3D Heat Equation Model Development and Simulation in a Controlled Environment

Abstract

This study presents a three dimensional analytical model for the heat equation with a laser induced Gaussian source term, based on the general solution provided by Evans. The model simulates transient temperature distributions in a metallic medium, with aluminum as the reference material, under varying laser parameters such as beam power, pulse duration, and beam radius. Results show strong agreement with theoretical expectations: temperature increases linearly with power, non-linearly with pulse duration, and inversely with beam radius. A decay in local temperature increase was also observed. Assumptions include constant material properties and ideal boundary conditions, making the model suitable for controlled environments. Future work will address more complex geometries, non-constant properties, and improved numerical efficiency.

1 Introduction

The heat equation describes how heat evolves over time and space within a system:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + Q(x,y,z,t) \tag{1}$$

Here, T is the temperature, $\alpha = \frac{k}{\rho C}$ is the thermal diffusivity, and $f(x,y,z,t)$ represents an internal heat source per unit volume. The thermal diffusivity α characterizes how quickly heat diffuses through the material, where:

- k is the thermal conductivity (W/m·K),
- ρ is the material density (kg/m^3),
- C is the specific heat capacity (J/kg·K).

In the absence of a source term ($Q = 0$), Equation (1) reduces to the homogeneous heat equation.

The heat equation relates the energy transferred to a system by heat and therefore provides a framework to understand and simulate thermal processes accurately. The model developed in this paper incorporates realistic conditions, including variable material properties, initial conditions, and a Gaussian laser pulse heat source.

2 Theoretical Background and Analytical Model development

2.1 Model development

The heat equation is a three-dimensional, second-order partial differential equation, as shown in Equation (1). $Q(x,y,z,t)$ can be written as any equation that describe the heat source term, in the current model it is described as a gaussian source, which is the most accurate way to model a standard laser pulse, however for plasma modeling a Dirac-delta approach will prove more accurate due to the high energy sources.
The gaussian source is written as follows:

$$Q(x,y,z,t) = I_0 \exp\left(-\frac{(x-x_0)^2+(y-y_0)^2}{w^2}\right)\cdot\exp\left(-\frac{z}{\delta}\right)\cdot\exp\left(-\frac{(t-t_0)^2}{\tau^2}\right) \quad (2)$$

- $I_0 = \frac{P}{\pi w^2}$ is the initial intensity of the laser
- $x - x_0$ is the point at which the laser hit on the x spatial direction
- $y - y_0$ is the point at which the laser hit on the y spatial direction
- z is the distance the laser penetrates through the material
- δ is the optical penetration depth which is the distance light travels within a material before its intensity is reduced to 37% (1/e) of its initial value at the surface
- τ is the time period at which the pulse is applied on.

As derived by *David J. Griffiths* in *Introduction to Electrodynamics* (Equation 8.6, p. 363), Poynting's Theorem states:

> The rate of change of electromagnetic energy within a volume is equal to the work done on the charges inside that volume, minus the net electromagnetic energy flux leaving the volume.

By normalizing Equation (2), the expression for the energy transferred into the system can be found using Poynting's Theorem. Since the model works for an insulated system, the net electromagnetic flux exiting the volume equates to zero.

$$W = E = \int_V \int_0^t Q(x,y,z,t)\, dt\, dV \quad (3)$$

Each integral evaluates to:

$$\int_{-\infty}^{\infty} \exp\left(-\frac{(x-x_0)^2}{w^2}\right) dx = w\sqrt{\pi}$$

$$\int_{-\infty}^{\infty} \exp\left(-\frac{(y-y_0)^2}{w^2}\right) dy = w\sqrt{\pi}$$

$$\int_0^\infty \exp\left(-\frac{z}{\delta}\right)dz = \delta$$

$$\int_{-\infty}^\infty \exp\left(-\frac{(t-t_0)^2}{\tau^2}\right)dt = \tau\sqrt{\pi}$$

By putting it all together the expression for the energy within the system is dervied.

$$E = I_0 w^2 \pi^{3/2} \delta \tau \tag{4}$$

Using Equation (2), this can become a source term solution by introducing a factor of $\frac{\mu_a}{\rho C}$ where μ_a is the absorption coefficient which is material dependent. That way the units are joules per second for the source term.

$$f(x,y,z,t) = \frac{I_0 \mu_a}{\rho C} \exp\left(-\frac{(x-x_0)^2+(y-y_0)^2}{w^2}\right) \cdot \exp\left(-\frac{z}{\delta}\right) \cdot \exp\left(-\frac{(t-t_0)^2}{\tau^2}\right) \tag{5}$$

The model will be is based on the general integral solution to the heat equation, as presented in *Partial Differential Equations* by Lawrence Evans [1], and by applying Equation (5) as the gaussian source term solution, the temperature distribution can be calculated as follows

$$T(x,y,z,t) = \int_{\mathbb{R}^3} G(x-y,t)T_0(y)\,dy + \int_0^t \int_{\mathbb{R}^3} \exp\left(-\frac{|x-y|^2}{4(t-t')}\right) f(x,y,z,t')\,dy\,dt', \tag{6}$$

where the laser source term $f(x,y,z,t)$ is defined as:

$$f(x,y,z,t') = \frac{\mu_a}{\rho c} I_0 \exp\left(-\frac{(x_1-x_0)^2+(y_1-y_0)^2}{w^2}\right) \exp\left(-\frac{z}{\delta}\right) \exp\left(-\frac{(t'-t_0)^2}{\tau^2}\right),$$

and the Green's function in the solution is:

$$G(x-y,t) = \frac{1}{(4\pi\alpha t)^{3/2}} \exp\left(-\frac{|x-y|^2}{4\alpha t}\right).$$

2.2 Boundary conditions

To develop a numerical solution, boundary conditions must be applied.
For the current model, a controlled environment in a perfect insulator is assumed.
The initial tempereature is assumed to be uniform throughout the object.

$$T(x,y,z,t=0) = T(x,y,z) = T_0$$

For the specific simulation, $T_0 = 20^\circ C$.
On the walls of the object, Newmann boundry conditions were applied such that

$$\frac{\partial T}{\partial S} = 0$$

Here S is normal to the surface of the cube.
The Newmann condition can also be assumed directly from the fact that this is a uniform distribution of heat at $t = 0$

2.3 Finite difference method

The definition of a derivative is as follows:

$$f'(x) = \lim_{\Delta x \to 0} \frac{\Delta f(x)}{\Delta x} \tag{7}$$

However, for computers, an infinitesimal $\to$ is impossible.
The aim is to discretize the continuous dependencies.

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x} \tag{8}$$

$$\tag{9}$$

$$x : x_i \quad x + \Delta x : x_{i+1} \quad \Delta x : h \tag{10}$$

Where x_i is the current position, x_{i+1} is the next position and h is the current step number. As h decreases, the derivative approximation becomes more accurate. Applying the Taylor expansion, we can estimate the estimated value of $f(x)$.

$$f(x) = f(a)(x-a) + f'(a)(x-a) + \frac{f''(a)(x-a)^2}{2!} + ... \tag{11}$$

$$x - a = h \qquad f'(x) \approx \frac{f(x_{i+1}) - f(x_i)}{h} \tag{12}$$

$$f'(x) \approx \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \tag{13}$$

Here $O(h)$ means that the next value in the series will be of order h.
By repeating the process, the second derivative can be obtained.

$$f''(x) = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{\Delta x^2} + O(h^2) \tag{14}$$

Where in this case $O(h^2)$ represents an error in the order of h^2

3 Numerical Algorithm to solve the 3D Heat equation

3.1 Step 1: Define the domain

Consider an even cube for simplicity.

$$\text{Length} = L_x = L_y = L_z$$

$$\text{Step distance} = dx = dy = dz = \frac{L}{N-1}$$

$$N = \text{Number of steps}$$

3.2 Step 2: Time step and simulation time

Initializing the time step dt and the running time of the simulation t

3.3 Step 3: Initilize temperature field

$$\text{At } t = 0 \quad T_{i_0,j_0,k_0} = T(x,y,z,0)$$

3.4 Step 4: Define the laser pulse source

Using the source I defined earlier

$$Q(x,y,z,t) = I_0 \exp\left(-\frac{(x_{i+1}-x_i)^2 + (y_{i+1}-y_i)^2}{w^2}\right) \cdot \exp\left(-\frac{z}{\delta}\right) \cdot \exp\left(-\frac{t-t_0}{\tau^2}\right)$$

Where all the parameters represent the same representation as before. $t_0 = 0$

3.5 Step 5: Time loop

3.5.1 a) Compute the laplacian $\nabla^2 T$

Using finite differentiation introduced earlier, the second derivitve has the following expression:

$$f''(x) \approx \frac{f(x_{i+1}) - 2f(x) + f(x_{i-1})}{h^2}.$$

Using that expresison

$$\nabla^2 T \approx \frac{T_{i+1,j,k} + T_{i-1} - 2T_{i,j,k}}{dx^2} + \frac{T_{i,j+1,k} + T_{i,j-1,k} - 2T_{i,j,k}}{dy^2} + \frac{T_{i,j,k+1} + T_{i,j,k-1} - 2T_{i,j,k}}{dz^2}$$

3.5.2 b) Compute The source term at time t

At this point in time we need to compute the source term $Q(x,y,z,t_{current})$ in each time, that the temperature is being evaluated. (note that it is applied for some period τ, it can be simplified by assuming it is only applied at t = 0, but thats not realistic).

3.5.3 c) Update the temperature using Euler's Method

Since $\frac{\partial T}{\partial t} = \alpha \nabla^2 T + Q(x,y,z,t)$ I can estimate the temperature as

$$T_{i,j,k}^{n+1} \approx T_{i,j,k}^{n} + dt(\alpha \nabla^2 T_{i,j,k} + Q(x,y,z,t))$$

3.5.4 d) Apply boundry conditions

While they are inculded in the analytic solution, they are not included in the algorithm. Therefore they must be included.

$$T_0 = 20^\circ C \quad \text{For all walls}$$

$$\frac{\partial T}{\partial S} = 0 \;\; \text{Newman boundary condition}$$

4 Simulation Results

The following section shows data generated by the model using Python, the simulation ran the model and varied Power, Legnth, Beam radius and duration, varying one parameters each time and keeping the others constant; that allowed to observe the relationships between the local temperature variances of the object to the parameter. The following table shows the default simulation parameters used.

Table 1: Default Simulation Parameters

Parameter	Value	Unit	Description
L	1	m	Domain length
P	1×10^6	W	Power input
w	1×10^{-4}	m	Beam width
τ	1×10^{-6}	s	Pulse duration
N	6	-	Number of grid points
t_{total}	1×10^{-4}	s	Total simulation time
ρ	2700	$\mathrm{kg\,m^{-3}}$	Material density
c	900	$\mathrm{J\,kg^{-1}\,K^{-1}}$	Specific heat capacity
k	237	$\mathrm{W\,m^{-1}\,K^{-1}}$	Thermal conductivity
T_0	20	°C	Initial temperature
α	$\frac{k}{\rho c}$	$\mathrm{m^2\,s^{-1}}$	Thermal diffusivity
μ_a	$0.1 \times L$	$\mathrm{m^{-1}}$	Absorption coefficient

It is important to note that μ_a is a property that varies between different materials; however, as a modeling choice it scales with L to allow the results to remain physically correct. For practical experiment μ_a one would need a material-specific value.

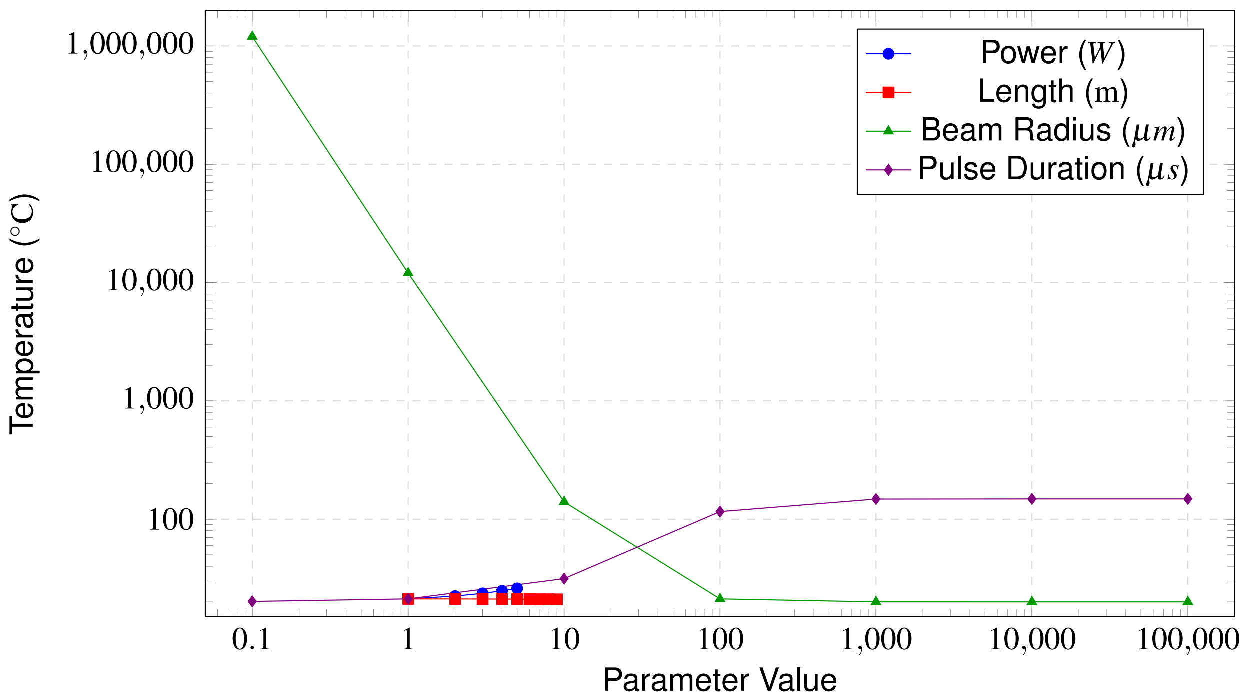

Figure 1: Local Temperature variances in power, length, beam radius, and pulse duration. *Power: Temperature increases linearly with power as expected. Length: Increased length reduces maximum temperature increase. Radius: Maximum temperature increases with reduced beam radius. Pulse duration: Longer pulses lead to higher temperatures until saturation.*

Table 2: Power (MW) vs Temperature (℃)

Power (MW)	Temperature (°C)
1.0	21.20
2.0	22.40
3.0	23.61
4.0	24.81
5.0	26.01

Table 3: Length vs Maximum Temperature

Power (MW)	Temperature (°C)
1.000	21.20
2.000	21.18
3.000	21.15
4.000	21.13
5.000	21.11
6.000	21.09
7.000	21.07
8.000	21.05
9.000	21.02

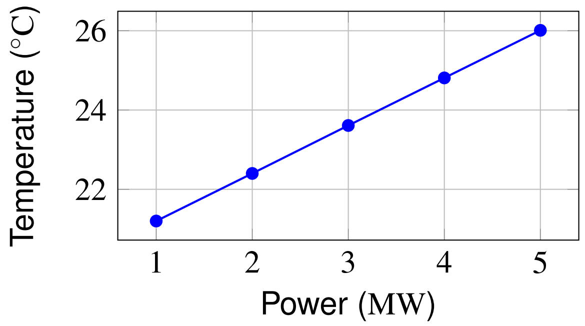

Figure 2: Power (MW) vs Temperature (°C) - plotted individually to show the linear relationship between the power and temperature

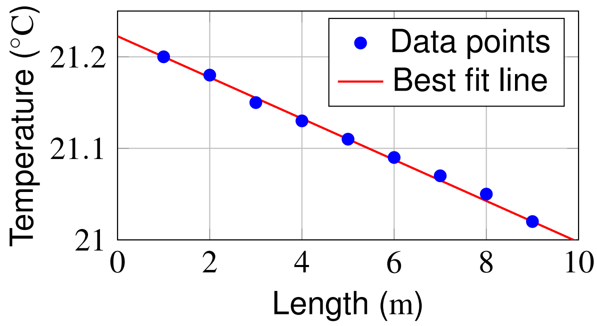

Figure 3: Length (m) Temperature (°C) plotted individually to show the relationship between length increase and temperature.

- Power (MW) vs Local Temperature (°C) - Linear increase of temperature due to power increaes. The result matches the expectation. From Equation (5) it is shown that $T \propto I0 \propto P$.
- Length (m) vs Local Temperature (°C) - As the length increases, the heat is distributed over a larger domain, resulting in a reducing temperature increase in the material. However, a slight increase in temperature is still observed, which can be attributed to the total energy being transferred into the material.
- Beam radius (µm) vs Local Temperature (°C) - For smaller beam radius, more energy is transferred locally, causing the maximum temperature to increase to very large values. As the beam radius increases, the local temperature reduces since the same amount of energy is transferred in larger domain (assuming power remains constant).

- Pulse Duration (µs) vs Temperature Increase - Result aligns with established physical theory, the local temperature values initially increase sharply with pulse duration. However, at 1000µs, the object reaches equilibrium. In practice, once equilibrium is reached, the object begins a phase change. This behavior is not reflected in the graph as the model does not account for phase transitions.

5 Discussion

The results from the previous section demonstrate that the model functions correctly as the outcomes are consistent with established physical theory. The model performs well under controlled conditions and offers valuable insight into how temperature varies with different parameters. Its potential applications are significant; from the model, other physical properties such as energy, laser wavelength, and more can be inferred. An immediate application is in welding. As shown in Figure 3, the maximum temperature increases substantially as the radius of the beam decreases. In practical terms, this allows us to estimate the temperature required to cut metals or other materials precisely and to control that temperature by adjusting the beam radius.

6 Future work

Currently, the model is limited to cubical systems. Future work will focus on extending the model to support different geometries and improving the underlying code. In the short term, this can be achieved by converting the model to cylindrical and spherical coordinate systems, allowing analysis of various symmetric shapes, particularly slabs, which are commonly used in optical applications. Additional improvements may include removing the Newman boundary condition and incorporating heat loss to the surrounding air, thereby allowing the model to simulate non-insulated systems. Another potential direction is to integrate the model with hydrodynamics, providing insight into fluid behavior within insulated materials as temperature varies. Also stability and error analysis are required to optimize the grid and time-step values to increase the accuracy and computational efficiency of the model.

7 Conclusions

In this study, a three-dimensional model of the heat equation was developed to simulate the local temperature response to variations in key parameters. The model incorporates the general solution of the heat equation presented by Lawrence Evans, with a Gaussian laser heat source term. Account for all essential parameters relevant to a laser system operating in a controlled environment.

The simulations used the physical properties of aluminum to represent a generic metallic material; however, the model is able to adapt to other materials by adjusting physical parameters. The results were consistent with established physical theory, which provides strong evidence for the validity of the model.

The simulation showed that the local temperature at the point of contact of the laser increases linearly with laser power (W), increases rapidly with the duration of the pulse (s) until saturation, and is inversely related to the radius of the beam (m) until saturation. An interesting trend was observed in relation to object length: as length increased, the temperature rise diminished nearly linearly, though the temperature continued to increase overall.

The model assumes constant thermal properties, a perfectly insulating boundary, and a simplified laser material interaction via a scaled absorption coefficient. Although appropriate for a controlled setting, these assumptions can limit the applicability of the model to systems with non-linear material behavior or complex geometries.

Future work may involve optimizing computational efficiency, implementing solvers in cylindrical or spherical coordinates, and incorporating stability/error analysis. These improvements could improve both accuracy and performance, particularly in applications with high precision or biological relevance.

8 References

References

[1] L. C. Evans, *Partial Differential Equations*, 2nd ed., American Mathematical Society, 2010, Section 2.3, p. 49.

[2] D. J. Griffiths, *Introduction to Electrodynamics*, 3rd ed., Prentice Hall, 1999, Equation 8.6, p. 363.