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Sensitivity computation of periodically excited dynamical systems

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Abstract In the optimization of continuous-time dynamical systems, it can be important to numerically calculate the parametric sensitivity of some long-time-averaged quantities in the system. These computations are challenging for the typical numerical methods in the presence of oscillations, which can originate from the internal structure of an autonomous dynamical system, or be caused by an external periodic excitation. The case of periodic excitation is motivated by the heat conduction of mechanical parts in engines, where the mean strength of heat fluctuation can be an important parameter in the engineering design. The authors investigate approaches to transform periodically excited systems into autonomous systems that are appropriate for sensitivity analysis. Least squares shadowing method is used for computing sensitivities, and the effect of the different kinds of transformations are compared to each other. The resulting numerical method is presented on the motivational example of heat conduction.

Keywords sensitivity · least squares shadowing · periodic excitation

1 Introduction

In modelling of engineering systems, it is a common situation to have a periodic load on the bodies in the model. When it is necessary to perform an optimization of the system, the presence of the oscillating excitation leads to a challenge to find appropriate numerical methods.

A typical method of optimisation is to compute the parametric sensitivity of the appropriately chosen objective function, which can be a basis of a numerical iteration. It is useful for a wide class of systems to calculate of the sensitivity of the trajectories by directly using

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the chain rule for the objective function. However, recent studies show [1,2,3], that for systems with periodic and chaotic attractors, this direct method can fail if the objective function contains long-time average of the solutions.

For avoiding these problems, the least squares shadowing (LSS) method was introduced by Wang and co-authors [4,3,5,6], based on the consequences of the shadowing lemma [7]. This method is applicable directly for autonomous ordinary differential equations (ODEs), but originally, the problems of our interest are described by non-autonomous partial differential equations (PDEs). The semi-discretisation can be performed carefully, but it is not trivial how to transform a non-autonomous system into an autonomous one to avoid divergence of the method.

In this paper, we analyse possible transformations by considering the effect on the calculation of the parametric sensitivity of long-time averaged objective functions. The other purpose of the paper is improving the least squares shadowing method appropriately for the periodically excited problems to reduce the error of the numerical method. For that, we use a more general norm than [3], and the tuning of the numerical parameters is analysed, as well.

The topic of the research is motivated by heat conduction problems from mechanical engineering. In engines working in stationary state, the solid parts are exposed to a heat cycle, thus, they suffer from periodic thermal excitation. This excitation creates a stationary oscillation in temperature in the parts, as well. The dependence on parameters and excitations can be often quite complicated [8,9,10,11,12]. Minimising the intensity of oscillations in the temperature is important to increase the lifetime of the machine.

We introduce a simple motivation problem of a periodically excited 1D heat conduction system. The effect of the excitation frequency on the heat fluctuation is analysed. The chosen global objective function is the long-time average of the intensity of the oscillations, which is averaged in space, as well. This example can be solved analytically, which provides a strong basis of checking the numerical results.

The paper is organised as follows. In Section 2, the motivation problem is presented. In Section 3, some parametric sensitivity concepts are summarised for solutions and for objective functions of autonomous systems. In Section 4, we investigate possible transformations of the periodically excited systems into autonomous systems. In Section 5, the numerical method of least squares shadowing [3] is improved and the numerical algorithm is presented. In Section 6, the presented methods are demonstrated on the motivation problem of heat conduction.

2 Motivation problem from thermal engineering

Let us consider a wall with a static thermal boundary condition at one side (model of the environment of the engine) and harmonic boundary condition at the other side (model of the inside of the engine connected to the heat cycle, see Figure 1). In this transfer problem, several types of boundary conditions could be assumed (e.g. prescribed temperature, prescribed heat flux, heat convection), but the essence of the problem does not change by applying a homogeneous boundary condition of prescribed temperatures at both boundaries.

Let L be the thickness of the wall, a is the thermal diffusivity, $\hat{\omega}$ is the angular frequency of the excitation and $\hat{T}_A$ is the amplitude of the excitation (see Figure 1). The 1D heat conduction equation of the form

$$\dot{\hat{T}}(\hat{x},\hat{t}) = a \cdot \frac{\mathrm{d}^2\hat{T}}{\mathrm{d}\hat{x}^2}(\hat{x},\hat{t}) \tag{1}$$

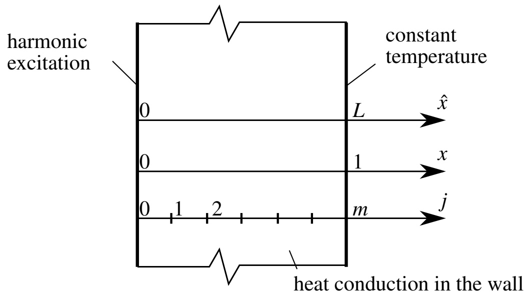

Fig. 1 Sketch of the motivation problem of Section 2. An infinite wall is subjected to a harmonically oscillating temperature load at one side, and the temperature is kept fixed at the another side. The task is to determine the sensitivity of the mean strength of temperature fluctuation in the wall. The distance through the wall is measured by the variable $\hat{x} \in [0,L]$. Its dimensionless form $x \in [0,1]$ in used Section 2, as well, and the discrete variable $j \in \{0,1,\dots m\}$ is used in Section 6 at the demonstration of the presented numerical methods.

is considered together with the boundary conditions

$$\hat{T}(0,\hat{t}) = \hat{T}_A \sin(\hat{\omega}\hat{t}), \qquad \hat{T}(L,\hat{t}) = 0, \tag{2}$$

and the initial condition

$$\hat{T}(\hat{x},0) = \hat{T}_I(\hat{x}), \tag{3}$$

where the $\dot{\hat{T}}$ denotes the derivative of the temperature with respect to the time $\hat{t}$, and the location along the wall is denoted by $\hat{x}$.

Let us transform the problem (1)-(3) into a dimensionless form by using the transformations

$$x := \frac{\hat{x}}{L}, \qquad t := \frac{\hat{t}a}{L^2}, \qquad T(x,t) := \frac{\hat{T}\left(xL, tL^2/a\right)}{\hat{T}_A}. \tag{4}$$

Then, (1) leads to the dimensionless PDE

$$\dot{T}(x,t) = \frac{\mathrm{d}^2 T}{\mathrm{d}x^2}(x,t), \tag{5}$$

and the boundary and initial conditions (2)-(3) become

$$T(0,t) = \sin(\omega t), \qquad T(1,t) = 0, \qquad T(x,0) = T_I(x) := \frac{\hat{T}_I(xL)}{\hat{T}_A}, \tag{6}$$

where

$$\omega := \frac{\hat{\omega}L^2}{a}. \tag{7}$$

is the dimensionless angular frequency. Instead of a, L and $\hat{\omega}$, the dimensionless ω can be chosen as a single optimisation parameter.

Our goal in the engineering problem is to *reduce the amplitude of the heat fluctuations in the wall*. For measuring the instantaneous strength heat fluctuation at a time instance t, let us choose the function

$$D(t) := \int_0^1 \left(T(x,t) - \langle T\rangle(x)\right)^2 \mathrm{d}x, \tag{8}$$

where the integral provides averaging through the thickness of the wall. Here $\langle T\rangle(x)$ denotes the long-time-averaged temperature at a location x, defined by

$$\langle T\rangle(x) := \lim_{t_1\to\infty} \frac{1}{t_1}\int_0^{t_1} T(x,t)\mathrm{d}t. \tag{9}$$

By averaging $D(t)$ in time, we get a mean strength of fluctuation,

$$\overline{D}(t_1) := \frac{1}{t_1}\int_0^{t_1} D(t)\mathrm{d}t = \frac{1}{t_1}\int_0^{t_1}\int_0^1 \left(T(x,t) - \langle T\rangle(x)\right)^2 \mathrm{d}x\mathrm{d}t. \tag{10}$$

To analyse long-time behaviour, the long-time average is calculated by

$$\langle D\rangle := \lim_{t_1\to\infty} \overline{D}(t_1) = \lim_{t_1\to\infty} \frac{1}{t_1}\int_0^{t_1}\int_0^1 \left(T(x,t) - \langle T\rangle(x)\right)^2 \mathrm{d}x\mathrm{d}t. \tag{11}$$

We have implicitly assumed, that the limits in (9) and (11) exist, which can be checked from the physical behaviour of the system.

If the value of ω is varied then the objective function $\langle D\rangle = \langle D\rangle(\omega)$ expresses the average strength of temperature fluctuations in the wall. To explore the effect of the parameter ω, we would like to determine the sensitivity

$$S(\omega) := \frac{\mathrm{d}\langle D\rangle(\omega)}{\mathrm{d}\omega}. \tag{12}$$

The calculation of this derivative is challenging for numerical methods because of the differentiation of the objective function with an improper integral inside (see the integration with respect to t_1 in (11)). This problem is the motivation for the subsequent analysis of this paper. Sections 3-5 contain the main results of the paper, and the developed methods are demonstrated on this motivation problem in Section 6.

3 Parametric sensitivity of autonomous systems

In this section, a short overview is presented on the parametric sensitivity of autonomous systems. These notions are important for the subsequent derivations.

3.1 Direct and generalised sensitivity of the solutions

Let us consider the set $U \subset \mathbb{R}^n$ of the phase variables, the set $P \subset \mathbb{R}$ of a single scalar parameter, and the smooth vector field $f : U \times P \to \mathbb{R}^n, (u,p) \to f(u,p)$. Let us denote the initial condition by $u_0 : P \to U, p \to u_0(p)$, which also depends smoothly on the parameter p. The family of the integral curves are denoted by $u : [0,\infty) \times P \to U, (t,p) \to u(t,p)$, and it satisfies the initial value problem

$$\begin{aligned} \dot{u}(t,p) := \partial_1 u(t,p) = f(u(t,p),p), \\ u(0,p) = u_0(p), \end{aligned} \tag{13}$$

where ∂_1 denotes the partial derivative with respect to the first variable.

If we require that the dependence on the parameter p is continuously differentiable then the *direct* parametric *sensitivity of the solution* can be defined by

$$u'(t,p) := \partial_2 u(t,p). \tag{14}$$

From (13)-(14), the initial value problem for u' is given by

$$\begin{aligned}\dot{u}'(t,p) &= \partial_1 f(u(t,p),p)\cdot u'(t,p)+\partial_2 f(u(t,p),p),\\ u'(0,p) &= \partial_1 u_0(p).\end{aligned} \tag{15}$$

If the typical time scale of the dynamics is also modified by the change of the parameters then the direct sensitivity (14) usually diverges in time and it does not express properly the effect of the parameters. A possible generalization of (14) can be created by considering the transformation $t \to \tilde{t}(t,p)$ of the time with

$$\partial_1 \tilde{t}(t,p_0) = 1, \qquad \partial_2 \tilde{t}(t,p) = \mu(t,p), \tag{16}$$

where $\mu(t,p) : [0,\infty)\times P \to \mathbb{R}^+$ measures the *time dilation* due to the change of parameters and $p_0 \in P$ is a chosen fixed parameter. By using this time transformation, the transformed solution is

$$\tilde{u}(t,p) := u(\tilde{t}(t,p),p). \tag{17}$$

Then, the *generalised* parametric *sensitivity of the solution* can be defined by the sensitivity of the transformed solution by

$$u^*(t,p) := \tilde{u}'(t,p), \tag{18}$$

which leads to

$$u^*(t,p) = \partial_2 u(t,p)+\mu(t,p)\cdot\partial_1 u(t,p) = u'(t,p)+\mu(t,p)\cdot f(u(t,p),p). \tag{19}$$

By differentiating (19), the initial value problem for u^* can be written into the form

$$\begin{aligned}\dot{u}^*(t,p) &= \partial_1 f(u(t,p),p)\cdot u^*(t,p)+\partial_2 f(u,p)+\dot{\mu}(t,p)\cdot f(u(t,p),p),\\ u^*(0,p) &= \partial_1 u_0(p)+\mu(0,p)\cdot f(u_0,p).\end{aligned} \tag{20}$$

Note that the time dilation function $\mu(t,p)$ is still undetermined, and it is not obvious how to chose it properly. For our purposes, the goal is to choose $\mu(t,p)$ in such a way that it cancels out the time dilation due to the parameter change (see Fig. 2). Such a time dilation function can be found either intuitively or it can be calculated by using a numerical method. One possible solution is the least squares shadowing (LSS) method introduced by Wang [3], which provides the time dilation μ and the sensitivity u^* simultaneously.

3.2 Direct and generalised sensitivity of the objective function

We consider an objective function $\langle Q\rangle : P \to \mathbb{R}$, which is defined by

$$\langle Q\rangle(p) := \lim_{t_1\to\infty}\frac{1}{t_1}\int_0^{t_1} Q(u(t,p),p)\mathrm{d}t, \tag{21}$$

where the objective function is obtained from a long-time integral average of the *instantaneous objective function* $Q : U\times P \to \mathbb{R}$. We restrict the analysis to those systems where the limit (21) exists. This condition is typically satisfied for systems with bounded solutions.

Our goal is to calculate the sensitivity

$$S(p) := \frac{\mathrm{d}\langle Q\rangle(p)}{\mathrm{d}p} = \frac{\mathrm{d}}{\mathrm{d}p}\lim_{t_1\to\infty}\frac{1}{t_1}\int_0^{t_1} Q(u(t,p),p)\mathrm{d}t, \tag{22}$$

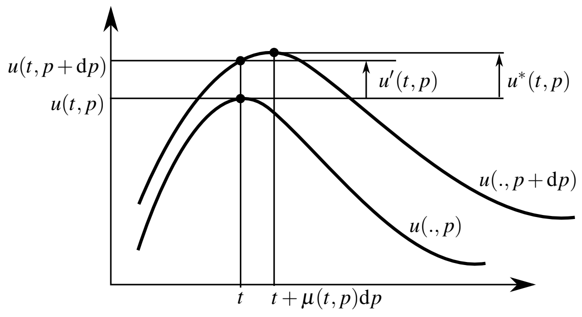

Fig. 2 Difference between the direct and the generalised parametric sensitivity. In the case of generalised sensitivity, the change of the trajectory is measured by shifting the time variable. The amount of this shift is described by the time dilation function $\mu(t,p)$. The figure demonstrates that by an appropriate choice of μ, the generalised sensitivity u^* can measure the effect of the parameter better than the direct sensitivity u'.

which expresses the sensitivity of $\langle Q \rangle (p)$ with respect to the parameter p. The straightforward idea is to calculate S from the sensitivity of Q.

The sensitivity of the instantaneous objective function Q can be calculated from the direct sensitivity method, through u',

$$Q'(u,p) := \partial_1 Q(u,p) \cdot u'(t,p) + \partial_2 Q(u,p), \tag{23}$$

or, from the generalised sensitivity method, through u^*,

$$Q^*(u,p) := \partial_1 Q(u,p) \cdot u^*(t,p) + \partial_2 Q(u,p). \tag{24}$$

If we swap the order of differentiation and the limit then the approximation of (22) can be obtained by using the direct sensitivity (23), and we get

$$S(p) \approx \check{S}(p) := \lim_{t_1\to\infty} \frac{1}{t_1} \int_0^{t_1} \Big(\partial_1 Q(u,p) \cdot u'(t,p) + \partial_2 Q(u,p) \Big) \mathrm{d}t, \tag{25}$$

if the limit exists. Or, if we use the generalised sensitivity from (24) then we obtain

$$\begin{aligned} S(p) \approx \hat{S}(p) := {} & \lim_{t_1\to\infty} \frac{1}{t_1} \int_0^{t_1} \partial_1 Q(u,p) \cdot u^*(t,p)\mathrm{d}t + \lim_{t_1\to\infty} \frac{1}{t_1} \int_0^{t_1} \partial_2 Q(u,p))\mathrm{d}t \\ & + \lim_{t_1\to\infty} \frac{1}{t_1} \int_0^{t_1} Q(u,p) \big(\dot{\mu}(t,p)\mathrm{d}t\big) + \lim_{t_1\to\infty} \left(-\frac{1}{t_1^2} \cdot \mu(t_1,p) \cdot \int_0^{t_1} Q(u,p)\mathrm{d}t \right), \end{aligned} \tag{26}$$

if the limit exists. The third term of (26) is obtained from integration by substitution (see (16) for the time transformation). The fourth term of (26) originates from the sensitivity of t_1 in the denominator (see (16), again). By simplifying (26), we get

$$\begin{aligned} S(p) \approx \hat{S}(p) := {} & \lim_{t_1\to\infty} \frac{1}{t_1} \int_0^{t_1} \Big(\partial_1 Q(u,p) \cdot u^*(t,p) + \partial_2 Q(u,p) + \dot{\mu}(t,p) \cdot Q(u,p) \Big) \mathrm{d}t \\ & - \left(\lim_{t_1\to\infty} \frac{1}{t_1} \mu(t_1,p) \right) \cdot \left(\lim_{t_1\to\infty} \frac{1}{t_1} \int_0^{t_1} Q(u,p)\mathrm{d}t \right). \end{aligned} \tag{27}$$

It is not obvious how accurate the approximation of S is by $\check{S}$ or $\hat{S}$. Generally, the change in the order of the limit and differentiation is not permissible. In the case of direct sensitivity, $\check{S}$ can be rather different from S if u' is not uniformly bounded (see [1] and [3] for demonstration). This is true for $\hat{S}$ as well if an arbitrary time dilation function μ is chosen. However, the shadowing lemma guarantees that for uniformly hyperbolic attractors, a uniformly bounded u^* and a corresponding μ can be found (see [13], [14], p. 50). In this case, $\hat{S} = S$ can be reached if the smoothness of the applied instantaneous objective function Q is ensured.

4 Sensitivity of systems with periodic excitation

In the sensitivity computation methods presented in Section (3), *autonomous* systems are considered. If we want to calculate the parametric sensitivity of non-autonomous systems then the differential equation have to be transformed appropriately into an autonomous system. This is not a trivial operation if the previous methods are to be used effectively.

4.1 The test problem

For a demonstration of the properties of the different methods, let us consider the following test problem,

$$\dot{y}(t,\omega) = -y + \sin(\omega t), \qquad\qquad y(0,\omega) \equiv y_0, \tag{28}$$

with $y \in \mathbb{R}$ and the instantaneous objective function $Q(y,\omega) = y^2$. We want to determine the sensitivity of the long-term integral-average of Q with respect to the parameter ω (see (21)-(22)).

The sensitivity of this simple test problem can be still determined analytically by direct calculation. After the decay of any transients, the solution of (28) tends to the particular solution

$$y_p(t) = \frac{1}{1+\omega^2}\sin(\omega t) - \frac{\omega}{1+\omega^2}\cos(\omega t). \tag{29}$$

Then, the objective function becomes

$$\langle Q \rangle(\omega) = \lim_{t_1\to\infty} \frac{1}{t_1}\int_0^{t_1} y^2(t)\mathrm{d}t = \frac{1}{2(1+\omega^2)}, \tag{30}$$

and its derivative gives the sensitivity

$$S(\omega) = \frac{\mathrm{d}\langle Q \rangle(\omega)}{\mathrm{d}\omega} = -\frac{\omega}{(1+\omega^2)^2}. \tag{31}$$

In the following subsections, we calculate the sensitivities $\check{S}$ or $\hat{S}$ according to (25)-(27) for different approaches to transform (28) into an autonomous system.

4.2 Methods for transformation into an autonomous system

There are more possible ways to convert systems with harmonic excitation into an autonomous system. The trivial method is to choose an additional state variable with $\tau(t,p) \equiv t$ as a dependent time variable. Then, the system (28) becomes

$$\begin{bmatrix} \dot{y} \\ \dot{\tau} \end{bmatrix} = \begin{bmatrix} -y+\sin(\omega\tau) \\ 1 \end{bmatrix}, \qquad \begin{bmatrix} y \\ \tau \end{bmatrix}(0,\omega) = \begin{bmatrix} y_0 \\ 0 \end{bmatrix}. \tag{32}$$

This choice has a few disadvantages. Firstly, the solution for τ is surely unbounded, secondly the parameter inside the terms $\sin(\omega t)$ results unbounded derivatives when computing the sensitivities in (14) and (18). The latter issue can be solved by choosing the *phase* of the excitation for the new variable $\tau(t,\omega) = \omega t$, then, the system (28) becomes

$$\begin{bmatrix} \dot{y} \\ \dot{\tau} \end{bmatrix} = \begin{bmatrix} -y+\sin\tau \\ \omega \end{bmatrix}, \qquad \begin{bmatrix} y \\ \tau \end{bmatrix}(0,\omega) = \begin{bmatrix} y_0 \\ 0 \end{bmatrix}. \tag{33}$$

If we want to produce the excitation from bounded auxiliary variables, a two-dimensional sub-system can be used, for example in the form

$$\begin{bmatrix} \dot{y} \\ \dot{\tau}_s \\ \dot{\tau}_c \end{bmatrix} = \begin{bmatrix} -y+\tau_s \\ \omega\tau_c \\ -\omega\tau_s \end{bmatrix}, \qquad \begin{bmatrix} y \\ \tau_s \\ \tau_c \end{bmatrix}(0,\omega) = \begin{bmatrix} y_0 \\ 0 \\ 1 \end{bmatrix}, \tag{34}$$

where $u = (y, \tau_s, \tau_c)$, $\tau_s(t,\omega) := \sin(\omega t)$ and $\tau_c(t,\omega) := \cos(\omega t)$. The excitation is produced by the linear oscillator in the phase plane of τ_s and τ_c. In this construction the perturbations in the initial conditions cause error not only in the phase shift, but in the amplitude of the excitation, as well. This error can be damped by adding a control term which pulls back the trajectory to the unit circle,

$$\begin{bmatrix} \dot{y} \\ \dot{\tau}_s \\ \dot{\tau}_c \end{bmatrix} = \begin{bmatrix} -y+\tau_s \\ \omega\tau_c - \delta\tau_s(\tau_s^2, +\tau_c^2-1) \\ -\omega\tau_s - \delta\tau_c(\tau_s^2, +\tau_c^2-1) \end{bmatrix}, \qquad \begin{bmatrix} y \\ \tau_s \\ \tau_c \end{bmatrix}(0,\omega) = \begin{bmatrix} y_0 \\ 0 \\ 1 \end{bmatrix}, \tag{35}$$

where $\delta > 0$ is a damping parameter.

All the systems (32)-(35) provide the same solution as the initial value problem (28). However, they behave differently when computing the parametric sensitivities presented in Subsection 3.1.

The presented transformations can be generalized to the case of several periodic excitation terms. Consider e.g. the following system

$$\dot{y}(t,\omega) = -y+\cos(2t)+\sin(\omega t)+\sin^3(t/\omega^2+1/3), \qquad y(0,\omega) \equiv y_0, \tag{36}$$

where the three excitation terms are modified by the parameter ω in a different way. In that case, we can generalize the transformation (33) by choosing three state variables for the phase of each excitation term: $\tau_1 = 2t$, $\tau_2 = \omega t$ $\tau_3 = t/\omega^2 + 1/3$. Then, the resulting autonomous system becomes

$$\begin{bmatrix} \dot{y} \\ \dot{\tau}_1 \\ \dot{\tau}_2 \\ \dot{\tau}_3 \end{bmatrix} = \begin{bmatrix} -y+\cos\tau_1+\sin\tau_2+\sin^3\tau_3 \\ 2 \\ \omega \\ 1/\omega^2 \end{bmatrix}, \qquad \begin{bmatrix} y \\ \tau_1 \\ \tau_2 \\ \tau_3 \end{bmatrix}(0,\omega) = \begin{bmatrix} y_0 \\ 0 \\ 0 \\ 1/3 \end{bmatrix}. \tag{37}$$

The transformations resulting to (34) and (35) can be applied to (36), as well. Then, two variables in the autonomous system can be introduced to each excitation term. Note that the periodic excitation terms are not restricted to be harmonic. However, a smooth periodic function can be transformed into a series of harmonic functions.

4.3 Failure of the direct sensitivity method

In this subsection, we demonstrate that the *direct* sensitivity method (15) computes incorrect sensitivities for the non-autonomous system (28) and for all corresponding autonomous systems (32)-(35) presented in the last subsection.

Let us first check the result of the direct sensitivity method in the case when the system (28) is not transformed to an autonomous system, but it is kept in its original non-autonomous form. Then, the single phase variable is $u = y$, the parameter is $p = \omega$, and the evolution equation (15) becomes

$$\dot{y}' = -y' + t\cos(\omega t). \tag{38}$$

The solution of this linear scalar differential equation can be written in the form $y'(t) = C_1 \sin(\omega t + c_1) + C_2 t\cos(\omega t + c_2) + C_3 \exp(-t)$, where the coefficients C_1, C_1, C_3, c_1, c_2 depend on ω and y_0. The second term is linearly growing, y' becomes unbounded, and the sensitivity in (25) does not exist.

Let us consider the different types of transformations in (32)-(35). In the case of (32), we have $u = (y, \tau)$ and $p = \omega$. By substituting them into the evolution equation (15) of the sensitivities, we get

$$\begin{bmatrix} \dot{y}' \\ \dot{\tau}' \end{bmatrix} = \begin{bmatrix} -1 & \omega\cos(\omega\tau) \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y' \\ \tau' \end{bmatrix} + \begin{bmatrix} \tau\cos(\omega\tau) \\ 0 \end{bmatrix}. \tag{39}$$

The solution for $\tau'(t)$ is constant, but the solution for y' is unbounded, because of the multiplier $\tau(t) \equiv t$ in the second term. Therefore, the term $\partial_1 Q \cdot u' = 2yy'$ diverges in (23), and thus, the limit in (25) does not exist. Consequently, the direct sensitivity method does not provide a relevant result for the system (28).

Let us now consider the next transformation possibility in (33). Then, (15) becomes

$$\begin{bmatrix} \dot{y}' \\ \dot{\tau}' \end{bmatrix} = \begin{bmatrix} -1 & \omega\cos\tau \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y' \\ \tau' \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{40}$$

Its solution for τ' is $\tau'(t) = \tau'_0 + t$, the solution for y' is divergent, and the limit (25) does not exist, again.

We could think that the divergent property is caused by the unbounded behaviour of τ in (32)-(33), but the similar effect is caused in the case of the formulation (34) of the excitation. By considering (34) with $u = (y, \tau_s, \tau_c)$, the equation (15) gives

$$\begin{bmatrix} \dot{y}' \\ \dot{\tau}'_s \\ \dot{\tau}'_c \end{bmatrix} = \begin{bmatrix} -1 & 1 & 0 \\ 0 & 0 & \omega \\ 0 & -\omega & 0 \end{bmatrix} \begin{bmatrix} y' \\ \tau'_s \\ \tau'_c \end{bmatrix} + \begin{bmatrix} 0 \\ \tau_c \\ -\tau_s \end{bmatrix}. \tag{41}$$

Because of $\tau_s(t) = \sin(\omega t)$ and $\tau_c(t) = \sin(\omega t)$, external resonance of the differential equation can be observed, and the solution of the exciting subsystem can be written into the form

$$\begin{aligned} \tau'_s(t) &= \tau'_{c0}\sin(\omega t) + \tau'_{s0}\cos(\omega t) + t\cos(\omega t) \\ \tau'_c(t) &= -\tau'_{s0}\sin(\omega t) + \tau'_{c0}\cos(\omega t) + t\sin(\omega t), \end{aligned} \tag{42}$$

where τ'_{s0} and τ'_{c0} are the initial conditions. The last terms with the t multipliers appear independently from the initial conditions, making the sensitivity y' unbounded. Then, (25) does not exist, again. The situation does not change even if the damped formulation (35) is applied.

We can conclude that the direct sensitivity method does not provide correct results in the case of this example of periodic excitation. The physical reasoning is clear: the typical time-scale of the system is tuned by the parameter ω and a small change of the parameter causes a phase shift of the oscillation which increases in time without a limit. The growth rate of this oscillation is *linear* due to the increasing phase difference. In chaotic systems, a similar issue occurs with an *exponential* growth of the sensitivities. That behaviour is caused by the existence of unstable Characteristic Lyapunov Vectors (see [6]).

4.4 Analytical solution by the generalised sensitivity method

The change of the time scale of the system due to parameters can be considered by the time dilation function μ of the generalised sensitivity method. However, one cannot find an appropriate μ for all transformations from (32)-(35).

In the case of the trivial formulation (32) of the excitation, we can modify (39) by using (20) instead of (15). Then, we get

$$\begin{bmatrix} \dot{y}^* \\ \dot{\tau}^* \end{bmatrix} = \begin{bmatrix} -1 & \omega\cos(\omega\tau) \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y^* \\ \tau^* \end{bmatrix} + \begin{bmatrix} \tau\cos(\omega\tau) \\ 0 \end{bmatrix} + \dot{\mu} \begin{bmatrix} -y+\sin(\omega\tau) \\ 1 \end{bmatrix}. \tag{43}$$

The second equation gives

$$\dot{\tau}^* = \dot{\mu}, \tag{44}$$

which expresses that τ^* and μ differ in an additive constant only. As we have seen in the previous subsection, the unbounded solutions for the sensitivities cause divergence in the sensitivity of the objective function. If we require τ^* to be bounded then μ has to be also bounded due to (44). But then, the term $\tau\cos(\omega\tau)$ causes divergence in the sensitivity y^*, and the sensitivity of the objective function does not exist. *That is, the trivial transformation* (32) *of the excitation cannot be used properly even with the generalised sensitivity method.*

Let us now apply the generalised sensitivity method to (33). Instead of (15), let us apply (20) to rewrite (40). Then, we get

$$\begin{bmatrix} \dot{y}^* \\ \dot{\tau}^* \end{bmatrix} = \begin{bmatrix} -1 & \cos\tau \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y^* \\ \tau^* \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \dot{\mu} \begin{bmatrix} -y+\sin\tau \\ \omega \end{bmatrix}. \tag{45}$$

As in the previous cases, our target is to find a time dilation function $\mu(t)$, for which the sensitivities y^* and τ^* are bounded. Let us consider the second equation of (41),

$$\dot{\tau}^* = 1 + \dot{\mu}\omega. \tag{46}$$

The simplest appropriate choice is $\dot{\mu}(t) = -1/\omega$, which makes τ^* constant, i.e. bounded. Let us check the value of the sensitivity computed by (27). By considering $\tau(t) = \omega t$ from the definition and $y(t) = y_p(t)$ from (29), the solution of (43) tends to the particular solution

$$y_p^*(t) = -\frac{2\omega}{(1+\omega^2)^2}\sin(\omega t) + \frac{1-\omega^2}{(1+\omega^2)^2}\cos(\omega t) \tag{47}$$

Then, the sensitivity (27) becomes

$$\hat{S}(\omega) = \lim_{t_1\to\infty} \frac{1}{t_1} \int_0^{t_1} \Big(2y(t)y(t)^* - \frac{1}{\omega}\cdot y^2(t)\Big)\mathrm{d}t + \frac{1}{\omega}\cdot\left(\lim_{t_1\to\infty}\frac{1}{t_1}\int_0^{t_1} y^2(t)\mathrm{d}t\right) = \\ = -\frac{\omega}{(1+\omega^2)^2}, \quad (48)$$

which gives back the exact result of (31).

That is, the intuitive choice $\dot{\mu}(t) \equiv -1/\omega$ is appropriate for obtaining the correct result of the test problem (28) by using the autonomous model (33).

The similar method is applicable also for (34). Then, the evolution of the sensitivities from (20) becomes

$$\begin{bmatrix} \dot{y}^* \\ \dot{\tau}_s^* \\ \dot{\tau}_c^* \end{bmatrix} = \begin{bmatrix} -1 & 1 & 0 \\ 0 & 0 & \omega \\ 0 & -\omega & 0 \end{bmatrix} \begin{bmatrix} y^* \\ \tau_s^* \\ \tau_c^* \end{bmatrix} + \begin{bmatrix} 0 \\ \tau_c \\ -\tau_s \end{bmatrix} + \dot{\mu} \begin{bmatrix} -y+\tau_s \\ \omega\tau_c \\ -\omega\tau_s \end{bmatrix}. \quad (49)$$

By using the value $\dot{\mu}(t) \equiv -1/\omega$, again, the lase term of (49) cancels the second term, which term caused the divergence in (41). Then, the particular solution of (49) for y^* coincides with (47). The computation of the generalised sensitivity (27) leads to (48), again.

The physical explanation behind the value $-1/\omega$ is that the long-time solution of (28) is periodic with the same frequency as the excitation. By changing the frequency of the excitation, the typical time scale of the long-time behaviour is also changed, and the connection is reciprocal. If the frequency is increased then the time dilation must be negative to follow the faster behaviour.

5 Numerical solution with least squares shadowing method

5.1 Improvement to the least squares shadowing method

The least squares shadowing (LSS) method was introduced by Wang and co-authors [3,5, 6]. The goal of the method is to find the *shadowing direction*, which corresponds to a a certain sensitivity $u^*(t)$ with special properties. By adding a perturbation in this direction, the perturbed trajectory remains uniformly close to the original trajectory (see [13] and [14], p. 50). The perturbation of the time scale corresponds to the time dilation function $\mu(t)$.

In the LSS method, the least squares distance between the original and perturbed trajectory is minimized to find the shadowing trajectory. In the terms of the sensitivity $u^*(t)$ and the time dilation function $\mu(t)$, it is required that the function

$$\Pi(u^*,\mu) := \lim_{t_1\to\infty}\frac{1}{t_1}\int_{t=1}^{t_1} \frac{1}{2}||u^*||^2 + \frac{1}{2}\alpha^2\dot{\mu}^2\mathrm{d}t \quad (50)$$

is minimal, while the functions satisfy the evolution equation

$$\dot{u^*}(t,p) = \partial_1 f(u,p)\cdot u^* + \partial_2 f(u,p) + \dot{\mu}(t,p)\cdot f(u,p) \quad (51)$$

from (20). Here, α is a constant parameter for the method and $||.||$ is the norm of the vector.

In the original method of Wang, $||.||$ means the simple two-norm, but for our purposes, it is now generalised to

$$||u^*|| := \sqrt{(u^*)^T G u^*}, \quad (52)$$

where G is a positive definite matrix, containing the weight factors for the different variables. If the entries of u originates from a physical model, and we have preliminary information of these variables then the form of G can be chosen intuitively to increase the accuracy of the method. For example, in the heat conduction problem in Section 6, the last entry of u comes from the periodic excitation, and all the other variables are temperatures. Then, by having different weights in G for the different kinds of variables, we can improve the performance of the numerical method.

5.2 Creating a time-discrete problem

For a time discretisation, the step size Δt and the number of time steps N is to be chosen. The time of integration is then given by $t_1 = N\Delta t$. Let the discrete approximation of the solution $u(t,p)$ be

$$u^i :\approx u(i\Delta t), \qquad i = 0\ldots N, \tag{53}$$

which are supposed to be calculated by usual time integration. The unknown values of the sensitivities and the time dilation at the discrete points are denoted by

$$v^i :\approx u^*(i\Delta t), \qquad i = 0\ldots N, \qquad \eta^i :\approx \dot{\mu}\left((i-1/2)\Delta t\right), \qquad i = 1\ldots N. \tag{54}$$

With these, (51) can be approximated by the discrete variables. By using trapezoid integration, we get

$$\frac{v^i - v^{i-1}}{\Delta t} = \frac{\partial_1 f(u^i,p)v^i + \partial_1 f(u^{i-1},p)v^{i-1}}{2} + \frac{\partial_2 f(u^i,p) + \partial_2 f(u^{i-1},p)}{2} + \\ + \eta^i \frac{f(u^i,p) + f(u^{i-1},p)}{2}, \qquad i = 1\ldots N. \tag{55}$$

This equation can be written into linear form,

$$C_1^{i-1} v^{i-1} + C_2^i v^i + C_3^i \eta^i + C_4^i = 0, \tag{56}$$

where the meaning of the constants are

$$C_1^i := \frac{I}{\Delta t} + \frac{\partial_1 f(u^i,p)}{2}, \qquad C_2^i := -\frac{I}{\Delta t} + \frac{\partial_1 f(u^i,p)}{2}, \tag{57}$$

$$C_3^i := \frac{f(u^i,p) + f(u^{i-1},p)}{2}, \qquad C_4^i := \frac{\partial_2 f(u^i,p) + \partial_2 f(u^{i-1},p)}{2}. \tag{58}$$

The function Π in (50) can also be approximated by the discrete values,

$$\Pi(u^*,\mu) \approx \frac{1}{N+1}\left(\sum_{i=0}^{N} \frac{1}{2}(v^i)^T G v^i + \sum_{i=1}^{N} \frac{1}{2}\alpha^2(\eta^i)^2\right). \tag{59}$$

This expression creates a constrained extreme value problem together with equations (56). The method of Lagrange multipliers is applied, and the function

$$\tilde{\Pi}(v^i,\eta^i,\lambda^i) := \sum_{i=0}^{N} \frac{1}{2}(v^i)^T G v^i + \sum_{i=1}^{N} \frac{1}{2}\alpha^2(\eta^i)^2 + \\ + \sum_{i=0}^{N} \lambda^i \left(C_1^{i-1} v^{i-1} + C_2^i v^i + C_3^i \eta^i + C_4^i\right) \tag{60}$$

is defined, where $\lambda^i, i = 1 \dots N$ denote the Lagrange multipliers. The solution for the minimum is given by the partial derivatives, i.e.

$$\frac{\partial \tilde{\Pi}}{\partial v^i} = 0, \qquad \frac{\partial \tilde{\Pi}}{\partial \eta^i} = 0, \qquad \frac{\partial \tilde{\Pi}}{\partial \lambda^i} = 0. \tag{61}$$

5.3 Steps of numerical solution

From calculating (61), we get the following set of equations,

$$\begin{aligned} G v^i + (C_2^i)^T \lambda^i + (C_1^i)^T \lambda^{i+1} &= 0, & i &= 0 \dots N, & (62)\\ \alpha^2 \eta^i + (C_3^i)^T \lambda^i &= 0, & i &= 1 \dots N, & (63)\\ C_1^{i-1} v^{i-1} + C_2^i v^i + C_3^i \eta^i + C_4^i &= 0, & i &= 1 \dots N. & (64) \end{aligned}$$

This creates a set of linear equations for the unknowns v^i, η^i, λ^i. The system can be simplified by using Gauss elimination, and after eliminating v^i and η^i variables, we obtain

$$-L^i \lambda^{i-1} - K^i \lambda^i - L^{i+1} \lambda^{i+1} + C_4^i = 0, \qquad i = 1 \dots N, \tag{65}$$

with the formal notation of $\lambda^0 := \lambda^{N+1} := 0$. Here the K^i and L^i matrices are given by

$$\begin{aligned} K^i &:= C_1^{i-1} G^{-1} (C_1^{i-1})^T + C_2^i G^{-1} (C_2^i)^T + \frac{1}{\alpha^2} C_3^i (C_3^i)^T, & (66)\\ L^i &:= C_1^{i-1} G^{-1} (C_2^{i-1})^T. & (67) \end{aligned}$$

In matrix form, (65) gives

$$\begin{bmatrix} K^1 & L^2 & & & \\ L^2 & K^2 & L^3 & & \\ & L^3 & \ddots & \ddots & \\ & & \ddots & K^{N-1} & L^N \\ & & & L^N & K^N \end{bmatrix} \begin{bmatrix} \lambda^1 \\ \lambda^2 \\ \vdots \\ \lambda^{N-1} \\ \lambda^N \end{bmatrix} = \begin{bmatrix} C_4^1 \\ C_4^2 \\ \vdots \\ C_4^{N-1} \\ C_4^N \end{bmatrix}, \tag{68}$$

which is a block-tridiagonal matrix with a block size n.

For this tridiagonal problem, a direct solution algorithm can be built easily. (A similar *block-cyclic reduction* method, see [15], p. 197.) First, the following matrices are calculated iteratively, for increasing index i,

$$\begin{aligned} \tilde{K}^1 &:= K^1, & & & (69)\\ \tilde{C}_4^1 &:= C_4^1, & & & (70)\\ \tilde{K}^i &:= K^i - L^{i-1} (\tilde{K}^{i-1})^{-1} L^{i-1}, & i &= 2 \dots N, & (71)\\ \tilde{C}_4^i &:= C_4^i - L^{i-1} (\tilde{K}^{i-1})^{-1} \tilde{C}_4^{i-1}, & i &= 2 \dots N. & (72) \end{aligned}$$

Then, the Lagrange multipliers λ^i can be calculated iteratively, for decreasing index i,

$$\begin{aligned} \lambda^{N+1} &= 0, & & & (73)\\ \lambda^i &= (\tilde{K}^i)^{-1} \left(\tilde{C}_4^i - L^i \lambda^{i+1} \right), & i &= N \dots 1. & (74) \end{aligned}$$

Then, from (63) and (64), the sensitivities and time dilations can be computed,

$$\eta^i = -\frac{1}{\alpha^2}(C_3^i)^T \lambda^i, \tag{75}$$

$$v^i = -G^{-1}\left((C_2^i)^T \lambda^i + (C_1^i)^T \lambda^{i+1}\right). \tag{76}$$

Finally, by using the rectangle rule for numerical integration of (27), we get

$$\hat{S}(p) \approx \frac{1}{N+1}\sum_{i=0}^{N}\left(\partial_1 Q(u^i,p)v^i + \partial_2 Q\right) + \frac{1}{N}\sum_{i=1}^{N}\left(\frac{Q(u^i,p)+Q(u^{i-1},p)}{2} - \overline{Q}\right)\eta^i \tag{77}$$

for the sensitivity of the objective function, where

$$\langle Q\rangle(p) \approx \overline{Q} := \frac{1}{N+1}\sum_{i=0}^{N} Q(u^i,p) \tag{78}$$

is the approximation of the objective function.

6 Application to the heat conduction problem

Now, the methods of Section 4-5 are applied to the motivation problem presented in Section 2. In case of this problem, the sensitivities can be determined analytically and compared to those of the numerical method.

6.1 Creating the semi-discrete model

As the applied numerical methods are based on ODEs, we create the semi-discretised approximation of the continuous problem described in Section 2. For more complex problems, the set of ODEs can be created by appropriate finite difference methods.

Let interval $x = [0,1]$ of the wall be divided into m equal sections, and let

$$T_j(t) \approx T\left(\frac{j}{m}, t\right), \qquad j = 0, \ldots m, \tag{79}$$

be a discrete approximation of the temperature distribution in (5). The temperature at the endpoints are fixed by the boundary conditions,

$$T_0(t) = \sin(\omega t), \qquad T_m(t) = 0. \tag{80}$$

The dynamics at the remaining points can be approximated by applying the central difference scheme

$$\frac{\mathrm{d}^2 T}{\mathrm{d}x^2}\left(\frac{j}{m}, t\right) \approx \frac{T_{j-1}(t) - 2T_j(t) + T_{j+1}(t)}{(j/m)^2} \tag{81}$$

to (5). The resulting $m-1$-dimensional ODE can be written in the form

$$\dot{T}_d(t) = m^2 H T_d(t) + m^2 \sin(\omega t) e_1, \tag{82}$$

where

$$T_d(t) := \begin{bmatrix} T_1(t) \\ T_2(t) \\ \vdots \\ T_{m-1}(t) \end{bmatrix}, \qquad H := \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \\ & & 1 & -2 \end{bmatrix}, \qquad e_1 := \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{83}$$

The initial condition (6) for the discrete system becomes

$$T_{dI} = \begin{bmatrix} T_I(1/m) \\ T_I(2/m) \\ \vdots \\ T_I((m-1)/m). \end{bmatrix} \tag{84}$$

From the discrete solution $T_d(t)$, let us determine the approximate value $D_d(t) \approx D(t)$. Based on (8), by using trapezoid integration, we get

$$D_d(t) = \frac{1}{m} \sum_{j=1}^{m-1} T_j(t) T_j(t) + \frac{1}{2m} \sin^2(\omega t). \tag{85}$$

The long-time average of the fluctuation can be defined in a similar manner to (11) as

$$\langle D_d \rangle := \lim_{t_1 \to \infty} \frac{1}{t_1} \int_0^{t_1} D_d(t) \mathrm{d}t. \tag{86}$$

In the subsequent calculations we use numerical methods to approximate

$$S_d(\omega) := \frac{\mathrm{d} \langle D_d \rangle (\omega)}{\mathrm{d}\omega}, \tag{87}$$

and if m is large enough then this is an appropriate approximation also for $S_d(\omega) \approx S(\omega)$.

6.2 Analytical reference solution

The solution of the linear ODE (82) can be written in the form

$$T_d(t) = T_{dH}(t) + T_{dP}(t), \tag{88}$$

where the T_{dH} homogeneous solution in the form

$$T_{dH}(t) := \exp(m^2 H t) \cdot (T_{dI} - A), \tag{89}$$

and the T_{dP} particular solution can be written in the form

$$T_{dP}(t) := A \cos(\omega t) + B \sin(\omega t). \tag{90}$$

By substituting (90) into (82) and by using harmonic balance for the terms with sine and cosine, we get

$$\begin{bmatrix} m^2 H & \omega I \\ -\omega I & m^2 H \end{bmatrix} \cdot \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ m^2 e_1 \end{bmatrix}, \tag{91}$$

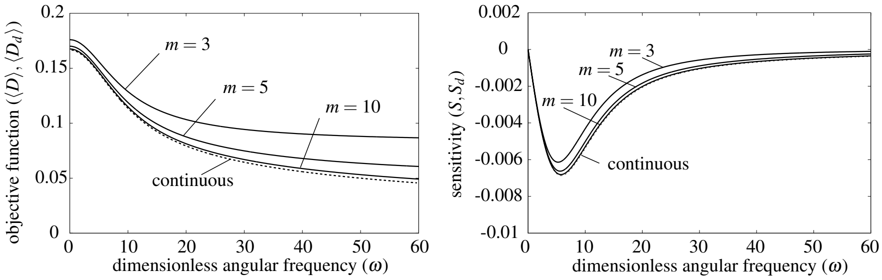

Fig. 3 Analytical solution for the objective function $\langle D\rangle(\omega)$ of the continuous test problem (dotted line) and for the objective function $\langle D_d\rangle(\omega)$ of the semi-discrete test problem (solid lines).
Analytical solutions for the sensitivity $S(\omega)$ of the continuous test problem (dotted line) and for the sensitivity $S_d(\omega)$ of the semi-discrete test problem (solid lines).

where

$$W(\omega) := \left(H^2 + \left(\frac{\omega}{m^2}\right)^2 I\right)^{-1}, \tag{92}$$

and I denotes the $m \times m$ identity matrix. Then, the solution for the constants A and B of the particular solution is

$$A = -\frac{\omega}{m^2} W e_1, \qquad\qquad B = -HW e_1. \tag{93}$$

Independently from the initial condition, the homogeneous solution (89) converges to zero because H has only negative real eigenvalues. Thus, for the long-time behaviour of the system, the particular solution can be considered only. Performing the calculations in (86), we obtain

$$\langle D_d\rangle = \frac{1}{2}\frac{1}{m}\left(A^T A + B^T B + \frac{1}{2}\right), \tag{94}$$

and after substituting A and B from (93), it can be simplified to

$$\langle D_d\rangle(\omega) = \frac{1}{2m} e_1^T W(\omega) e_1 + \frac{1}{4m}. \tag{95}$$

This result is shown in the left panel of Fig. 3 for different values of m. It can be shown numerically that by increasing m, this discrete approximation $\langle D_d\rangle$ tends to the continuous objective function

$$\langle D\rangle(\omega) = \frac{1}{\sqrt{8\omega}} \cdot \frac{\sinh\sqrt{2\omega} - \sin\sqrt{2\omega}}{\cosh\sqrt{2\omega} - \cos\sqrt{2\omega}} \tag{96}$$

(see the left panel of Fig. 3 denoted by a dashed line). The formula (96) can be derived by using the form of the homogeneous continuous solution (see [16], p.146.) and by using the Rayleigh-Krulov functions (see e.g. [17], p. 205). The steps of the derivation are similar to those of the discrete case $\langle D_d\rangle$, but the derivation is lengthy. Thus, only the result is presented here as a curiosity.

It is hard to analytically express the sensitivity $S_d(\omega) := \mathrm{d}\langle D_d\rangle/\mathrm{d}\omega$, but it can be calculated for a reasonable value of m by using a computer algebra software. The results can be seen in the right panel of Fig. 3, denoted by solid lines. The sensitivity $S(\omega)$ computed from (96) is denoted by a dashed line in the right panel of Fig. 3.

6.3 Numerical solution by the least square shadowing method

By using the method from (33) to create an autonomous system, the differential equation (82) can be written into the general form $\dot{u} = f(u, p)$ from (13) with

$$u = \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{m-1} \\ \tau \end{bmatrix} = \begin{bmatrix} T_d \\ \tau \end{bmatrix}, \qquad f(u,p) = \begin{bmatrix} m^2 H T_d + m^2 \sin\tau e_1 \\ \omega \end{bmatrix}, \tag{97}$$

and $p = \omega$. Then, the objective function $Q = D_d$ from (85) becomes

$$Q(u,p) = \frac{1}{m}\sum_{j=1}^{m-1} T_j T_j + \frac{1}{2m}\sin^2\tau. \tag{98}$$

The partial derivatives of (97) and (98) result in

$$\partial_1 f(u,p) = \begin{bmatrix} m^2 H & m^2 \cos\tau e_1 \\ 0 & 0 \end{bmatrix}, \qquad \partial_2 f(u,\omega) = e_m := \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}, \tag{99}$$

$$\partial_1 Q(u,p) = \begin{bmatrix} \frac{2}{m}T_1 & \frac{2}{m}T_2 & \dots \frac{2}{m}T_{m-1} & \sin\tau\cos\tau \end{bmatrix}, \qquad \partial_2 Q(u,p) = 0. \tag{100}$$

Suppose that the discrete approximation

$$u^i = \begin{bmatrix} T_d^i \\ \tau^i \end{bmatrix} \approx \begin{bmatrix} T_d(i\Delta t) \\ \tau(i\Delta t) \end{bmatrix} \tag{101}$$

is known from the numerical solution of the semi-discretised problem (82). Then, we want to determine the sensitivity (87) by using the least square shadowing method from Section 5.

The vector of the sensitivities is given by

$$u^* = \begin{bmatrix} T_d^* \\ \tau^* \end{bmatrix}, \tag{102}$$

and the computation of the matrices (58) gives

$$\begin{aligned} C_1^i &= \begin{bmatrix} \frac{I}{\Delta t} + \frac{1}{2}m^2 H & \frac{1}{2}m^2\cos\tau^i e_1 \\ 0 & \frac{1}{\Delta t} \end{bmatrix}, \\ C_2^i &= \begin{bmatrix} -\frac{I}{\Delta t} + \frac{1}{2}m^2 H & \frac{1}{2}m^2\cos\tau^i e_1 \\ 0 & -\frac{1}{\Delta t} \end{bmatrix}, \\ C_3^i &= \begin{bmatrix} \frac{1}{2}m^2 H \left(T_d^i + T_d^{i-1}\right) + \frac{1}{2}m^2\left(\sin\tau^i + \sin\tau^{i-1}\right) e_1 \\ \omega \end{bmatrix}, \\ C_4^i &= e_m. \end{aligned} \tag{103}$$

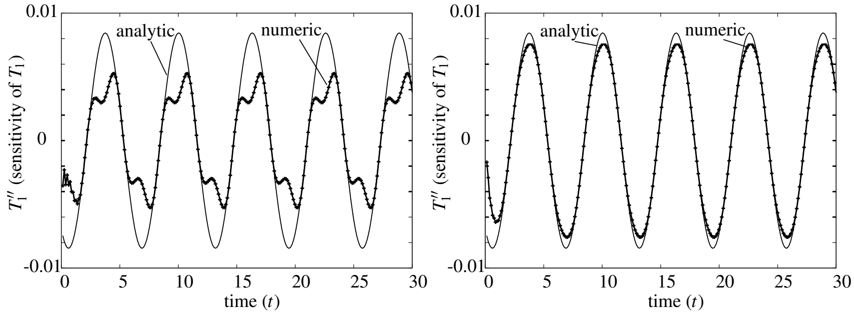

Fig. 4 Coordinate v_1^i of the sensitivity of the trajectory, by using the parameters $m = 30$, $\alpha = 1$, $n_{div} = 50$, $n_{per} = 8$, $\omega = 5$. Left panel: for small value of $\beta = 3$, there is a significant error in the sensitivity. Right panel: by increasing the parameter to $\beta = 20$, we get a better approximation.

Let us choose a diagonal matrix G for the norm (52). In the main diagonal of G, let us choose a uniform 1 weight for the temperature sensitivities, and let the weight for the time phase τ be denoted by β^2. Then, we have the weighting matrix $G = \mathrm{diag}(1, 1, \ldots, 1, \beta^2)$, and we simply get

$$G^{-1} = \mathrm{diag}(1, 1, \ldots, 1, 1/\beta^2). \tag{104}$$

Now, we have all of the expressions to compute the sensitivities according to the algorithm described in the previous subsection. The parameters α and β are to be chosen for the least squares shadowing method, and Δt, N are chosen to have the appropriate time grid.

6.4 Results and the effect of numerical parameters

The parameter $p = \omega$ is related to the time scale of the dynamics. Therefore, the numerical parameters Δt and N can be chosen effectively by using dimensionless parameters containing ω. Let us introduce the numerical parameters

$$n_{div} := \frac{2\pi}{\omega \Delta t} \qquad \text{and} \qquad n_{per} := \frac{N \Delta t \omega}{2\pi}. \tag{105}$$

The parameter n_{div} expresses the number of time steps during a period of oscillation (number of *div*isions in a period), and n_{per} expresses the number of oscillations covered by the calculations (number of *per*iods); both are real numbers. Now, we have the parameter set $(\alpha, \beta, n_{div}, n_{per})$ to modify the behaviour of the algorithm.

The results obtained from some parameter settings can be seen in the subsequent figures. All numerical computation were performed with $m = 30$ for the spatial discretization. The presented effects of the parameters do not ensure general tendencies of the numerical method, which would need a further throughout mathematical analysis. Instead, we are intended to demonstrate the importance of tuning these numerical parameters and to explore some typical tendencies in the case of the current example of the heat conduction problem.

In Figure 4, we can see the the first component of the sensitivity v^i of the trajectories along the time (see (54)) for a chosen parameter $\omega = 5$. By increasing the parameter β typically reduces the error of this quantity. Increasing β also reduces the oscillations in the rate of time dilation (see Figure 5).

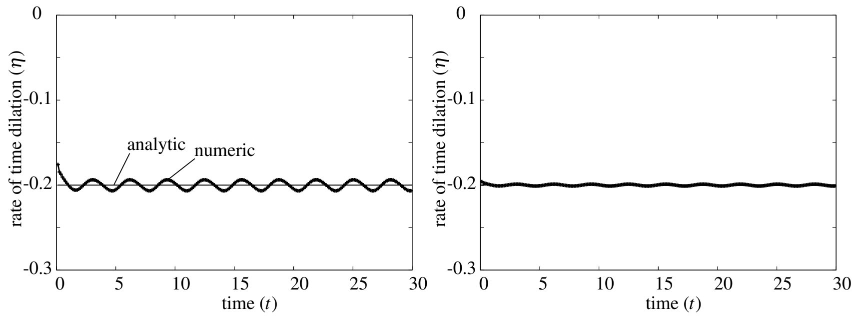

Fig. 5 Rate of time dilation η^i, by using the parameters $m = 30$, $\alpha = 1$, $n_{div} = 50$, $n_{per} = 8$, $\omega = 5$. Left panel: for $\beta = 3$, the numerical oscillation is still large, but it remains around the analytical value $-1/\omega$. Right panel: for $\beta = 20$, the amplitude of the oscillation is small around the analytical value.

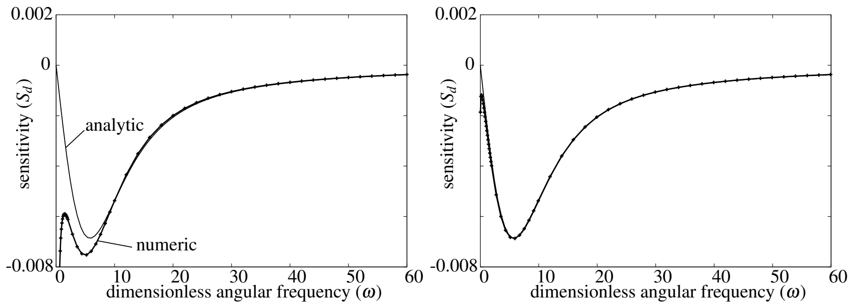

Fig. 6 Computation of the sensitivities at $m = 30$. Left panel: *inappropriately* chosen parameters ($\alpha = 1$, $\beta = 10$, $n_{div} = 8$, $n_{per} = 5$), which cause significant error for small values of ω (low frequencies). Right panel: *appropriately* chosen parameters ($\alpha = 0.1$, $\beta = 100$, $n_{div} = 20$, $n_{per} = 50$).

If the sensitivity is computed for the whole range of the angular frequency ω, we get the graphs in Figure 6. The appropriate setting of $(\alpha, \beta, n_{div}, n_{per})$ can be used to reduce the error for small ω values.

The relative error of the method can be seen in Figure 7 depending on the different numerical parameters. The arrows show the increase of the current parameter through the curves. The error is large for ω values near zero, but it decreases fast, especially for the properly set parameters.

It is found that the error becomes smaller if the value of α is decreased (see the top-left panel of Fig. 7). The very large value of α pulls the values of η^i to zero. However, increasing the value of β makes the computation more accurate (see the top-left panel of Fig. 7), by minimizing the τ' sensitivities of the phase shift. From the bottom-left and bottom-right panel of Figure 7, we can conclude that increasing of the number of the time steps decreases the error, either by increasing n_{div} or n_{per}. However, increasing n_{div} has diminishing returns (bottom-left panel of Fig. 7), and further decrease of the error can be achieved by increasing n_{per}.

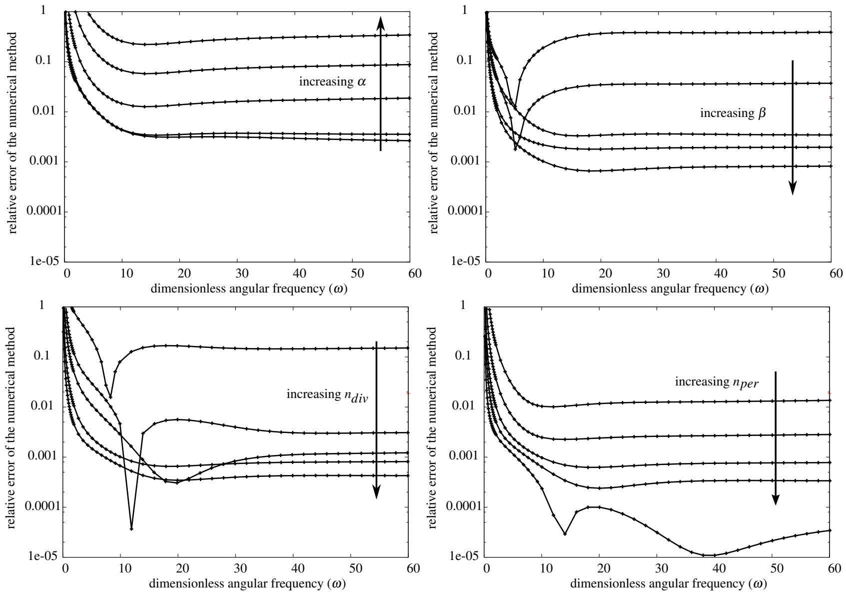

Fig. 7 Effect of the parameters on the relative error of the method, $m = 12$ in all cases. Top-left panel: effect of α with $\beta = 1$, $n_{div} = 100$, $n_{per} = 20$ and $\alpha \in \{0.01, 0.1, 1, 5, 20\}$. Top-right panel: effect of β with $\alpha = 0.1$, $n_{div} = 100$, $n_{per} = 20$ and $\beta \in \{0.5, 0.8, 1, 10, 200\}$. Bottom-left panel: effect of n_{div} with $\alpha = 0.1$, $\beta = 200$, $n_{per} = 20$ and $n_{div} \in \{3, 10, 20, 100, 300\}$. Bottom-right panel: effect of n_{per} with $\alpha = 0.1$, $\beta = 200$, $n_{div} = 100$ and $n_{per} \in \{1, 5, 20, 50, 200\}$.

7 Conclusion

We investigated the computation of parametric sensitivity of dynamical systems with a periodic excitation, which is motivated by heat conduction problems from mechanical engineering.

By using a simple test example, we demonstrated that sensitivity calculation by using the direct sensitivities of the trajectories leads to an incorrect result when considering long-time-averaged objective functions in the presence of periodic excitations. Moreover, the method of generalised sensitivity fails, as well, when we use the trivial transformation of the system to an autonomous differential equation. We analysed several approaches and showed that this transformation should be performed carefully enable the computation of accurate sensitivities.

The method of least squares shadowing can be used to compute the parametric sensitivities numerically, but we improved the method to obtain a greater freedom to choose the numerical parameters. This makes it possible to perform the calculations more effectively in the case of badly conditioned differential equations transformed from non-autonomous systems.

We demonstrated the results on the example of an 1D heat conduction problem with periodic excitation. We obtained several numerical parameters that affect the accuracy of the computation. The numerical result showed good agreement with the reference analytical solution.

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