Pseudospectral Methods for Thermodynamics of Thin Films at Nanoscale

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1. Introduction
In this article, two new classes of numerical approximation solution of time dependent initial boundary value problems in three dimensions are proposed. The first class is based on weak formulation of the problem, whereas the second class uses the explicit substitution of the derivatives for basis functions. In both cases, the physical domain is transformed into the parent domain. Non-classical basis functions are introduced. For the first class of methods, weak formulation is derived, whereas the discrete representation of the problem is proposed for the second class of methods. A fully second-order finite difference discretization in time is used. The three consecutive time steps model is then solved explicitly, by using a preconditioned conjugate gradient method. The schemes are illustrated through examples which are used to investigate the heat transfer in sub-microscale thin films. Comparisons are made with available literature.

2. Classes of weak and strong formulations
There are two ways that collocation (spectral/pseudospectral) methods can be used to solve PDE's in a complicated geometry, without including basis functions that are special to the geometry and, therefore, unwieldy and inefficient to use. The first class of methods is based on the derivation of the weak formulation of the problem [4], while the second class of methods is based on the explicit derivative matrix entries of the trial functions [2,5]. Although many classical polynomial approximations based on Chebyshev and Legendre polynomials are used, there are few works that use non-classical polynomial approximations [6].

Our concern in this paper is to propose two combined spectral-finite difference method to the model problem. We look for a solution that is periodic in all space dimensions. We employ the spectral collocation method based on equally spaced three dimensional mesh grids in each direction. In the first class of methods, we derive the continuous weak formulation of problem. Then by using basis functions for space discretization and finite difference scheme for time discretization, we obtain the discrete weak formulation of problem. In the second class, we first map the physical domain onto parent domain. Then, the explicit substitution of derivatives that appear in partial differential equation are applied. Again, we use finite difference scheme for time discretization, while spectral discretization method will be used to deal with space dimensions. This kind of treatment leads to an algebraic symmetric system of equations. A preconditioned conjugate gradient (PCG) method will be used to find numerical solutions.

In this paper, we consider the physical domain to be a thin film, where the thickness is at the sub-microscale, i.e.

\[ \Omega = \{(x, y, z)| 0 \leq x, y \leq L \& 0 \leq z \leq \varepsilon \}. \]

Here, \( \varepsilon \) is of order 0.01 \( \mu \)m and \( L \) is an order of 0.1 mm.

Consider the following time dependent third order partial differential equation under some known specific initial and boundary conditions

\[
\frac{1}{\alpha} \left( \frac{\partial U}{\partial t} + \tau_s \frac{\partial ^3 U}{\partial z^3} \right) = \nabla ^2 U + \tau_c \left( \frac{\partial ^2 U}{\partial x^2} + \frac{\partial ^2 U}{\partial y^2} \right) + \tau_r \frac{\partial ^2 U}{\partial z^2} + S,
\]

where \( \alpha = \frac{\kappa}{\rho C_p} \).

The initial conditions are assumed to be:

\[
U(x, y, z, 0) = f(x, y, z),
\]
\[
\frac{\partial U}{\partial t}(x, y, z, 0) = g(x, y, z),
\]

where the functions \( f \) and \( g \) are given. We assume that the boundary conditions are periodic:

\[
U(0, y, z, t) = U(L, y, z, t) = U_1,
\]
\[
U(x, 0, z, t) = U(x, L, z, t) = U_2,
\]
\[
U(x, y, 0, t) = U(x, y, L, t) = U_3,
\]
where \( U_1, U_2 \) and \( U_3 \) are given and assumed to be constants. We also assume that the solution of the above initial and boundary value problem is smooth.

The novel heat transport model is different from traditional heat diffusion equation, i.e., it has a third order mixed derivative of temperature with respect to time and space, and a second order derivative of temperature with respect to time [5,6]. These new terms are due to the behavior of the microstructures of thin films, or micro objects such as special kind of dielectrics, Si semiconductors, laser micro-machining, laser patterning, laser processing of diamond films from carbon-ion implanted copper substrates, and laser surface hardening [1].

3. Time Splitting Scheme

In order to have a fully second-order scheme in terms of central difference formulas, we approximate the first and second derivative of temperature with respect to time about \( \left[ \frac{t_{n+1}}{2} \right] \) as:

\[
\left. \frac{\partial U}{\partial t} \right|_{i,j,k}^{n+1} \approx \frac{U_{i,j,k}^{n+1} - U_{i,j,k}^{n-1}}{2\Delta t},
\]

\[
\left. \frac{\partial^2 U}{\partial t^2} \right|_{i,j,k}^{n+1} \approx \frac{U_{i,j,k}^{n-1} - 2U_{i,j,k}^{n} + U_{i,j,k}^{n+1}}{(\Delta t)^2},
\]

where

\[
U_{i,j,k}^{n} = U(x_i, y_j, z_k, t_n, \Delta t).
\]

4. Numerical Results

Here we consider the temperature rise in a sub-nanoscale gold film. The proper heat source was chosen [6]. The boundary conditions were assumed to be insulated. Such boundary conditions arise from the case that the gold thin film is subjected to a short-pulse laser irradiation. Hence, one may assume no heat losses from the film surfaces in the short-time response [6]. The discrete system (for both approaches) is used to compute approximation solution to the problem. In the \( xyz \) coordinate, the differential equation is collocated at the equally spaced \( 16 \times 16 \times 16, 20 \times 20 \times 20, 32 \times 32 \times 32 \) and \( 40 \times 40 \times 40 \) with a time increment of 0.05 fs. The convergent solution \( U_{i,j,k}^{n+1} \) was obtained if in the preconditioned conjugate gradient procedure the convergent criterion

\[
\max_{1 \leq i,j,k \leq N-1} \left| U_{i,j,k}^{n+1} - U_{i,j,k}^{n} \right| < \frac{1}{2} \times 10^{-12},
\]

was satisfied. For the time dependent problem as it was expected, the rate of convergence is \( \Delta t^2 \).

Figure 1 gives the temperature rise on the surface of the gold film using four different meshes. From this figure, it has seen that the temperature rises to a maximum at about 0.278 ps and then it goes down. From Figure 1, it is clear that when the mesh sizes decrease one can obtain more accurate results.

![Temperature rise on the surface of the gold thin film using four different meshes and a time increment of 0.05 fs.](image)

References