Stability and Grid Convergence Analysis of the 3D Heat Equation with Laser Source

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Abstract

This report presents the numerical solution of the three-dimensional heat equation under laser heating using an explicit FTCS finite difference scheme. Stability and convergence analyses were conducted to verify the physical validity and numerical robustness of the model. The stability analysis confirmed the model's behavior within the theoretical FTCS stability limits, while an unexpected non-linear relationship between relative error and domain size was observed—indicating a diffusion length scale around 3 cm. The convergence study demonstrated a rate of approximately 1.24 with an excellent goodness-of-fit ($R^2 \approx 1$), supporting the reliability of the numerical method. These findings lay the groundwork for extending the model to more complex geometries and integrating machine learning approaches for efficient temperature prediction in laser–material interactions.

1 Introduction

The three-dimensional (3D) heat conduction problem involves understanding how heat distributes throughout a material over time. By incorporating additional physical parameters and accounting for complex geometries, more realistic solutions can be obtained that align more closely with both theoretical predictions and experimental observations.

Accurate and stable numerical solutions are essential in laser-based heating applications, where localized thermal distributions critically impact both the effectiveness of the process and its operational safety. In such cases, precise modeling of heat diffusion is required to capture the effects of time-varying, spatially localized sources.

This study implements a finite difference scheme based on the Forward Time-Centered Space (FTCS) method to solve the 3D heat conduction equation. A time step stability analysis was performed to ensure compliance with the theoretical stability condition:

$$\Delta t \leq \frac{\Delta z^2}{6\alpha}, \tag{1}$$

where Δz is the spatial grid size in the z-direction, corresponding to the laser penetration depth, and α is the thermal diffusivity. In addition, a grid convergence study was conducted to evaluate the numerical accuracy of the method. The observed convergence rate was $p = 1.24 \pm 0.08$ with a coefficient of determination $R^2 \approx 1$, indicating strong agreement with theoretical expectations and confirming a linear behavior of the error with respect to grid refinement.

2 Theory

2.1 The model

Using a general solution to the heat equation as developed by Evans [**?**], and assuming a Gaussian laser heat source, the temperature field $T(x,y,z,t)$ is given by:

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

where:

- $T(x,y,z,t)$ is the temperature at position (x,y,z) and time t,
- $G(x-y,t)$ is the 3D Green's function of the heat equation, defined as:

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

- α is the thermal diffusivity of the material,
- $T_0(y)$ is the initial temperature distribution,
- $f(y,t')$ is the source term representing the Gaussian laser pulse, given by:

$$f(x,y,z,t') = \frac{\mu_a}{\rho c} I_0 \exp\left(-\frac{(x-x_0)^2+(y-y_0)^2}{w^2}\right) \exp\left(-\frac{z}{\delta}\right) \exp\left(-\frac{(t'-t_0)^2}{2\sigma^2}\right), \tag{4}$$

with the following parameters:

- μ_a — absorption coefficient (m^{-1})
- ρ — material density $(\mathrm{kg\,m^{-3}})$,
- c — specific heat capacity $(\mathrm{J\,kg^{-1}\,K^{-1}})$,
- I_0 — peak laser intensity $(\mathrm{W/m^2})$,
- (x_0, y_0) — beam center in the xy-plane (m),
- w — beam radius (m) ,
- δ — laser penetration depth (m),
- t_0 — pulse center time (s),
- σ — pulse duration parameter (s).

A more detailed derivation of the source term can be found in my previous work [2], where the temporal decay was modeled as exponential. Here, I adapt it to a Gaussian temporal decay to better represent the laser pulse characteristics.

2.2 Forward Time-Centered Space (FTCS) time step stability condition

The Forward Time-Centered Space (FTCS) method is a finite difference scheme commonly used to numerically solve the heat equation. As demonstrated in Equation (1), the stability of this explicit method requires the time step Δt to satisfy the condition:

$$\alpha \Delta t \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right) \leq \frac{1}{2d},$$

where d is the spatial dimension. Since the penetration depth in the z-direction is much smaller than the characteristic lengths in x and y (i.e., $\Delta z \ll \Delta x, \Delta y$), the term $\frac{1}{\Delta z^2}$ dominates. Hence, the stability condition simplifies to:

$$\frac{\alpha \Delta t}{\Delta z^2} \leq \frac{1}{6}. \tag{5}$$

Rearranging gives:

$$\Delta t \leq \frac{\Delta z^2}{6\alpha}.$$

2.3 Convergence rate

To determine the convergence rate of the simulation, the relationship between the relative error and grid spacing h was utilized:

$$\text{Relative Error} \propto h^p, \tag{6}$$

where p is the convergence rate. Taking the base-10 logarithm of both sides yields a linear relationship:

$$\log_{10}(\text{Relative Error}) = p \log_{10}(h) + C, \tag{7}$$

where C is a constant. The relative error is calculated as $|T_{\text{ref}} - T_{\text{current}}|$, where T_{ref} is the reference solution at the finest grid, and T_{current} is the solution at the current grid size. By plotting $\log_{10}(\text{Relative Error})$ against $\log_{10}(h)$, the slope of the resulting line corresponds to the convergence rate p.

3 Methods

The heat equation was solved using an explicit FTCS finite difference scheme with a standard second-order central difference approximation for the Laplacian operator, as described in [2]. For completeness, the discrete Laplacian is given by

$$\nabla^2 T_{i,j,k} \approx \frac{T_{i+1,j,k} - 2T_{i,j,k} + T_{i-1,j,k}}{\Delta x^2} + \frac{T_{i,j+1,k} - 2T_{i,j,k} + T_{i,j-1,k}}{\Delta y^2} + \frac{T_{i,j,k+1} - 2T_{i,j,k} + T_{i,j,k-1}}{\Delta z^2} \tag{8}$$

and the discrete forward temperature increase is

$$T_{i,j,k}^{n+1} = T_{i,j,k}^{n} + \Delta t \left(\alpha \nabla^2 T_{i,j,k} + f(x,y,z,t) \right). \tag{9}$$

This report focuses on the stability and convergence analysis of this method applied to the 3D heat diffusion problem under laser heating.

4 Results

4.1 Stability Analysis

The stability analysis, conducted following the approach outlined in Section 3.2, demonstrated that the model behavior is consistent with theoretical predictions. For time steps Δt smaller than the stability limit, the solution remains stable and physically reasonable. However, as Δt approaches the critical value $\Delta t_{\max}$, the temperature values increase rapidly, eventually diverging to non-physical values. The heat map shown on the right shows the spatial temperature distribution on the material's surface; however, due to the extreme temperature rise near $\Delta t_{\max}$, the visualization cannot accurately represent the full extent of the temperature increase.

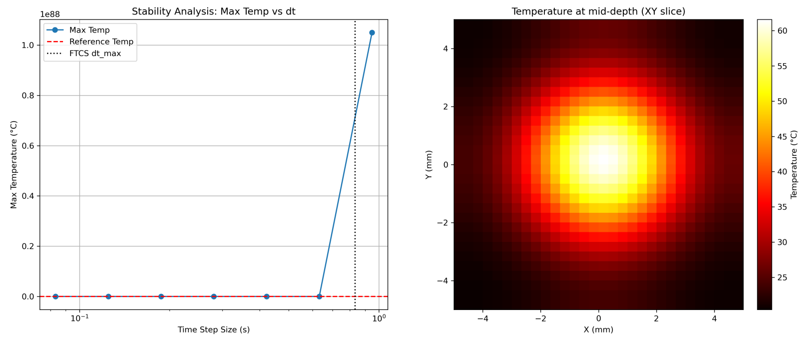

Figure 1: Temperature values diverge as $\Delta t \rightarrow \Delta t_{max}$

4.1.1 Relative error analysis

An interesting relationship emerged during the stability analysis when varying the domain length to optimize visualization of the results. It was observed that the relative temperature errors also varied with length. By increasing the length and plotting the relative error (%) versus length (cm), a nonlinear relationship was revealed: as the length increased, the relative error initially grew, but beyond approximately 3 cm, the relative error stabilized and showed little variation.

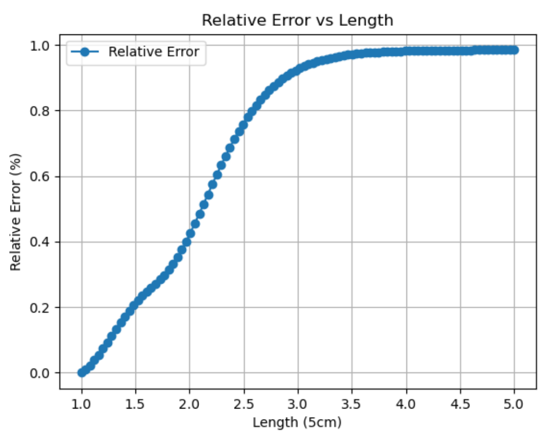

Figure 2: Non linear relationship between relative error (%) and length (cm
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Table 1: Max Temperature and Relative Error for Lengths 1–5 cm

Length (cm)	Max Temp (℃)	Relative Error
1.0	1335.28	0.0000
2.0	800.02	0.4009
3.0	103.84	0.9222
4.0	23.95	0.9821
5.0	20.18	0.9849

The relative error increases sharply up to approximately 3 cm, after which it stabilizes near 98%. This plateau suggests that beyond 3 cm, further increases in the domain size have a diminishing effect on the relative error, indicating that boundary effects become negligible and the temperature distribution achieves a more uniform state.
This behavior supports the hypothesis that the heat diffusion length scale in the material is roughly 3 cm, beyond which the numerical solution behaves consistently and maintains physical accuracy.
Therefore, a 3 cm domain can be considered the minimum effective size for which the error remains essentially constant.

4.2 Convergence Analysis

The results of the convergence analysis closely follow the theoretical prediction, exhibiting an almost perfect linear relationship with $R^2 \approx 1$. The observed convergence rate of $p \approx 1.24 \pm 0.07$ suggests that the numerical solution converges to the true solution slightly faster than the expected first-order rate. This improved convergence may be attributed to the smoothness of the Gaussian source term in the model. The following plot and table illustrate the expected linear relationship between grid spacing and relative error, along with the key statistical parameters obtained from fitting the data.

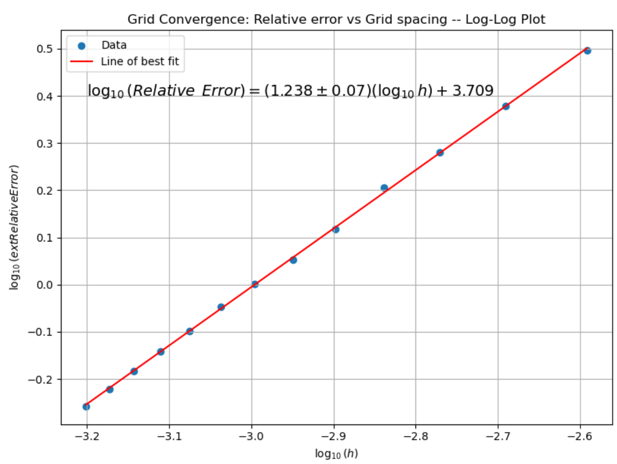

Figure 3: Linear relationship as expected from theory

Table 2: Statistical properties of the log-log convergence fit.

Data fitting values	**Value**
Order of convergence (slope)	1.238
Intercept	3.709
R^2 value	0.9998
Standard error of slope	0.0069

5 Future Work

Since the model has now been confirmed to have physical validity, the next steps involve generalizing it to cylindrical and spherical coordinate systems to accommodate the common symmetries encountered in laser applications. Following that, the focus will shift to generating large amounts of simulation data to train a machine learning model. The goal is for the ML model to predict temperature distributions based on input parameters, eliminating the need to run the full simulation each time.

A machine learning model capable of accurately predicting temperature in complex geometries could have numerous applications, including plasma modeling and medical treatments, by significantly reducing runtime and computational cost.

6 Discussion

The stability analysis confirmed that the explicit FTCS finite difference scheme is stable within the theoretical stability limit for the time step size. As the time step approaches the critical threshold, the solution begins to diverge, demonstrating the expected instability. This validation is crucial for ensuring the numerical scheme reliably simulates the physical heat diffusion process under laser heating conditions.

The convergence analysis showed a near-linear relationship between the logarithm of the error and grid refinement, with a convergence rate of approximately $p = 1.24 \pm 0.07$ and an excellent fit of $R^2 \approx 1$. This result aligns with theoretical predictions and suggests the numerical solution rapidly approaches the true physical solution as the grid is refined. The slightly higher than expected convergence rate may be attributed to the smooth Gaussian heat source function, which reduces numerical error.

An intriguing observation was made regarding the relative error behavior with increasing domain length. The relative error increased sharply up to around 3 cm and then plateaued near 98%. This behavior suggests that boundary effects diminish, and the temperature distribution stabilizes. Consequently, the 3 cm domain can be considered the minimum effective size for accurate and physically meaningful simulation results. This finding has important implications for simulation design, as smaller domains introduce significant errors while larger domains offer diminishing returns in accuracy at increased computational cost.

7 Conclusion

The model was physically verified, and the stability analysis confirmed that it remains stable within the FTCS (Forward Time Centered Space) stability conditions. An unexpected finding was the non-uniform relationship between relative error and domain size. Specifically, domains smaller than approximately 3 cm exhibited high relative errors, while increasing the domain beyond this threshold resulted in negligible improvement, despite higher computational cost. This suggests a characteristic diffusion length scale around 3 cm.

The convergence analysis showed that the model follows the expected theoretical trend, with a convergence rate of $p \approx 1.24 \pm 0.07$ and an excellent linear fit of $R^2 \approx 1$, indicating that the numerical solution approaches the true physical solution with grid refinement.

Future work will focus on extending the model to cylindrical and spherical coordinate systems and using machine learning to predict temperature distributions from input parameters, aiming to reduce simulation time and expand applicability to complex geometries.

8 References

References

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

[2] Tommer Weizmann. A more detailed derivation of the source term and the finite difference application in the simulation. GitHub repository. 2025. Available from: https://github.com/TommerWeizmann/heat-transfer-model

[3] Primer Computational Mathematics. FTCS method [Internet]. 2025. Available from: https://primer-computational-mathematics.github.io/book/c_mathematics/numerical_methods/7_FTCS.html