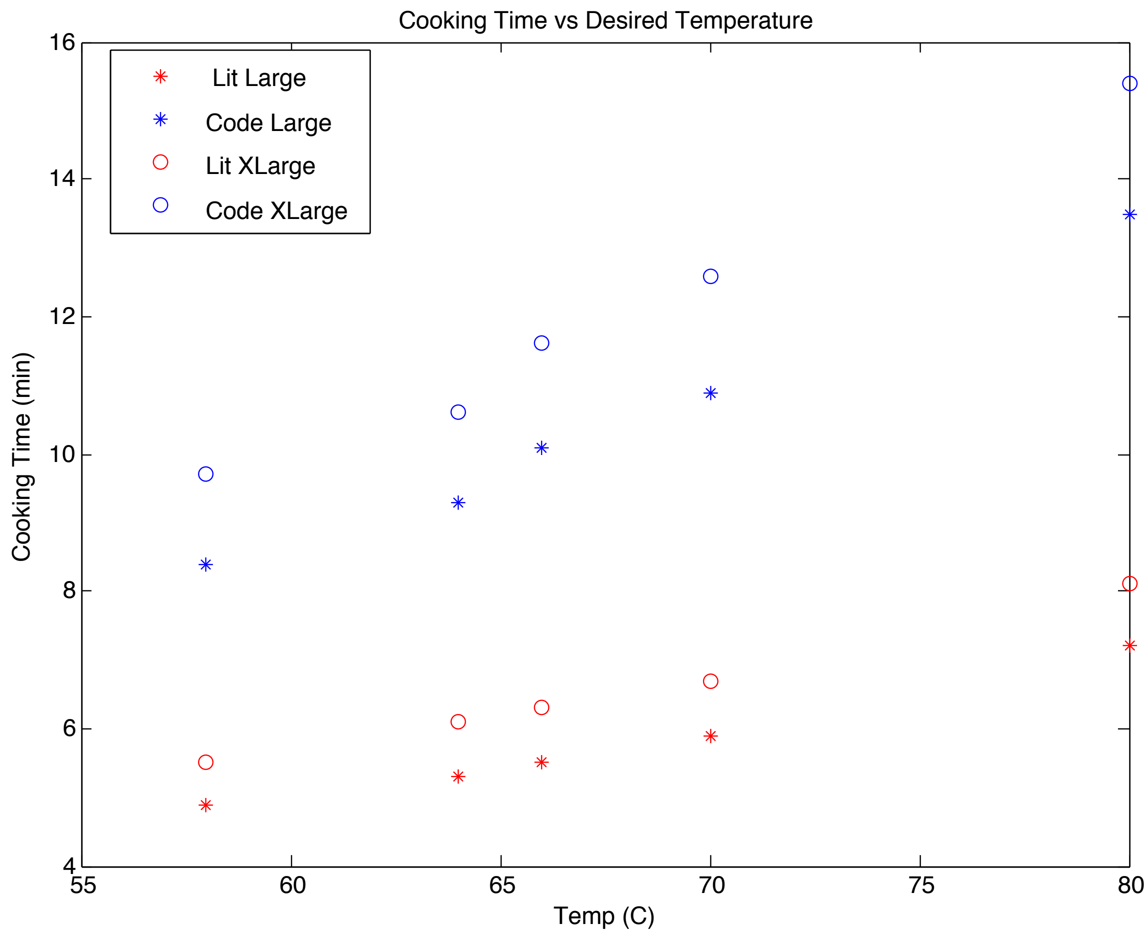

Potential Applications

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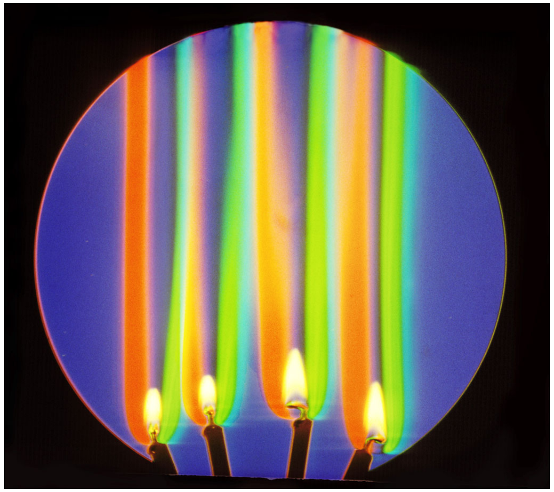

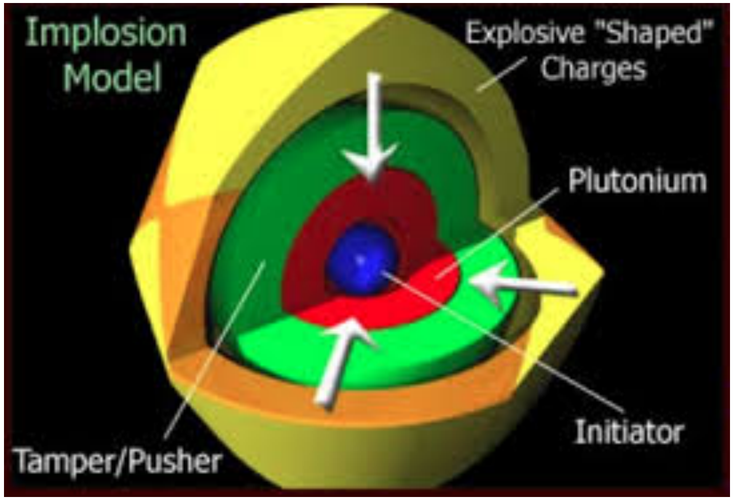

Questions/References/Acknowledgments

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Any questions?

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Peter Barham The Science of Cooking, Springer, 2001 ISBN-10: 3540674667, ISBN-13: 978-3540674665

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