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Semi-analytic approximation of the temperature field resulting from moving heat loads

D.W.M. Veldman, R.H.B. Fey, H.J. Zwart, M.M.J. van de Wal, J.D.B.J. van den Boom, H. Nijmeijer

Abstract

Moving heat load problems appear in many manufacturing processes, such as lithography, welding, grinding, and additive manufacturing. The simulation of moving heat load problems by the finite-element method poses several numerical challenges, which may lead to time consuming computations. In this paper, we propose a 2D semi-analytic model in which the problem in two spatial dimensions is decoupled into three problems in one spatial dimension. This decoupling significantly reduces the computational time, but also introduces an additional error. The method is applied to a wafer heating example, in which the computational time is reduced by a factor 10 at the cost of a 4% error in the temperature field.

Key phrases: Moving heat source
Finite elements
Wafer heating

1. Introduction

Moving heat load problems occur in many manufacturing processes, such as welding [1–8], grinding [9,10], metal cutting [11,12], laser hardening of metals [13,14], and additive manufacturing [15–18]. More recently, moving heat load problems are also studied in precision engineering because of their emerging relevance in lithography systems for the semiconductor industry. Because this is still an emerging problem only a few introductory references are available [19–21]. In the lithography application, it is customary to consider a two-dimensional (2D) spatial domain (see [20,21]), whereas three-dimensional (3D) spatial domains are typical for the other applications.

The basis of the theory for moving heat sources was developed by Rosenthal [1,22], who observed that when the path of the heat load is long enough, the temperature distribution around the source soon becomes constant. Assuming constant material properties, Rosenthal developed closed-form analytic expressions for these quasi-stationary temperature fields resulting from point, line, and plane heat sources. Although Rosenthal’s analysis provides valuable estimates, transient effects and position or temperature-dependent coefficients are important in many applications. In these situations the problem is solved by Finite Element (FE) analysis (see for example [2,3,16]).

Solving a moving heat load problem by the FE method poses several numerical challenges. One problem is that by fixing the coordinate frame to the heat load we obtain a convection-diffusion problem. It is well known that the FE discretization of such problems may result in spurious oscillations [23]. Spurious oscillations can be prevented in two ways. In the first approach, the mesh size in the direction of the velocity of the moving load is chosen smaller than $2D/\nu$, where $D$ [m$^2$/s] denotes the thermal diffusivity of the material and $\nu$ [m/s] denotes the velocity of the moving load [23]. Note that this approach is computationally demanding when the velocity $\nu$ is high. In the second approach, upwinding schemes [23,24] are used. These schemes prevent spurious oscillations at the cost of an increased discretization error.

Another problem is that the area in which the heat load is applied is typically small. This makes both the spatial and temporal discretization of such problems computationally demanding. For example, Zhang et al. [15] report that for a Gaussian heat distribution, the mesh size should be at least twice as small as the radius of the heat distribution and at least two time steps are needed for the time that the heat load travels along one element.

Because of these considerations, many problems require a small mesh size. For a static mesh, this mesh size needs to be used in the whole region through which the heat load travels, which results in models with many Degrees of Freedom (DOFs). To keep the number of DOFs limited, adaptive meshing strategies have been
proposed [3,4,17], which lead to significant reduction in computational effort. Note that these schemes require some cost for updating the mesh and that the temporal discretization remains challenging, since the adaptive mesh will keep the mesh size near the source small.

For problems with constant coefficients, spatial discretization can be avoided by semi-analytic methods [5–8,25]. In these methods, the temperature field is expressed as the convolution of the fundamental solution of the heat equation and the applied heat load. The convolution over space can typically be solved analytically, so that only numerical evaluation of the convolution over time remains. This is still a computationally intensive operation when the solution is evaluated on a fine grid.

In this paper, we propose a novel semi-analytic approximation method to reduce the computational cost of 2D transient moving load problems with constant coefficients. We construct a semi-analytic approximation in which we decouple the problem in two spatial dimensions into three problems in one spatial dimension. This significantly reduces the computational cost, especially on fine grids. The proposed method is demonstrated by an example from precision engineering, more specifically for a wafer heating problem.

The remainder of this paper is structured as follows. In Section 2, the semi-analytic approximation for the temperature field is introduced on an infinite domain. In Section 3, we give a physical interpretation of the semi-analytic approximation. In Section 4, we discuss the modeling of edge effects and repetitive scanning patterns, which are typically encountered in lithography and additive manufacturing. In Section 5, we apply the developed techniques in a wafer heating example. In Section 6, the conclusions are presented and the results are discussed.

2. Semi-analytic approximation

2.1. Problem formulation

We consider heat conduction in a thin infinite plate with thickness $H$ [m] and constant material properties (see Fig. 1). The heat losses to the surrounding media at the top and bottom of the plate are proportional to the temperature with constant heat transfer coefficients $h_{\text{top}}$ and $h_{\text{bot}}$ [W/m$^2$K], respectively. Because the plate is thin, the temperature gradient along the thickness of the plate can be neglected. The resulting temperature field $T_{2D} = T_{2D}(x,y,t)$ [K] relative to a reference temperature $T_s$ satisfies the heat equation, see for example [22]

$$\rho c \frac{\partial T_{2D}}{\partial t} = k \left( \frac{\partial^2 T_{2D}}{\partial x^2} + \frac{\partial^2 T_{2D}}{\partial y^2} \right) - (h_{\text{top}} + h_{\text{bot}}) T_{2D} + Q,$$

where $\rho$ [kg/m$^3$] is the mass density, $c$ [J/kg K] the heat capacity, $k$ [W/mK] the thermal conductivity, and $Q$ [W/m$^2$] the applied heat load. We will consider (1) on the unbounded domain $(x,y) \in \mathbb{R}^2$ with zero initial conditions $T_{2D}(x,y,t=0) = 0$.

We assume that the heat load $Q$ is of the form

$$Q(x,y,t) = X(x)Y(y - vt)Q(t),$$

where $X(x) \geq 0$ [1/m] describes the shape of the applied heat load in the $x$-direction, $Y(y) \geq 0$ [1/m] describes the shape of the applied heat load in the $y$-direction, $v$ [m/s] denotes the velocity of the moving load and $Q(t) \geq 0$ [W] is the net amount of heat applied at time $t$. Note that the uniform heat load applied in a rectangular area shown in Fig. 1 can be written in this form by taking block functions for $X(x)$ and $Y(y)$. Such a heat load has been considered in laser hardening [14] and will also be considered in the lithography example in Section 5. Also the Gaussian heat distribution considered in many applications (see for example [2,3,15,18]) is of the form in (2). Observe that $Q$ moves with a constant velocity $v$ in positive $y$-direction.

When we divide (1) by $\rho c H$, we obtain

$$\frac{\partial T_{2D}}{\partial t} = D \left( \frac{\partial^2 T_{2D}}{\partial x^2} + \frac{\partial^2 T_{2D}}{\partial y^2} \right) - hT_{2D} + \Theta,$$

where $D = k/\rho c > 0$ [m$^2$/s] denotes the thermal diffusivity, $h = (h_{\text{top}} + h_{\text{bot}})/(\rho c H) \geq 0$ [1/s], and $\Theta = Q/(\rho c H)$ [K/s] can be written as

$$\Theta(x,y,t) = X(x)Y(y - vt)\Theta(t),$$

where $\Theta(t) = Q(t)/(\rho c H)$ [m$^2$/K].

The fundamental solution of (3) (i.e. the response of the homogeneous equation (3) with $\Theta \equiv 0$ resulting from the initial condition $T_{2D}(x,y,t=0) = T_0\delta(x,y)$, with $T_0 = 1$ [m$^2$ K]) is given by

$$T_0 \Phi_{2D}(x,y,t) = T_0 e^{-ht} \Phi(x,y,t),$$

where $\Phi(x,y,t)$ denotes the fundamental solution of the heat equation in one spatial dimension

$$\Phi(x,t) = \frac{1}{\sqrt{4 \pi D t}} \exp \left( -\frac{x^2}{4 D t} \right).$$

This can be checked by differentiating (5) to time and using that $\Phi(x,t)$ is the solution to the one-dimensional (1D) heat equation (i.e. $\frac{\partial^2 \Phi}{\partial x^2} = \frac{\partial^2 \Phi}{\partial t^2}$). Since we are assuming zero initial conditions, Duhamel’s principle [26] asserts that

$$T_{2D}(x,y,t) = \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi_{2D}(x',y',\tau) \Theta(x-x',y-y',\tau - \tau) \, dx' \, dy' \, d\tau.$$

When we substitute (4) and (5) in this equation, we find that

$$T_{2D}(x,y,t) = \int_0^t f(y,t,\tau)N(x,\tau) \, d\tau,$$

where we have introduced

$$f(y,t,\tau) = \int_{-\infty}^{\infty} e^{-ht} \Phi(y',\tau) Y(y - y' - v(t - \tau)) \Theta(t - \tau) \, dy',$$

$$N(x,\tau) = \int_{-\infty}^{\infty} \Phi(x',\tau) X(x - x') \, dx'.$$

2.2. The approximate solution

We will introduce an approximate solution by simplifying the integral in (8). Note that the only factor in (8) that depends on $x$ is $N(x,\tau)$. In our semi-analytic approximation, we move this factor outside the integral.
To this end, we approximate \( N(x, \tau) \) by a first-order Taylor series expansion around \( \tau = \tau^* \), where \( \tau^* \) does not depend on \( \tau \) and is not determined yet

\[
N(x, \tau) = N(x, \tau^* + (\tau - \tau^*)) \approx N(x, \tau^*) + (\tau - \tau^*) \frac{\partial N}{\partial \tau}(x, \tau^*).
\]  

(11)

When we substitute this approximation back into (8), we obtain a semi-analytic approximation \( \hat{T}_{2D} \) of the true field temperature \( T_{2D} \) as

\[
\hat{T}_{2D}(x, y, t) = T_{ID}(y, t)N(x, \tau^*)
\]

\[
+ \left( T_{ID}^{(1)}(y, t) - \tau^* T_{ID}(y, t) \right) \frac{\partial N}{\partial \tau}(x, \tau^*).
\]

(12)

where

\[
T_{ID}(y, t) = \int_0^t f(y, t, \tau) \, d\tau.
\]

(13)

\[
T_{ID}^{(1)}(y, t) = \int_0^t \tau f(y, t, \tau) \, d\tau.
\]

(14)

The error in the semi-analytic approximation \( \hat{T}_{2D} \) originates from the Taylor series approximation of \( N(x, \tau) \) in (11), which can be expressed as (see e.g. [27])

\[
\frac{1}{2} (\tau - \tau^*)^2 \frac{\partial^2 N}{\partial \tau^2}(x, \tau^*).
\]

(15)

where \( \tau^* \) is an (un)known point between \( \tau \) and \( \tau^* \). Assuming the difference between \( \tau \) and \( \tau^* \) is small, we may approximate the error in \( \tau^* \) by \( \tau \), so that (15) becomes the first higher-order term that is omitted in the Taylor expansion (11).

Based on (15) with \( \tau^* \) replaced by \( \tau \), the error in the semi-analytic approximation is estimated as

\[
R_{ID}(y, t, \tau) = \frac{\partial N}{\partial \tau}(x, \tau^*)
\]

(16)

where

\[
R_{ID}(y, t, \tau) = \frac{1}{2} \int_0^t (\tau - \tau^*)^2 f(y, t, \tau) \, d\tau.
\]

(17)

We choose \( \tau^* \) to minimize \( R_{ID} \), so we compute

\[
\frac{\partial R_{ID}}{\partial \tau^*} = -\int_0^t (\tau - \tau^*) f(y, t, \tau) \, d\tau = -T_{ID}^{(1)}(y, t) + \tau^* T_{ID}(y, t),
\]

(18)

where \( T_{ID}^{(1)} \) and \( T_{ID} \) are as in (13) and (14), respectively. We thus see that we should choose \( \tau^* \)

\[
\tau^* = \tau^*(y, t) = \frac{T_{ID}^{(1)}(y, t)}{T_{ID}(y, t)}.
\]

(19)

Note that this choice of \( \tau^* \) cancels the second term on the Right Hand Side (RHS) of (12), so that the semi-analytic approximation becomes

\[
\hat{T}_{2D}(x, y, t) = T_{ID}(y, t) N(x, \tau^*(y, t)).
\]

(20)

We note that the semi-analytic approximation \( \hat{T}_{2D} \) is well-defined with \( \tau^* \) defined by (19). To see this, recall that \( Y \) and \( \Theta \) are nonnegative, so that (9) shows that \( f \) is nonnegative. Hence 

\[
\frac{\partial R_{ID}}{\partial \tau^*} = T_{ID}(y, t) > 0
\]

and the choice of \( \tau^* \) in (19) indeed minimizes \( R_{ID} \). Furthermore, the definition of \( T_{ID}^{(1)} \) in (14) shows that

\[
0 \leq T_{ID}^{(1)}(y, t) \leq \int_0^t f(y, t, \tau) \, d\tau = t T_{ID}(y, t).
\]

(21)

When \( T_{ID}(y, t) > 0 \), we may divide the above inequalities by \( T_{ID}(y, t) \), from which we find

\[
0 \leq \tau^*(y, t) \leq t.
\]

(22)

In case \( T_{ID}(y, t) = 0 \), (21) shows that \( T_{ID}^{(1)}(y, t) = 0 \). Now (12) shows that \( T_{2D}(x, y, t) = 0 \) for any choice of \( \tau^* \). So when the quotient in (19) is not well-defined, the value of \( \tau^* \) does not influence the resulting semi-analytic approximation \( T_{2D} \).

Since the integral expressions in (10), (13), and (14) can generally not be solved explicitly, it will be convenient to express \( N(x, \tau), T_{ID}(y, t), \) and \( T_{ID}^{(1)}(y, t) \) as the solutions of Partial Differential Equations (PDEs) in one spatial dimension. Using that \( \phi(x, \tau) \) is the fundamental solution for the heat equation in one spatial dimension, we see that \( N(x, \tau) \) in (10) is in fact the solution to the initial value problem

\[
\frac{\partial N}{\partial \tau} = D \frac{\partial^2 N}{\partial x^2}, \quad N(x, 0) = X(x),
\]

(23)

and by looking back at (9) that \( T_{ID} \) in (13) is the solution to the PDE

\[
\frac{\partial T_{ID}}{\partial t} = D \frac{\partial^2 T_{ID}}{\partial x^2} - h T_{ID} + Y(y - vt) \Theta(t),
\]

(24)

with zero initial conditions. To see how we can compute \( T_{ID}^{(1)}(y, t) \) as the solution of a PDE, note that (14) can be rewritten as

\[
T_{ID}^{(1)}(y, t) = t T_{ID}(y, t) - T_{ID}^{(1)}(y, t),
\]

(25)

where

\[
T_{ID}^{(1)}(y, t) = \int_0^t (t - \tau) f(y, t, \tau) \, d\tau.
\]

(26)

The integral in (26) can be interpreted as the solution to the PDE

\[
\frac{\partial T_{ID}^{(1)}}{\partial t} = D \frac{\partial^2 T_{ID}^{(1)}}{\partial x^2} - h T_{ID}^{(1)} + t Y(y - vt) \Theta(t),
\]

(27)

with zero initial conditions.

We thus compute the semi-analytic approximation \( \hat{T}_{2D} \) in (20) by the following steps

1. Discretize (23) to find \( N(x, \tau) \).
2. Discretize (24) to find \( T_{ID}(y, t) \).
3. Discretize (27) to find \( T_{ID}^{(1)}(y, t) \).
4. Compute \( T_{ID}^{(1)} \) from (25).
5. Compute \( \tau^* \) from (19).
6. Compute \( \hat{T}_{2D}(x, y, t) \) from (20).

Note that this procedure requires to solve three PDEs in one spatial dimension ((23), (24) and (25)), whereas (3) is a PDE in two spatial dimensions. This means the procedure to compute \( \hat{T}_{2D} \) will be much more efficient than computing \( T_{2D} \) by discretizing (3). For example, when we consider the rectangular grid in Fig. 2 with \( N_x \) grid points in the x-direction and \( N_y \) gridpoints in the y-direction, the spatial discretization of (3) yields \( N_x N_y \) Ordinary Differential Equations (ODEs) whereas the spatial discretization of (24) and (25) only leads to \( N_x + 2 N_y \) ODEs.

In some cases, a closed form analytic expression for the solution for \( N(x, \tau) \) can be obtained by computing the integral in (10) directly. A closed form analytic expression for \( T_{ID}(y, t) \) and \( T_{ID}^{(1)}(y, t) \) in (13) and (14) is impossible to obtain for most practical situations.

It is important to note that, at a certain level of accuracy, the truncation of the Taylor series in (11) introduces an error that cannot be reduced further by refining the 1D mesh. To reduce this error, more terms in the Taylor series expansion (11) should be
considered, which leads to higher-order approximations. Because the semi-analytic approximation $\tilde{T}_{2D}$ in (20) is based on the first-order Taylor series approximation in (11), $\tilde{T}_{2D}$ in (20) will be called the first-order semi-analytic approximation. The nth-order semi-analytic approximation follows by substitution of an nth-order Taylor series approximation for $N(x, \tau)$ around $\tau = t'$ in (8). In particular, the second-order semi-analytic approximation is found by adding (16) to the first-order semi-analytic approximation $\tilde{T}_{2D}$ in (20). The computation of an $n$-th order ($n \geq 2$) semi-analytic approximation is addressed in Appendix A.

3. Physical properties and interpretation

The (first-order) semi-analytic approximation $\tilde{T}_{2D}$ defined in the previous section is built from three functions: $T_{1D}$, $N$, and $\tau$. These three functions have a clear physical interpretation in terms of the original problem.

For the physical interpretation, note that integrating $N(x, \tau)$ in (10) over $x$ gives

$$\int_{-\infty}^{\infty} N(x, \tau) \, dx = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi(x - x', \tau) \Phi(x'') \, dx' \, dx'',$$

where we applied a change of variables $x'' = x - x'$ and changed the order of integration. Since the integral of $\Phi(x, \tau)$ from $x = -\infty$ to $x = +\infty$ equals 1, we see that

$$\int_{-\infty}^{\infty} N(x, \tau) \, dx = \int_{-\infty}^{\infty} X(x) \, dx,$$

where we used $\tau > 0$. Integrating the formula for $T_{2D}$ in (8) over $x$ and using (13) and (29), we see that

$$\int_{-\infty}^{\infty} T_{2D}(x, y, t) \, dx = T_{1D}(y, t) \int_{-\infty}^{\infty} X(x) \, dx.$$

By integrating (20) over $x$ using (29), we also find

$$\int_{-\infty}^{\infty} \tilde{T}_{2D}(x, y, t) \, dx = \tilde{T}_{1D}(y, t) \int_{-\infty}^{\infty} X(x) \, dx.$$

Since the RHS of (30) is equal to the RHS of (31), we see that $T_{1D}$ is chosen such that the internal energy of the semi-analytic approximation on lines in $x$-direction $\rho c H \int_{-\infty}^{\infty} T_{2D} \, dx$ is matched with the internal energy of the exact solution along lines in the $x$-direction $\rho c H \int_{-\infty}^{\infty} T_{2D} \, dx$. In particular, (29) shows that the shape functions $N(x, \tau)$ describing the dependence on $x$ are normalized such that the integral over $x$ is constant.

We can find a physical interpretation of $N$ and $\tau$ when we assume that $Y(y - vt) = \delta(y - vt)$ is a Dirac delta and $\Theta(t) = 1$. In this case the heat load is applied on a line in the $x$-direction (see Fig. 3) and does not vary over time.

To find a physical interpretation for $N$, we think about which profiles we would expect to see in the $x$-direction on a line $y = y_0$. As observed by Goldak et al. [2], the heat transport into the $y$-direction may be neglected when the velocity $v$ is high. Looking back at the original problem (3), this means that we neglect the term $D(\partial^2 T_{2D}/\partial y^2)$. On a line $y = y_0$, we thus expect that the profiles $N_{y_0}(x, t)$ in the $x$-direction are solutions of

$$\frac{\partial N_{y_0}}{\partial t} = D \frac{\partial^2 N_{y_0}}{\partial x^2} - h N_{y_0} + X(x) \delta(y_0 - vt).$$

For zero initial conditions at $t \to -\infty$, the solution to this equation is

$$N_{y_0}(x, t) = e^{\langle y_0/v - t \rangle} \left\{ \begin{array}{ll} 0 & \text{for } t < y_0/v \text{ or } t \to y_0/v, \\ N(x, t - y_0/v) & \text{for } t \to y_0/v, \end{array} \right.$$

where $N$ is the solution of (23). The factor $e^{\langle y_0/v - t \rangle}$ does not depend on $x$, so that it does not change the shape profiles that are observed in the $x$-direction and therefore the profiles in the $x$-direction we expect to see are indeed snapshots from $N(x, \tau)$.

For the interpretation of $\tau = t'(y, t)$, it will be convenient to introduce a coordinate frame fixed to the heat load defined by $(x, \zeta, t) = (x, y - vt, t)$. (34) Now observe that the semi-analytic approximation in (20) uses $N(x, \tau)$ as the profile in the $x$-direction. Furthermore, the expected profile in (33) is $N(x, t - y_0/v)$. We thus expect $\tau$ to be

$$\tau_{\text{phys}} = t - y_0/v = -\zeta_0/v, \quad (\zeta_0 < 0),$$

where $\zeta_0 = y_0/v$. The expression for $\tau_{\text{phys}}$ in (35) in fact describes the time since the heat load has arrived at $y = y_0$. This can be seen from Fig. 3: since the heat load is located at $y = vt - t_0$ (because $Y(y - vt) = \delta(y - vt)$), the time the heat load arrives at $y_0$ is $t_0 = y_0/v$. At time $t$, the time since the heat load has arrived at $y = y_0$ is $t - t_0 = t - y_0/v$, which is precisely $\tau_{\text{phys}}$.

This interpretation is indeed closely related to the formula for $\tau$ in (19). For $\Theta(t) = 1$ and $Y(y - vt) = \delta(y - vt)$, it easy to see from (9) that $f(y, \zeta, t, \tau) = f(\zeta + vt, t, \tau)$ is only a function of $\zeta$ and $\tau$. Using this observation we can then compute

$$\lim_{\tau \to \tau(\zeta + vt, t, \tau)} = \frac{2D}{v^2 + 4D \tau} \frac{\zeta}{\sqrt{v^2 + 4D \tau}},$$

where the integrals have been computed directly in MAPLE [28]. By expanding (36) in a first order Taylor expansion in $1/v$ around $1/v = 0$, we see that the expression in (36) approaches $|\zeta|/|v|$ for $v \to \infty$. Since the choice of the line $y = y_0$ was arbitrary in the derivation of $\tau_{\text{phys}}$, we may write $y$ instead of $y_0$ in (35) and we find that $\tau_{\text{phys}} = -|\zeta| + |v| \tau$ for $|\zeta| < v$. We conclude that $\tau$ may be interpreted as the time since the heat load has arrived when $Y(y - vt) = \delta(y - vt), \Theta(t) \equiv 1$, and $v$ is large.
4. Edge effects and repetitive scanning patterns

4.1. Edge effects

The results so far have been derived for a heat source moving in an infinite domain. However, in a practical situation such as the example in Section 5 we typically have a bounded domain.

Assuming the solution \( T_{gr} = T_{gr}(x, y, t) \) (for which we can compute a semi-analytic approximation using the approach from Section 2) on the infinite domain \((x, y) \in \mathbb{R}^2\) is available, we discuss how we can construct solutions on the bounded domain.

The effect of one straight edge with a perfectly insulated or zero temperature boundary condition can be included by the method of images \([1,29]\). Fig. 4 (\( \partial T/\partial n = 0 \), i.e. perfectly insulated edge) and Fig. 5 (\( T = 0 \) at the edge) illustrate how the part of \( T_{gr} \) that falls outside the domain of interest is mirrored in the edge and then added or subtracted from \( T_{gr} \) to obtain the solution on the bounded domain.

For the wafer heating application, we are interested in using these reflection type of arguments for a circular domain with radius \( R \) and with perfectly insulated edges. To this end \( T_{gr} \) is written in cylindrical \((r, \theta)\)-coordinates defined by \( x = r \cos(\theta) \) and \( y = r \sin(\theta) \). To approximate the solution on the bounded domain \( r < R \), we propose to reflect in the edge \( r = R \) along radial lines according to the formula

\[
T(r, \theta, t) = T_{gr}(r, \theta, t) + T_{gr}(R^2/r, \theta, t). \tag{37}
\]

It is important to note that (37) does not give the exact solution on the bounded domain \( r < R \), in contrast to the reflection along a straight edge. To make this more precise, note that for \( T \) in (37) to give the exact solution we need that (1) \( T \) should satisfy the boundary condition and (2) the reflected part \( T_{gr}(R^2/r, \theta, t) \) should be a solution of the heat Eq. (3) with zero source term. To check the boundary condition, we compute

\[
\frac{\partial T}{\partial r} \bigg|_{r=R} = \frac{\partial T_{gr}}{\partial r} \bigg|_{r=R} - \frac{R^2}{r^2} \frac{\partial^2 T_{gr}}{\partial r^2} \bigg|_{r=R} = 0, \tag{38}
\]

so that \( T \) in (37) indeed satisfies the perfectly insulated boundary condition. However, the reflected part \( T_{gr}(R^2/r, \theta, t) \) is not a solution of the homogeneous heat equation

\[
\frac{\partial T}{\partial r} = D \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} \right) - hT, \tag{39}
\]

but instead satisfies

\[
\frac{\partial T}{\partial r} = D \frac{r^2}{R^2} \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} \right) - hT. \tag{40}
\]

Note, however, that close to the edge \( r = R \) the factor \( r^4/R^4 \approx 1 \), meaning that \( T \) is ‘almost’ a solution of the heat equation (39) near the edge. Since \( T_{gr} \rightarrow 0 \) for \( r \rightarrow \infty \), we see that the reflected part \( T \rightarrow 0 \) when \( r \rightarrow 0 \), meaning that \( T \) will trivially satisfy (39) in the center of the disc \( r = 0 \). Combining these two observations we see that the reflection formula is accurate when \( T \) is close to zero in the region where \( r^4/R^4 \) is significantly different from 1.

4.2. Repetitive scanning patterns

The fact that we have been considering solutions on the infinite domain \((x, y) \in \mathbb{R}^2\) is particularly useful when we are dealing with repetitive patterns, which occur in many applications such as additive manufacturing and lithography. As an example consider the expose pattern in Fig. 6, where the same heat load is applied to each of the 64 rectangles (fields), repeated in different locations in space and time. This means that the applied heat load can be written in the form

\[
Q(x, y, t) = \sum_{i=1}^{N} Q_{ji}(x, y - \nu(t - \tau_i)), t - \tau_i), \tag{41}
\]

where \( Q_{ji}(x, y, t) \) denotes the heat load applied in one field which is repeated \( N_j \) times, \( \psi_i : \mathbb{R}^2 \rightarrow \mathbb{R}^2 \) describes the translation and rotation in space, and \( \tau_i \) describes a shift in time. Since (2) on the infinite domain is linear and rotation, translation, and time invariant,
the temperature response resulting from the heat load in (41) can be obtained from the superposition principle as
\[ T(x, y, t) = \sum_{i=1}^{N_1} T_0(\psi(x, y - v(t - t_i)), t - t_i), \]  
(42)
where \( T_0(x, y, t) \) is the response resulting from \( Q_0(x, y, t) \). This formula shows that we can cheaply obtain the solution \( T \) on the infinite domain, since we only need to compute the response \( T_0 \) for one field. We then obtain the solution on the bounded domain by applying the reflection arguments from Section 4.1.

We thus propose the following computational procedure to compute the temperature response for repetitive scanning patterns:

1. Compute the solution for one field \( T_0(x, y, t) \) resulting from \( Q_0(x, y, t) \) on the infinite domain \((x, y) \in \mathbb{R}^2\).
2. Use (42) to obtain the solution \( T \) resulting from the complete heat load \( Q \) in (41) on the infinite domain \((x, y) \in \mathbb{R}^2\).
3. Use the reflection arguments from Section 4.1 to obtain the solution on the bounded domain.

This procedure is computationally much more efficient than discretizing (1) for the complete heat load \( Q \). The most important reason is that the area through which the heat load \( Q_0 \) travels is much smaller than the area through which the complete heat load \( Q \) travels. This means that the computation of \( T_0 \) requires a fine mesh in a much smaller area than would be required to compute the response for the complete heat load \( Q \). Another advantage is that \( Q_0 \) is applied during a shorter period of time than \( Q \), so that the cost for the temporal discretization is also reduced. Finally, if we use the semi-analytic approximation discussed in Section 2, the heat load applied in one field only \( N_x + 2N_y \) ODEs need to be discretized instead of \( N_x N_y \) ODEs.

5. Example

We illustrate our method for a lithography example from the semiconductor industry. In this example, we consider the exemplary expose pattern in Fig. 6. Each of the 64 fields in the figure (fields) are scanned consecutively by a uniform heat load applied in a smaller rectangular area (the slit). The scanning of one field is shown in Fig. 7. We use the method from Section 4 to obtain the complete temperature field, so we will first focus on the computation of the response for one field \( T_0 \), which we will then use to assemble the complete temperature field \( T \). The considered parameter values used to generate the results are given in Table 1.

To verify the accuracy of the semi-analytic approximation, we compare the solution \( T_0 \) to FE solutions on several grids. We discretize (1) using rectangular 4-node bilinear quadrilateral elements. Around the area in which the heat load is applied we use square elements with length \( L_x \) [m] and farther away from the heat load we increase the element size to efficiently approximate the solution on the infinite domain. Starting from the coarsest mesh considered for \( L_x = 6.4 \) mm shown in Fig. 7, we subdivide each element into four smaller ones until we reach \( L_x = 0.1 \) mm. For an FE simulation with \( L_x = 0.1 \) mm on the domain in Fig. 7 with perfectly insulated edges, the temperature increase on the edges is below 0.33% of the maximal temperature that occurs during the simulation, indicating that solutions computed on this domain will closely resemble the infinite domain solutions. The heat load is applied between \( t = 0 \) and \( t = t_1 = 0.115 \) s and the time in the simulation runs from \( t = 0 \) to \( t = 3 \) s, so that also the passive cooling that occurs after the heat load has been applied is included in the simulation. The code for the spatial discretization is written in MATLAB, and the time integration is done using MATLAB's ODE solver ode15s with the default tolerances (relative tolerance of \( 10^{-3} \) and absolute tolerance of \( 10^{-16} \)).

The semi-analytic approximation \( T_{SD} \) is computed on the same grids as the FE solutions. The heat load in Fig. 7 can be written in the form (4): we set \( X(x) \) equal to \( 1/L \) for \( x \in [-L/2, L/2] \) and zero otherwise, \( Y(\zeta) \) equal to \( 1/W \) for \( \zeta \in [-W/2, W/2] \) and zero otherwise, and \( Q(t) \) is equal to \( 1 \) [W] for \( 0 \leq t \leq t_1 \) and zero afterwards. For the considered \( X(x) \), we can determine a closed-form analytic expression for \( N(x, t^*) \) from (10), resulting in
\[ N(x, t^*) = \frac{1}{2\pi} \left[ \text{erf} \left( \frac{x + L/2}{\sqrt{4Dt^*}} \right) - \text{erf} \left( \frac{x - L/2}{\sqrt{4Dt^*}} \right) \right], \]  
(43)
where erf denotes the error function. To compute \( T_{SD}(y, t) \) and \( T_{SD}^{(y)}(y, t) \) we discretize (24) and (27), where we use the same grid in the \( y \)-direction as for the 2D FE solution. The spatial discretization is programmed in MATLAB and uses 2-node linear elements and the temporal discretization is again done by MATLAB’s ode15s with the default tolerances. It is important to note that for larger grid sizes the discretization introduces spurious oscillations (see [23]) in \( T_{SD}(y, t) \) and \( T_{SD}^{(y)}(y, t) \), which can result in negative values of \( t^* \). Since (43) is only defined for \( t^* > 0 \), we set \( N(x, t^*) = N(x, 0) = X(x) \) when negative values of \( t^* \) appear. Since
negative values of \( t' \) only appear when \( T_{1D} \) is small. Eq. (20) shows that this does not affect the semi-analytic approximation much.

Fig. 8 shows the relative error in the temperature field for the FE solution and the first- and second-order semi-analytic approximation. The FE solution with \( L_e = 0.1 \) mm is used as reference. The relative error is computed by taking the maximum over space and time of the absolute value of the error, divided by the maximum of the reference solution over space and time. The error in FE solution decreases at a constant rate, but the error in the first-order semi-analytic approximation stops decreasing at \( L_e = 1.6 \) mm. At this point, the error in the first-order semi-analytic approximation is no longer dominated by discretization errors but by the error introduced by the truncation of the Taylor series approximation in (11). This limits the accuracy of the first-order semi-analytic approximation to about 4%. For the second-order semi-analytic approximation, the error stops decreasing at \( L_e = 0.4 \) mm and the accuracy is limited to about 1.5%.

Fig. 9 shows the snapshot of the error profile of the first-order semi-analytic approximation at the moment \( t = t_m = 0.1036 \) s at which the maximal error is observed. The relative error in Fig. 9 is computed by dividing the observed error by the maximal temperature observed during the simulation for the FE model with element size \( L_e = 0.1 \) mm. We see that the maximal relative error is indeed below 4% and that the error occurs near the left and right side of the field, so near \( x = \pm L/2 \). The location of the maximal error is in agreement with the leading term of the error in the first-order semi-analytic approximation in (16), which contains the factor \( \dfrac{x}{C_6} \). Since \( N(x,t) \) is the solution of (23), we indeed expect that \( \dfrac{x}{C_6} \) is the largest near discontinuities in the initial condition \( N(x,0) = X(x) \), which are indeed located at \( x = \pm L/2 \). Note that for smoother initial conditions \( X(x) \), such as a Gaussian heat distribution, smaller errors as well as faster convergence may be expected when adding higher order terms.

We expect that the second-order semi-analytic approximation, which is obtained by adding (16) to the first-order semi-analytic approximation, will be more accurate, which is confirmed by Fig. 8. Since the coefficient \( R_{10}(y,t,t') \) is nonnegative because of (17), the expected error profile in the \( x \)-direction for the first-order semi-analytic approximation will be proportional to \( \dfrac{x}{C_6} \). Fig. 10a now shows the observed error profile in the first-order semi-analytic approximation in the \( x \)-direction \( \tilde{T}_{1D}(x,y_m,t_m) - T_{1D}(x,y_m,t_m) \) and Fig. 10b shows the expected error profile in the \( x \)-direction \( \dfrac{x}{C_6} \), where \( y_m = 32 \) mm and \( t_m = 0.1036 \) are such that maximal error occurs at the line \( y = y_m \) at time \( t = t_m \). Indeed, the shape of both profiles is very similar. This suggests that the expression in (16) gives a good indication of the observed error. Fig. 8 confirms that when we compute the second-order approximation by adding the term \( R_{10} \dfrac{x}{C_6} \) in (16) to the first-order approximation, the relative error is reduced to 1.5%.

Fig. 11 shows the CPU running times needed to obtain the temperature field for the FE solution and the first- and second-order semi-analytic approximations. At \( L_e = 1.6 \) mm, the first-order semi-analytic approximation is computed almost 10 times faster than the FE solution, while a similar accuracy is obtained, see Fig. 8. Computing the second-order semi-analytic approximation increases the computational cost because one additional PDE in one spatial dimension must be solved and because the time integration using MATLAB’s ode15s now requires stricter tolerances.

**Fig. 8.** The relative \( L^\infty \) error in the temperature field for varying mesh sizes \( L_e \) in the FE solution and the first- and second-order semi-analytic approximation.

**Fig. 9.** A snapshot of the error in the first-order semi-analytic approximation (computed for an element size of \( L_e = 0.1 \) mm) at the moment \( t = t_m = 0.1036 \) s the maximal error occurs (the heat load is applied in the solid rectangle which scans the dashed rectangle in the direction of the arrow).
Field on a 0.5 mm mesh is practically impossible in a direct FE model, because the computation time exceeds several days, whereas the method from Section 4.2 only takes less than 200 s to compute the solution in 2000 time steps.

6. Conclusions and discussions

We have introduced a semi-analytic approximation for the calculation of the 2D temperature field resulting from a moving heat load, by decoupling the problem in two spatial dimensions into three problems in one spatial dimension. Especially on fine meshes, this leads to a significant reduction in computational time compared to a conventional 2D FE analysis. This reduction in computational time comes at the cost of an error that, for a certain level of accuracy, cannot be reduced further by refining the 1D mesh, but can be reduced by computing higher order semi-analytic approximations (see Appendix A). The semi-analytic approximation was initially derived for an infinite domain, but edge effects can be included. This is particularly useful for the efficient simulation of repetitive scanning patterns that are typically encountered in lithography and additive manufacturing applications. In the presented wafer heating example, the first-order semi-analytic approximation reduces the time to compute the temperature field resulting from the scanning of a single field by a factor 10 compared to a standard FE approach with similar 4%-accuracy. For the second-order semi-analytic approximation this error is reduced to 1.5%. However, a much larger amount of CPU time is saved by assembling the response for the real exposure pattern using superposition, see Fig. 12, where the conventional FE approach leads to excessive CPU times.

As stated before, the proposed method introduces an additional error that at a certain accuracy level cannot be decreased by refining the 1D mesh size. However, the 4% error achieved for the first-order semi-analytic approximation in the wafer heating example is acceptable for two reasons: (1) the temperature field itself is not of interest, but only the displacements induced by it. For the considered example, the 4% error in the first-order semi-analytic approximation of the temperature field leads to a 0.4% error in the resulting displacements; (2) efficient simulation of the moving heat load problem is especially important when the model is used in a feedback control loop or for model-based controller design. In these cases, the feedback controller creates some robustness to modeling errors.

For the considered example, the difference between the 4%-accuracy of the first-order semi-analytic approximation and the 1.5%-accuracy of the second-order semi-analytic approximation is relatively small. So, for the considered rectangular uniform shape of the heat load considering more terms in the Taylor series approximation (11) does not rapidly increase the accuracy of the semi-analytic approximation. On the other hand, for an element size of $L_e = 0.8$ mm, the second-order approximation is still computed 10 times faster than an FE solution with similar accuracy, so that higher-order approximations may be valuable. Moreover, for a smoother shape $X(x)$ of the heat load in the $x$-direction increasing the order of the semi-analytic approximation may lead to faster convergence.

In the derivation of the approximation, we assumed that the heat load is of the form (2), with $X(x) \geq 0, Y(y) \geq 0$, and $Q(t) \geq 0$. The assumption that $X(x), Y(y)$, and $Q(t)$ are nonnegative is not very restrictive. Consider for example the case where $\dot{Q}(t)$ does not satisfy this assumption. In that case we can always write $\dot{Q}(t)$ as the difference of two nonnegative functions

$$\dot{Q}(t) = \dot{Q}^+(t) - \dot{Q}^-(t),$$

where $\dot{Q}^+(t) = \dot{Q}(t)$ when $\dot{Q}(t) > 0$ and zero otherwise, and $\dot{Q}^-(t) = -\dot{Q}(t)$ when $\dot{Q}(t) < 0$ and zero otherwise. Since the functions $\dot{Q}^+(t)$ and $\dot{Q}^-(t)$ are nonnegative, we can compute the approximation when we replace $\dot{Q}(t)$ in (1) by $\dot{Q}^+(t)$ and by $\dot{Q}^-(t)$. Since the PDE in (3) is linear, we may subtract the response for $\dot{Q}^-(t)$ from the response for $\dot{Q}^+(t)$ to find the response for $\dot{Q}(t)$. A similar procedure can be applied when $X(x)$ or $Y(y)$ are not nonnegative.

Finally, we note that the method can be generalized to a 3D spatial domain $(x,y,z) \in \mathbb{R}^3$. It is shown in Appendix B that the problem can be decoupled into four 1D problems, when the applied heat load can be written as

$$Q_{3D}(x,y,z,t) = X(x)Y(y - vt)Z(z)\dot{Q}(t).$$
In this case, the potential reduction in computational cost is even larger than the reduction for the two-dimensional problem considered in this paper.

**Conflict of interest**

Authors declare that there is no conflict of interest.

**Appendix A. Higher order approximations**

The accuracy of the approximation can be increased by considering higher-order terms in the Taylor series approximation of \( N(x, τ) \) in (11). So instead of the first-order expansion in (11), we consider an \( n \)-th order Taylor series expansion (\( n > 2 \))

\[
N(x, τ) \approx \sum_{k=0}^{n} \frac{(τ - τ^0)^k}{k!} \frac{∂^k N}{∂τ^k}(x, τ^0).
\]

(A.1)

Substitution of this expansion in (8) leads to an approximation

\[
\tilde{T}^{(n)}_{2D}(x, y, t) = \sum_{k=0}^{n} A^{(k)}_{2D}(y, t, t^0) \frac{1}{k!} \frac{∂^k N}{∂τ^k}(x, τ^0),
\]

(A.2)

where

\[
A^{(k)}_{2D}(y, t, t^0) = \int_0^t (τ - t^0)^k f(y, t, τ) dτ.
\]

(A.3)

We see in particular that now derivatives of \( N(x, τ) \) w.r.t. \( τ \) up to order \( n \) are needed. When an analytic expression for \( N(x, τ) \) can be obtained, these can be determined easily. However, when no analytic expression for \( N(x, τ) \) is available, obtaining these derivatives may be difficult. To illustrate the problem, we derive a PDE for \( \frac{∂^n N}{∂τ^n} \).

Because of the PDE for \( N(x, τ) \) in (23), we see that \( \frac{∂^n N}{∂τ^n} = D \frac{∂^n X}{∂τ^n} \).

The initial condition in (23) now gives that

\[
\frac{∂N}{∂τ} \bigg|_{τ=0} = D \frac{∂^2 X}{∂τ^2}.
\]

(A.4)

However, the blockfunction \( X(x) \) considered in the example is clearly not twice differentiable, so that the RHS in the equation above is not well defined. In particular, we see that \( \frac{∂^2 N}{∂τ^2} \) will behave wildly near \( τ = 0 \), meaning that it is difficult to construct a numerical approximation of \( \frac{∂^n N}{∂τ^n} \) near \( τ = 0 \). This becomes even more problematic for higher order derivatives.

We will not change the definition of \( τ(t, y) \) in (19) for the higher order approximations, meaning in particular that \( A^{(k)}_{ID}(y, t, t^0) = 0 \).

To see how we can compute the coefficients \( A^{(k)}_{ID}(y, t, t^0) \), we make a binomial expansion of the factor \( (τ - τ^0)^k \) to obtain

\[
A^{(k)}_{ID}(y, t, t^0) = \int_0^t (τ - t^0)^k f(y, t, τ) dτ
= \sum_{p=0}^{k} \binom{k}{p} (τ - t^0)^{k-p} (-1)^p T^{(p)}_{ID}(y, t),
\]

(A.5)

where

\[
T^{(p)}_{ID}(y, t) = \int_0^t (τ - t)^p f(y, t, τ) dτ.
\]

(A.6)

Now we recognize \( T^{(p)}_{ID}(y, t) \) as the solution to the one-dimensional PDE

\[
\frac{∂T^{(p)}_{ID}}{∂τ} = D \frac{∂^2 T^{(p)}_{ID}}{∂y^2} - hT^{(p)}_{ID} + p^2 Y(y - vt) Θ(t),
\]

(A.7)

with zero initial conditions. Now the procedure to compute the \( n \)-th order approximation \( \tilde{T}^{(n)}_{2D} \) is the following:

1. Determine a closed form analytic expression for \( N(x, τ) \) by solving (10) directly and compute the first \( n \) derivatives w.r.t. \( τ \) of this expression.

2. Discretize the PDE in one spatial dimension in (A.7) for \( p = 0, 1, \ldots, n \) to find \( \tilde{T}^{(p)}_{1D}(y, τ) \).

3. Compute \( τ^*(y, t) \) from (19) (note that \( T_{1D} = T^{(0)}_{1D} \) and \( T^{(1)}_{1D} = T^{(1)}_{1D} - T^{(1)}_{1D} \)).

4. Compute \( A^{(k)}_{ID}(y, t, τ^*) \) for \( k = 0, 2, 3, \ldots, n \)

5. Compute \( \tilde{T}^{(n)}_{2D}(y, x, t) \) from (A.2).

In particular, we need to solve \( n + 1 \) PDEs in one spatial dimension in step 2 to compute the \( n \)-th order approximation.

**Appendix B. Three-dimensional spatial domain**

For the heat conduction problem in three spatial dimensions with moving source, we want to approximate the temperature field \( T_{3D}(x, y, z, t) \) that satisfies

\[
\frac{∂T_{3D}}{∂τ} = k \left( \frac{∂^2 T_{3D}}{∂x^2} + \frac{∂^2 T_{3D}}{∂y^2} + \frac{∂^2 T_{3D}}{∂z^2} \right) + Q_{3D},
\]

(B.1)

where \( ρ, c, k \) are the density, heat capacity, and thermal conductivity, respectively, and \( Q_{3D} \) is the applied heat load that is assumed to be of the form (45). Note that it is not natural to model the cooling to the environment as in (1), since such cooling will enter through boundary conditions in the 3D problem.

It is convenient to divide (B.1) by \( ρc \) to obtain

\[
\frac{∂T_{3D}}{∂τ} = D \left( \frac{∂^2 T_{3D}}{∂x^2} + \frac{∂^2 T_{3D}}{∂y^2} + \frac{∂^2 T_{3D}}{∂z^2} \right) + Θ_{3D},
\]

(B.2)

where

\[
Θ_{3D}(x, y, z, t) = X(x)Y(y - vt)Z(z)Θ(t),
\]

(B.3)

with \( Θ(t) = \hat{Q}(t)/ρc \).

The fundamental solution for (B.2) is

\[
Φ_{3D}(x, y, z, t) = Φ(x, τ)Φ(y, τ)Φ(z, τ),
\]

(B.4)

where \( Φ(x, τ) \) is given by (6). Now similarly as for the 2D problem, the solution to the 3D problem is given by the convolution of the fundamental solution in (B.4) and the applied heat load in (B.3), so that

\[
T_{3D}(x, y, z, t) = \int_{−∞}^{∞} f(y, t, τ) N(x, z, τ) dτ,
\]

(B.5)

where

\[
f(y, t, τ) = \int_{−∞}^{∞} Φ(τ') N(x, τ')Y(y - τ' - vt) Θ(τ - τ') dτ',
\]

(B.6)

\[
N(x, z, τ) = \int_{−∞}^{∞} \int_{−∞}^{∞} Φ(x', τ)Φ(z', τ)X(x - x')Z(z - z') dx' dτ'.
\]

(B.7)

Similarly as before, we approximate \( N(x, z, τ) \) in a Taylor series around \( τ = τ^0 \) as

\[
N(x, z, τ) ≈ N(x, z, τ^0) + (τ - τ^0) \frac{∂N}{∂τ} \bigg|_{(x,z,τ^0)}
\]

(B.8)

Substitution of the approximation (B.8) and (B.5) leads to the approximation.
\[ T_{\text{3D}}(x, y, z, t) = T_{\text{ID}}(y, t) \mathcal{N}(x, z, t') \]  
(B.9)

when we choose the expansion point \( t' \) as

\[ t'(y, t) = \frac{T_{\text{ID}}(y, t)}{T_{\text{ID}}(y, t')} , \]  
(B.10)

where

\[ T_{\text{ID}}(y, t) = \int_0^t f(y, t, \tau) \, d\tau, \]  
(B.11)

\[ T_{\text{ID}}^{(1)}(y, t) = \int_0^t \tau f(y, t, \tau) \, d\tau. \]  
(B.12)

Similarly as discussed for the 2D problem, \( T_{\text{ID}}(y, t) \) and \( T_{\text{ID}}^{(1)}(y, t) \) can be computed by solving two PDEs in one spatial dimension.

To compute \( N(x, z, \tau) \), note that (B.7) can be rewritten as

\[ N(x, z, \tau) = N_s(x, \tau)N_s(z, \tau), \]  
(B.13)

where

\[ N_s(x, \tau) = \int_{-\infty}^{\infty} \Phi(x', \tau)X(x - x') \, dx', \]  
(B.14)

\[ N_s(z, \tau) = \int_{-\infty}^{\infty} \Phi(z', \tau)Z(z - z') \, dz'. \]  
(B.15)

Now we recognize \( N_s \) and \( N_s \) as the solutions of the initial value problems

\[ \frac{\partial N_s}{\partial \tau} = D \frac{\partial^2 N_s}{\partial x^2}, \quad N_s(x, 0) = X(x), \]  
(B.16)

\[ \frac{\partial N_s}{\partial \tau} = D \frac{\partial^2 N_s}{\partial z^2}, \quad N_s(z, 0) = Z(z). \]  
(B.17)

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