Deep Learning for Physical Systems
Assignment 4

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Deliver a report of this assignment containing the answers to the questions listed here. UPLOAD to CANVAS in the Assignments section by March 26, 2024 (until 11 : 59 PM EST).

This assignment deals with a problem on heat conduction in double-layered structures, when exposed to ultra-short pulsed laser.

1. Parabolic Two Temperature Model (PTTM)

Ultrashort-pulsed lasers have been widely applied in biology, chemistry, medicine, physics, and optical technology due to their high efficiency, high power density, minimal collateral material damage, lower ablation thresholds, high precision production ability, and high-precision control of heating times and locations in thermal processing of materials. For an ultrashort-pulsed laser, the heating involves high-rate heat flow from electrons to lattices in picosecond domains. Based on the phonon-electron interaction, Qiu and Tien [2, 3, 4] followed earlier, similar models by Kagnaov et al. [6] and Anisimov et al. [7] and proposed a parabolic two-step (two-temperature) energy transport method between phonons and electrons in metal at the microscale where energy is induced by ultrashort-pulsed laser heating. The model is expressed as follows:

$$C_e T_e \frac{\partial T_e}{\partial t}(x,t) = \frac{\partial}{\partial x}\left(k_e \frac{\partial T_e}{\partial x}\right) - G\left[T_e(x,t) - T_l(x,t)\right] + S(x,t), \tag{1}$$

$$C_l \frac{\partial T_l(x,t)}{\partial t} = G\left[T_e(x,t) - T_l(x,t)\right]. \tag{2}$$

For double-layered structure, the equations look like:

$$C_e^{(m)} T_e^{(m)} \frac{\partial T_e^{(m)}}{\partial t} = \frac{\partial}{\partial x}\left(k_e^{(m)} \frac{\partial T_e^{(m)}}{\partial x}\right) - G^{(m)}\left[T_e^{(m)} - T_l^{(m)}\right] + S^{(m)}(x,t), \tag{3}$$

$$C_l^{(m)} \frac{\partial T_l^{(m)}}{\partial t} = G^{(m)}\left[T_e^{(m)} - T_l^{(m)}\right], \tag{4}$$

where the heat source is given as:

$$S^{(m)}(x,t) = 0.94 \frac{1-R}{t_p \delta} J \exp\left[-\frac{x}{\delta} - 2.77\left(\frac{t-2t_p}{t_p}\right)^2\right], \tag{5}$$

with the initial condition, and insulated boundary condition as:

$$T_l^{(m)}(x,0) = T_e^{(m)}(x,0) = T_0, \tag{6}$$

$$\left.\frac{\partial T_e^{(1)}}{\partial x}\right|_{(0,t)} = \left.\frac{\partial T_l^{(1)}}{\partial x}\right|_{(0,t)} = 0, \tag{7}$$

$$\left.\frac{\partial T_e^{(2)}}{\partial x}\right|_{(x_L,t)} = \left.\frac{\partial T_l^{(2)}}{\partial x}\right|_{(x_L,t)} = 0, \tag{8}$$

and the perfectly thermal-contact interfacial condition at $x = x_l$ as

$$T_e^{(1)}(x_l,t) = T_e^{(2)}(x_l,t), \quad k_e^{(1)}\frac{\partial T_e^{(1)}}{\partial x} = k_e^{(2)}\frac{\partial T_e^{(2)}}{\partial x}. \tag{9}$$

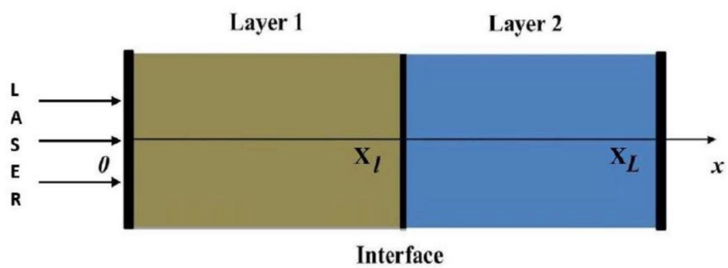

Figure 1: Schematic diagram for a double-layered film.

Here, $m = 1, 2$ represent the first layer $(0 \leq x \leq x_l)$ and the second layer $(x_l \leq x \leq x_L)$, respectively, and $0 \leq t \leq t_T$. T_0 is the ambient temperature, $C_e^{(m)}T_e^{(m)} = C_{e0}^{(m)}T_e^{(m)}/T_0$, and $k_e^{(m)} = k_{e0}^{(m)}T_e^{(m)}/T_l^{(m)}$, where $C_{eo}^{(m)}$ and $k_{eo}^{(m)}$ are constant heat capacity and conductivity, respectively. The insulated boundary condition arises from the fact that there are no heat losses from the film surfaces in the short time response. To come up with numerical methods for such kinds of systems, especially for higher dimensions, is very complicated. Physics-Informed Neural Networks (PINNs) [1] can be a solution to such issues.

2. Non Local Two Temperature Model (Weakly Nonlocal)

When the results for the electron temperature from the PTTM is plotted for the excitation surface (shown in Figure 2), it can be seen that there are some differences between the experimental value and the results obtained from the model. This is because the characteristic length scale becomes comparable with the mean free path of the heat carriers (such as in nano-scale characteristic length), due to the non-local effects which are not incorporated in the PTTM.

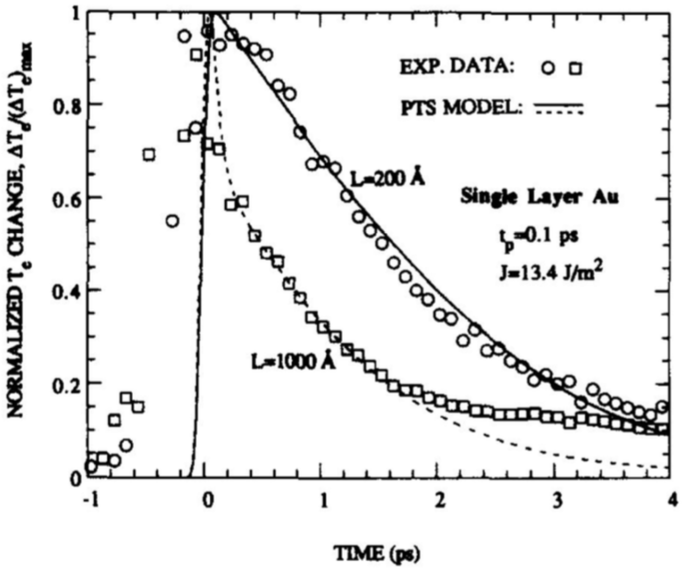

Figure 2: Experimental data from [5].

For the above reasons, Sobolev [8] has recently generalized the PTTM and the hyperbolic two-temperature model (HTTM) to a Non-Local Two-Temperature Model (NTTM), which takes into account the time and space non-local effects. These effects occur when the relaxation time becomes more effective (such as in low temperature) and when the characteristic length scale becomes comparable with the mean free path of heat carriers (such as in nanoscale characteristic length). The NTTM is given by:

$$q(x,t) + \tau \frac{\partial q(x,t)}{\partial t} = -k\frac{\partial T_1(x,t)}{\partial x} + l_e^2 \frac{\partial^2 q(x,t)}{\partial x^2}, \tag{10}$$

$$C_e \frac{\partial T_e(x,t)}{\partial t} = -\frac{\partial q(x,t)}{\partial x} + G[T_l(x,t) - T_e(x,t)] + S(x,t), \tag{11}$$

$$C_l \frac{\partial T_l(x,t)}{\partial t} = G[T_e(x,t) - T_l(x,t)], \tag{12}$$

where τ, l_e, C_e, and T_e are the relaxation time, mean free path, specific heat, and temperature for electrons; C_l and T_l are the specific heat and temperature for lattice; G is the electron-lattice coupling factor; k is the thermal conductivity of the material; and S is the heat source term. The values for τ are very hard to determine and do not have fixed values in the literature. PINNs may be used to overcome this issue. The experimental data for the electron temperature from the NTTM is uploaded as two files. The thermal properties of gold and chromium to be used are given in Table 1 [4].

Tasks:

You may use TensorFlow or PyTorch, or JAX for completing the tasks.

1. Device a way to use PINNs to solve the Parabolic Two Temperature Model. Compare with solutions given in [4].

2. Device a way to solve the NTTM problem, using the physics and as well as the experimental data. Compare with results given in [5]. Also compare with results that you got in Task 1. Are the new results justified? Why or why not?

Table 1: Thermal properties of gold and chromium.

Parameters	**Gold**	**Chromium**
G (Wm^{-3}K^{-1})	2.6×10^{16}	42×10^{16}
C_{e0} (Jm^{-3}K^{-1})	2.1×10^{4}	5.8×10^{4}
C_l (Jm^{-3}K^{-1})	2.5×10^{6}	3.3×10^{6}
k (Wm^{-1}K^{-1})	315	94

References

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