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Using Exact Particular Solutions and Modal Reduction in Topology Optimization of Transient Thermo-Mechanical Problems

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Abstract. Design of transient thermo-mechanical systems is a challenging task often encountered during the design of high precision machines and instrumentation. Topology optimization can provide valuable insight during the design process, however, for large scale problems the backward time integration required to obtain adjoint sensitivity information is undesired. Previous work has illustrated how the introduction of a reduced modal basis allows to eliminate the backward time integration to obtain the adjoint variables. In order to reduce computational effort further, additional reduction approaches are considered. The focus is specifically on design cases where the relevant heat loads can be expressed or approximated analytically by combinations of harmonic, polynomial or exponential functions of time. Using the method of undetermined coefficients, an exact particular solution is obtained using the full system. Then, the corresponding homogenous solution is expressed using a reduced modal basis, for which a relatively small set of modes is required to obtain an accurate approximation. For the cases where the time component of the heat loads are expressed by the considered analytical functions, the backward time integration is eliminated from the calculation of the design sensitivities, while the forward integration is handled by convolutions.

Keywords: Thermo-mechanical · Model order reduction · Analytical solution · Adjoint sensitivities · Transient problems

1 Introduction

This paper focusses on topology optimization of transient thermo-mechanical problems. These problems are, for instance, encountered during the design of high precision machines and instrumentation. Small temperature fluctuations and the resulting mechanical deformations may have significant impact on a machine's performance. Developing solutions to minimize these thermal deformations is a challenging task, especially when considering transient behavior.

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Often, the resulting designs require complex material layouts in combination with active thermal management and control [1,2]. Therefore, topology optimization is considered to support in the design of high performance thermo-mechanical systems.

Topology optimization has been investigated for several thermo-mechanical design problems in the past. Considering steady-state designs, there is the early work related to thermoelastic structures by Rodrigues and Fernandes [3]. Furthermore, the design of thermo-mechanical actuation by Sigmund [4], and recently different problem formulations for thermo-elastic problems were evaluated by Deaton and Grandi [5]. Besides steady-state designs, there have been investigations into transient thermo-mechanical designs as well. For example, the material design considering transient problems by Turteltaub [6], the design of thermo-mechanical actuators considering transient effects by Li *et al.* [7], and design of structures with minimal thermally triggered displacements using material penalization by Van de Ven *et al.* [8]. One of the drawbacks involved in transient topology optimization is the computational effort related to numerical time integration. Due to the sequential nature of the time integration possibilities to parallelize the numerical integrations are limited. Moreover, when considering topology optimization of transient systems, an additional backward time integration is required to determine the adjoint sensitivities. All state information is stored during the forward time integration, resulting in storage issues for large-scale systems. When considering topology optimization, a full evaluation of the performance as well as the sensitivities is required during each iteration. By overcoming the necessity to perform both forward and backward time integration, the computational costs of topology optimization for large-scale, transient thermo-mechanical systems is greatly reduced.

To overcome these limitations and improve the computation efficiency of the evaluation of the transient response and its sensitivities, model order reduction is applied. The goal is to maintain a high-quality approximation of the system's response and its sensitivities, by evaluating a system of lower dimensionality. Multiple approaches are available to construct the representative system of lower dimensionality, which are often based on constructing an effective basis to describe the systems behavior. In context of topology optimization, different approaches have been investigated: modal superposition [9,10], proper orthogonal decomposition [11,12], and Ritz vectors [13–15]. A detailed overview and comparison of the available approaches for model order reduction in the context of transient thermo-mechanical systems has been discussed by Hooijkamp and Van Keulen [10].

In this paper, we present an extension of the previously mentioned work of Hooijkamp and Van Keulen for designs subjected to fast transient or localized thermal loads. We focus on specific cases where the considered thermal loads can be expressed or approximated by analytical functions, i.e. harmonic, polynomial or exponential functions, of time. For these cases, the discretized heat equations are solved using the method of undetermined coefficients [16], by assuming a particular satisfying the linear system of equations. The complete system is used for the calculation, providing an exact particular solution. For the homogenous solution we introduce model order reduction using a modal basis, similar to [10], allowing us to eliminate the backward and forward integration from the sensitivity analysis.

The next section describes the considered transient thermo-mechanical problem with the considered modal superposition. This is followed by the derivation of the particular and homogeneous solutions, where the reduction is introduced for the homogenous solution. Section 5 illustrates the method for a one-dimensional case, for which the design sensitivities are derived in Sect. 6. The article concludes with a brief discussion and conclusion.

2 Thermo-Mechanical System

For the considered thermo-mechanical system we assume small temperature fluctuations with respect to a known reference temperature. This allows to assume linear material behavior and linearize the effects of convective and radiation boundary conditions. The heat equation is discretized with N degrees of freedom and written as:

$$\boldsymbol{C}_{\mathrm{T}}\dot{\boldsymbol{\theta}}[t] + \mathbf{K}_{\mathrm{T}}\boldsymbol{\theta}[t] = \boldsymbol{q}[t], \tag{1}$$

where $\boldsymbol{\theta}$ describes the temperature fluctuation as function of time with respect to a reference temperature, and its nodal time derivative $\dot{\boldsymbol{\theta}}$. The heat capacity and conductivity matrices are respectively indicated with $\boldsymbol{C}_{\mathrm{T}}$ and $\boldsymbol{K}_{\mathrm{T}}$. Any contribution by convection and/or radiation will be introduced in the conductivity matrix $\boldsymbol{K}_{\mathrm{T}}$ and the right-hand side is modified accordingly. The thermal load is represented by $\boldsymbol{q}[t]$ and is assumed to be a known, time-dependent function. Finally, the initial temperature distribution of the system at $t = 0$ is given as $\boldsymbol{\theta}[t = 0] = \boldsymbol{\theta}^0$.

The mechanical system is assumed to behave much faster compared to the thermal system and any mechanical loads are assumed to change slowly over time. Thus, inertial and damping effects are neglected in the mechanical system. Consequently, only one-way coupling from the thermal to the mechanical domain is considered, which is simply obtained through linear thermal expansion:

$$\begin{aligned} \boldsymbol{K}_{\mathrm{M}}\boldsymbol{u}[t] &= \boldsymbol{f}[t] + \boldsymbol{f}_{\mathrm{T}}[t], \\ &= \boldsymbol{f}[t] + \boldsymbol{A}\boldsymbol{\theta}[t], \end{aligned} \tag{2}$$

where $\boldsymbol{u}$ represents the nodal displacement degrees of freedom and $\boldsymbol{K}_{\mathrm{M}}$ the mechanical stiffness matrix. The introduced thermal load $\boldsymbol{f}_{\mathrm{T}}$ is introduced into the mechanical system through the coupling matrix $\boldsymbol{A}$.

2.1 Modal Superposition

Thermal mode superposition expresses the transient behavior of the system as a superposition of its eigenvectors and corresponding eigenvalues (i.e. thermal modes and time constants). The thermal modes and time constants are determined by the eigenvalue problem of the heat equation Eq. (1) using $\boldsymbol{\theta} = \boldsymbol{\phi}\mathrm{e}^{-\lambda t}$ as eigenfunction:

$$(\boldsymbol{K}_{\mathrm{T}} - \lambda_k \boldsymbol{C}_{\mathrm{T}})\, \boldsymbol{\phi}_k = \mathbf{0}, \tag{3}$$

with $\boldsymbol{\phi}_k$ and λ_k the eigenvector and its eigenvalue of the k^{th} mode respectively. The thermal time constants are defined as $\tau_k = \lambda_k^{-1}$. The N eigenmodes are ordered based on their time constants: $\tau_1 \geq \tau_2 \geq \ldots \geq \tau_k \geq \ldots \geq \tau_N$ and have the following orthonormality relations:

$$\begin{aligned} \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \boldsymbol{\phi}_l &= \delta_{kl}, \\ \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{K}_{\mathrm{T}} \boldsymbol{\phi}_l &= \frac{1}{\tau_k} \delta_{kl}. \end{aligned} \tag{4}$$

The transient behavior can be expressed as superposition of all N thermal modes:

$$\boldsymbol{\theta}[t] = \sum_{k=1}^{N} \boldsymbol{\phi}_k \eta_k[t], \tag{5}$$

with η_k the time-dependent modal amplitudes, which are obtained from N decoupled first order differential equations:

$$\dot{\eta}_k[t] + \frac{1}{\tau_k}\eta_k[t] = \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{q}[t], \qquad \eta_k[0] = \eta_k^0 = \phi_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \boldsymbol{\theta}^0. \tag{6}$$

For a general excitation $\boldsymbol{q}[t]$ the modal amplitudes are obtained by evaluating the convolution integral either analytically or numerically:

$$\eta_k[t] = \eta_k^0 \mathrm{e}^{-\frac{t}{\tau_k}} + \int_0^t q_k[\gamma] \mathrm{e}^{-\frac{t-\gamma}{\tau_k}} \,\mathrm{d}\gamma. \tag{7}$$

2.2 Modal Reduction

The thermal (and mechanical) response of the system is approximated by selecting only a subset of available thermal modes:

$$\boldsymbol{\theta}[t] \approx \hat{\boldsymbol{\theta}}[t] = \sum_{\boldsymbol{m}} \boldsymbol{\phi}_m \eta_m[t], \tag{8}$$

such that the subset has a length $R \ll N$. The key of the method is to select a small as possible set of modes, that still provides a high-quality approximation of the thermo-mechanical response. Most commonly, faster thermal modes are truncated:

$$\hat{\boldsymbol{\theta}}[t] = \sum_{m=1}^{R} \boldsymbol{\phi}_m \eta_m[t]. \tag{9}$$

However, alternative methods for mode truncation or mode selection may be used as well [17,18].

2.3 Modal Reduction with Analytical Solutions

Modal reduction provides a straightforward method to reduce the calculation of the response of a thermo-mechanical system. However, when considering localized heat loads, often we require a relatively large modal basis to accurately represent the localized response within the complete system. To improve the representation of the response, we seek to enrich the selected modal basis to more accurately capture the local effects of the considered loads.

When the applied loading $\boldsymbol{q}[t]$ can be described or approximated by time dependent analytical functions, we are able to enrich the chosen modal basis by *exact* particular solutions of the governing system of ODEs (Eq. (1)). We search for the exact solution given by the homogeneous $\boldsymbol{\theta}_{\mathrm{h}}[t]$ and the particular solution $\boldsymbol{\theta}_{\mathrm{p}}[t]$ such that:

$$\boldsymbol{\theta}[t] = \boldsymbol{\theta}_{\mathrm{h}}[t] + \boldsymbol{\theta}_{\mathrm{p}}[t]. \tag{10}$$

This holds for systems where all loads are initialized at $t = 0$. For loads that initialize at a later point in time $t = t^{\star}$, additional homogenous and particular solutions are introduced using superposition:

$$\boldsymbol{\theta}[t] = \boldsymbol{\theta}_{\mathrm{h}}[t] + \boldsymbol{\theta}_{\mathrm{h}}[t - t^{\star}] + \boldsymbol{\theta}_{\mathrm{p}}[t] + \boldsymbol{\theta}_{\mathrm{p}}[t - t^{\star}]. \tag{11}$$

The remainder of this work just considers systems where all loads initialize at $t = 0$, as the method is identical and should be repeated for any loads that initialize at later moments in time.

A particular solution is determined for all components of the considered loading. Using superposition, the contributions of the particular solutions for to n load components, are given as a summation of overall all n corresponding particular solutions:

$$\boldsymbol{\theta}_{\mathrm{p}}[t] = \sum_{i=1}^{n} \boldsymbol{\theta}_{\mathrm{p},i}[t]. \tag{12}$$

These particular solutions can be obtained when the components of the load are separable in a spatial distribution and a time dependent component. Three basic load components can be identified and are given in Table 1 with their corresponding particular solutions. The undetermined coefficients represent a temperature distribution corresponding to the considered component of the applied loading. The remaining coefficients are obtained by solving the system of equations that is obtained after substitution of the particular solution into the heat Eq. (1).

With the solutions available for all particular solutions, we are able to determine the homogenous solution. We express the homogenous solution using thermal modes and their corresponding time constants:

$$\boldsymbol{\theta}_{\mathrm{h}}[t] = \sum_{k=1}^{N} \nu_k \mathrm{e}^{-\frac{t}{\tau_k}} \boldsymbol{\phi}_k, \tag{13}$$

with ν_k as modal amplitudes. Here ν_k has a similar interpretation as the modal participation η_k, however, these amplitudes only relate to the homogenous part

Table 1. Forms of the considered load components $\boldsymbol{q}_i[t]$ in $\boldsymbol{q}[t]$ and the corresponding structure of the particular solution. The coefficients $\boldsymbol{A}$ represent time-invariant spatial distributions. The coefficients $\boldsymbol{a}, \boldsymbol{b}$ are to be determined by substitution. Table adopted from [16].

Form of load component $\boldsymbol{q}_i[t]$	Form of particular solution $\boldsymbol{\theta}_{\mathrm{p}}$
$\boldsymbol{A}\cos(\omega t)$ and/or $\boldsymbol{A}\sin(\omega t)$	$\boldsymbol{a}\cos(\omega t) + \boldsymbol{b}\sin(\omega t)$
$\boldsymbol{A}t^n$	$\sum_n \boldsymbol{a}_n t^n$
$\boldsymbol{A}\mathrm{e}^{\omega t}$	$\boldsymbol{a}\mathrm{e}^{\omega t}$

of the solution. The amplitudes are determined using the initial conditions at $t = 0$, for which we also require the particular solution at $t = 0$:

$$\boldsymbol{\theta}[t=0] = \boldsymbol{\theta}_{\mathrm{h}}[t=0] + \sum_{i=1}^{n} \boldsymbol{\theta}_{\mathrm{p},i}[t=0] = \boldsymbol{\theta}^0 \tag{14}$$

Substituting the expression of the homogeneous solution (Eq. (13)) and evaluating at $t = 0$, we find:

$$\sum_{k=1}^{N} \nu_k \boldsymbol{\phi}_k = \left(\boldsymbol{\theta}^0 - \sum_{i=i}^{n} \boldsymbol{\theta}_{\mathrm{p},i}[t=0] \right). \tag{15}$$

A set of decoupled equations are found by multiplying each side by $\boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}}$ and apply the property of the normalization of the eigenmodes $\boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \boldsymbol{\phi}_l = \delta_{kl}$ (Eq. (4)):

$$\nu_k = \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \left(\boldsymbol{\theta}^0 - \sum_{i=1}^{n} \boldsymbol{\theta}_{\mathrm{p},i}[t=0] \right). \tag{16}$$

If all eigensolutions are considered the homogenous and particular solutions provide an exact solution to the transient response:

$$\boldsymbol{\theta}[t] = \sum_{k=1}^{N} \nu_k \mathrm{e}^{-\frac{t}{\tau_k}} \boldsymbol{\phi}_k + \sum_{i=1}^{n} \boldsymbol{\theta}_{\mathrm{p},i}[t]. \tag{17}$$

Modal reduction (Eq. 8) is introduced for *only* the homogenous part of the solution, while keeping the particular solution exact. Similar to modal reduction, we truncate the faster thermal modes from the homogenous solution to obtain an approximate response:

$$\boldsymbol{\theta}[t] \approx \sum_{k=1}^{R} \nu_k \mathrm{e}^{-\frac{t}{\tau_k}} \boldsymbol{\phi}_k + \sum_{i=1}^{n} \boldsymbol{\theta}_{\mathrm{p},i}[t]. \tag{18}$$

Thus, we have introduced a modal approximation for only the homogenous part of the solution. Therefore, we introduce an approximation error during the initial part of the transient response, as this is given by an approximated homogenous solution. However, we have introduced an exact solution for the considered loading, and thereby provide additional temperature fields to accurately capture the localized effects of the considered forcing. Moreover, the truncated terms of the homogeneous solution decay exponentially, as they are governed by $\mathrm{e}^{(-t/\tau_k)}$. Therefore, the error introduced by truncating faster modes will decay from the response.

Note that besides superposition of the thermal modes for the homogeneous solution, it is possible to apply mode acceleration to improve the approximation of the homogenous solution. For modal acceleration the contribution of the truncated modes in assumed instantaneously, i.e. their effects are introduced by a static contribution. Allowing to improve the quality of the approximation of the thermal response [10]. Including mode acceleration in the approximation of the homogenous solution allows to further improve the response to the initial conditions and the initial contributions of the particular solutions at $t = 0$.

3 One-Dimensional Example

To illustrate the method the following system is considered:

$$\boldsymbol{C}_{\mathrm{T}}\dot{\boldsymbol{\theta}}[t] + \boldsymbol{K}_{\mathrm{T}}\boldsymbol{\theta}[t] = \boldsymbol{q}\sin(\omega t), \tag{19}$$

where we assume the excitation contains a spatial distribution $\boldsymbol{q}$ which varies in time by $\sin(\omega t)$. Initially the structure is assumed at rest with zero temperature, thus $\boldsymbol{\theta}^0 = 0$. For illustration purposes we consider a one-dimensional bar, illustrated in Fig. 1, however the same approach holds for two and three-dimensional cases. The left side is kept at $\theta = 0$, the right side is isolated, and the excitation is applied at the middle node.

We now separate the solution into a homogenous and particular solution, as Eq. (10). For the considered load, the homogenous and particular solution:

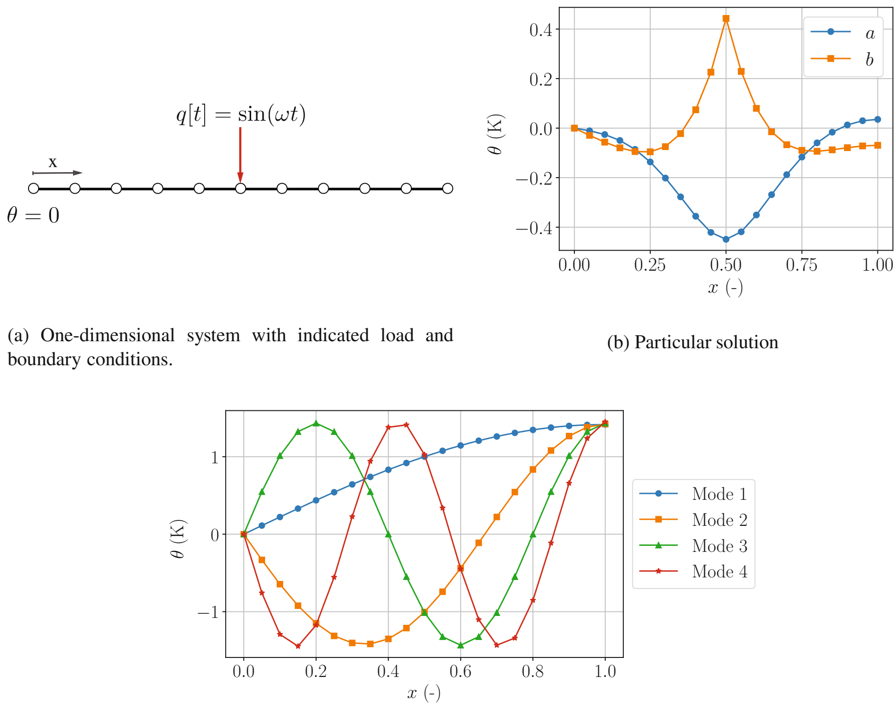
$$\begin{aligned}\boldsymbol{\theta}_{\mathrm{h}}[t] &= \sum_{k=1}^{N} \nu_k \mathrm{e}^{-\frac{t}{\tau_k}} \boldsymbol{\phi}_k \\ \boldsymbol{\theta}_{\mathrm{p}}[t] &= \boldsymbol{a}\cos(\omega t) + \boldsymbol{b}\sin(\omega t).\end{aligned} \tag{20}$$

Substitution into the discretized heat equation:

$$\boldsymbol{C}_{\mathrm{T}}\left(-\omega \boldsymbol{a}\sin(\omega t) + \omega \boldsymbol{b}\cos(\omega t)\right) + \boldsymbol{K}_{\mathrm{T}}\left(\boldsymbol{a}\cos(\omega t) + \boldsymbol{b}\sin(\omega t)\right) = \boldsymbol{q}\sin(\omega t), \tag{21}$$

provides the following set of equations that are solved together to determine the spatial distributions $\boldsymbol{a}$ and $\boldsymbol{b}$:

$$\begin{bmatrix} \boldsymbol{K}_{\mathrm{T}} & \omega \mathbf{C}_{\mathrm{T}} \\ -\omega \boldsymbol{C}_{\mathrm{T}} & \boldsymbol{K}_{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{bmatrix} = \begin{bmatrix} 0 \\ \boldsymbol{q} \end{bmatrix}. \tag{22}$$



(c) First four modes of the system

Fig. 1. Illustration of a one-dimensional bar with the applied boundary conditions (a), and the resulting temperature distributions corresponding to the particular solution (b). The first four thermal modes are visualized in (c).

The obtained fields $\boldsymbol{a}$ and $\boldsymbol{b}$ provide additional temperature distributions, similar to thermal modes, that represent the applied forcing, as illustrated in Fig. 1b. These fields are able to capture the localized behavior introduced by the applied loading. This is difficult to capture with a low number of thermal modes, due to the non smoothness of the resulting temperature field. For comparison, the first four thermal modes are given in Fig. 1c. The modal amplitudes corresponding to the homogenous solution are given by:

$$\begin{aligned} \nu_k &= \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \left(\boldsymbol{\theta}^0 - \boldsymbol{\theta}_{\mathrm{p}}[t=0] \right) \\ &= \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \left(\boldsymbol{\theta}^0 - \boldsymbol{a} \right) \end{aligned} \tag{23}$$

The full, exact solution becomes:

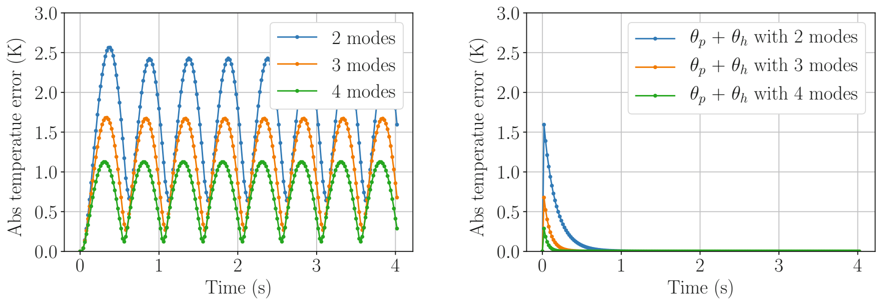
$$\boldsymbol{\theta}[t] = \sum_{k=1}^{N} \nu_k \mathrm{e}^{-\frac{t}{\tau_k}} \boldsymbol{\phi}_k + \boldsymbol{a} \cos(\omega t) + \boldsymbol{b} \sin(\omega t), \tag{24}$$

We now introduce modal reduction for only the homogenous solution to approximate the response:

$$\boldsymbol{\theta}[t] \approx \hat{\boldsymbol{\theta}}[t] = \sum_{k=1}^{R} \nu_k \mathrm{e}^{-\frac{t}{\tau_k}} \boldsymbol{\phi}_k + \boldsymbol{a}\cos(\omega t) + \boldsymbol{b}\sin(\omega t), \tag{25}$$

where the selected subset of modes has a length $R \ll N$.

Figure 2 compares the error with respect to the exact solution for systems with basic modal reduction (Fig. 2a) and the error when extending the basis with the obtained particular solution (Fig. 2b). For both approaches the absolute error compared to the solution using a full basis is evaluated for each node and summed. The comparison is presented using 2, 3 and 4 thermal modes. The first four modes of the system are illustrated in Fig. 1c. We observe that for a sinusoidal loading the error remains present throughout the complete time frame when using modal reduction. However, by introducing the particular solution and only representing the homogenous solution by modal reduction, we are able to capture the response considerably accurately. We now observe an exponentially decaying error during the initial response to the loading, which decreases when adding additional thermal modes into the basis of the homogenous response.



(a) Error using a reduced modal basis.

(b) Error using an exact particular solution and a reduced homogeneous solution.

Fig. 2. Illustration of the difference in absolute temperature for both reduction approaches. The temperature differences are calculated with respect to the exact solution containing a full modal basis. Figure (a) applies a modal reduction for 2, 3, and 4 thermal modes in the reduced set of modes. In Figure (b) the reduction contains the exact particular solution and the homogenous solution is approximated using 2, 3, and 4 thermal modes.

4 Sensitivity Analysis

In general, the optimization problem for a discretized thermo-mechanical system can be written as:

$$
\begin{aligned}
\min_{\boldsymbol{s}} \quad & f[\boldsymbol{s}, \boldsymbol{\theta}, \boldsymbol{u}, t], \\
\text{s.t} \quad & h[\boldsymbol{s}, \boldsymbol{\theta}, \boldsymbol{u}, t] = 0, \\
& g[\boldsymbol{s}, \boldsymbol{\theta}, \boldsymbol{u}, t] \leq 0, \\
& 0 < s_i^{\min} \leq s_i \leq s_i^{\max},
\end{aligned} \tag{26}
$$

with f the objective function, s_i the design variables with lower and upper bounds $s_i^{\min}$, $s_i^{\max}$, and h, g equality and inequality constraints. The objective function can depend on design variables $\boldsymbol{s}$, time t, and both thermal and mechanical responses given respectively by $\boldsymbol{\theta}[t]$ and $\boldsymbol{u}[t]$. Often, a response function $r[\boldsymbol{s}]$ is defined as performance over time, captured by the time integral:

$$
r[\boldsymbol{s}] = \int_{t_0}^{t_{\mathrm{E}}} P[\boldsymbol{s}, \boldsymbol{\theta}, \boldsymbol{u}, t] \mathrm{d}t, \tag{27}
$$

with t_0 and t_{E} the start and end time of the considered time frame, and P the considered function of interest, for example a difference with a reference displacement or temperature.

In this work, the objective and constraint functions are expressed using the homogenous and particular solutions of the considered system, where mode superposition has been introduced to reduce the homogenous response of the solution. Therefore, the considered response function is also an approximation:

$$
r[\boldsymbol{s}] \approx \hat{r}[\boldsymbol{s}] = \int_{t_0}^{t_{\mathrm{E}}} \hat{P}[\boldsymbol{s}, \hat{\boldsymbol{\theta}}, \hat{\boldsymbol{u}}, t] \mathrm{d}t. \tag{28}
$$

To find the sensitivities of the design, we differentiate the approximated response with respect to the design variables $\boldsymbol{s}$:

$$
\frac{\mathrm{d}\hat{r}}{\mathrm{d}s_i} = \int_{t_0}^{t_{\mathrm{E}}} \frac{\partial \hat{P}}{\partial s_i} + \frac{\partial \hat{P}}{\partial \hat{\boldsymbol{u}}} \frac{\mathrm{d}\hat{\boldsymbol{u}}}{\mathrm{d}s_i} + \frac{\partial \hat{P}}{\partial \hat{\boldsymbol{\theta}}} \frac{\mathrm{d}\hat{\boldsymbol{\theta}}}{\mathrm{d}s_i} \mathrm{d}t. \tag{29}
$$

To avoid computation of expensive derivatives and derivatives to system responses, we apply the adjoint variable method to calculate the sensitivities of the response. An additional advantage of using the analytical expressions for the thermal response, is the ability to eliminate backward time integration, which is required in standard adjoint formulations. For the adjoint sensitivities, the response function is augmented by the governing equations related to the particular and homogeneous solutions, as well as the eigenvalue problem and its normalization. Therefore, Eq. (28) is augmented with Eqs. (3), (4), (22), (23) and (25):

$$
\begin{aligned}
\hat{r}^{\star} = \hat{r} + \int_{t_0}^{t_{\mathrm{E}}} & \boldsymbol{\eta}^{\mathrm{T}} \left(\boldsymbol{K}_{\mathrm{u}} \boldsymbol{u} - \boldsymbol{f}[t] - \boldsymbol{A}\boldsymbol{\theta}[t] \right) \\
& + \boldsymbol{\lambda}^{\mathrm{T}}[t] \left(\boldsymbol{\theta}[t] - \sum_{k=1}^{R} \nu_k \mathrm{e}^{-t/\tau_k} \boldsymbol{\phi}_k - \boldsymbol{a}\cos(\omega t) - \boldsymbol{b}\sin(\omega t) \right) \mathrm{d}t \\
& + \sum_{k=1}^{R} \mu_k \left[\nu_k - \boldsymbol{\phi}^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \left(\boldsymbol{\theta}^0 - \boldsymbol{a} \right) \right] \\
& + \sum_{k=1}^{R} \boldsymbol{\gamma}_k^{\mathrm{T}} \left[\left(\boldsymbol{K}_{\mathrm{T}} - \frac{1}{\tau_k} \boldsymbol{C}_{\mathrm{T}} \right) \boldsymbol{\phi}_k \right] \\
& + \sum_{k=1}^{R} \chi_k \left(\frac{1}{2} - \frac{1}{2} \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \boldsymbol{\phi}_k \right), \\
& + \boldsymbol{\alpha}^{\mathrm{T}} \left(\boldsymbol{K}_{\mathrm{T}} \boldsymbol{a} + \omega \boldsymbol{C}_{\mathrm{T}} \boldsymbol{b} \right) + \boldsymbol{\beta}^{\mathrm{T}} \left(-\omega \boldsymbol{C}_{\mathrm{T}} \boldsymbol{a} + \boldsymbol{K}_{\mathrm{T}} \boldsymbol{b} - \boldsymbol{q}[t] \right),
\end{aligned}
\tag{30}
$$

with $\boldsymbol{\eta}, \boldsymbol{\lambda}, \mu_k, \boldsymbol{\gamma}_k, \chi_k, \boldsymbol{\alpha}$, and $\boldsymbol{\beta}$ the adjoint variables. Note that the formulation of the adjoint sensitivities is shown for a case subjected to a sinusoidal excitation. When other components are available in the loading, both the particular solution as well as the formulation of the adjoint sensitivities need to be modified accordingly. Similarly, minor modifications are required to include mode acceleration within the formulation of the adjoint variables.

To determine the adjoint variables, the sensitivities of the augmented performance measure are evaluated. Now, the adjoints are chosen such that the derivatives with respect to the system responses $\hat{\boldsymbol{u}}, \hat{\boldsymbol{\theta}}$, the thermal modes and time constants $\boldsymbol{\phi}_k$, τ_k, the modal amplitudes of the homogenous solution ν_k and both coefficients of the particular solution $\boldsymbol{a}, \boldsymbol{b}$ drop out. This results in the following adjoint equations:

$$
\begin{aligned}
\boldsymbol{\eta}[t] &= -\boldsymbol{K}_{\mathrm{u}}^{-1} \frac{\partial \hat{P}}{\partial \boldsymbol{u}}[t], \\
\boldsymbol{\lambda}[t] &= \boldsymbol{\eta}[t]^{\mathrm{T}} \boldsymbol{A} - \frac{\partial \hat{P}}{\partial \hat{\boldsymbol{\theta}}}[t], \\
\mu_k &= \int_{t_0}^{t_{\mathrm{E}}} \boldsymbol{\lambda}^{\mathrm{T}}[t] \mathrm{e}^{-t/\tau_k} \boldsymbol{\phi}_k \mathrm{d}t,
\end{aligned}
\tag{31}
$$

and an augmented system of equations related to the eigenvalue problem:

$$
\begin{bmatrix} \left(\boldsymbol{K}_{\mathrm{T}} - \frac{1}{\tau_k} \boldsymbol{C}_{\mathrm{T}} \right) & -\boldsymbol{C}_{\mathrm{T}} \boldsymbol{\phi}_k \\ -\boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\gamma}_k \\ \chi_k \end{bmatrix} = \begin{bmatrix} \int_{t_0}^{t_{\mathrm{E}}} \boldsymbol{\lambda}^{\mathrm{T}}[t] \nu_k \mathrm{e}^{-t/\tau_k} \mathrm{d}t + \mu_k \boldsymbol{C}_{\mathrm{T}} \left(\boldsymbol{a} - \boldsymbol{\theta}^0 \right) \\ \int_{t_0}^{t_{\mathrm{E}}} \boldsymbol{\lambda}^{\mathrm{T}}[t] \nu_k t \mathrm{e}^{-t/\tau_k} \mathrm{d}t \end{bmatrix}, \tag{32}
$$

and finally a system of equations corresponding similar to finding the undetermined coefficients of the particular solution:

$$
\begin{bmatrix} \boldsymbol{K}_{\mathrm{T}} & -\omega \boldsymbol{C}_{\mathrm{T}} \\ \omega \boldsymbol{C}_{\mathrm{T}} & \boldsymbol{K}_{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix} = \begin{bmatrix} \int_{t_0}^{t_{\mathrm{E}}} \boldsymbol{\lambda}^{\mathrm{T}}[t] \cos(\omega t) \mathrm{d}t - \sum_{k=1}^{R} \mu_k \boldsymbol{\phi}_k^{\mathrm{T}} \boldsymbol{C}_{\mathrm{T}} \\ \int_{t_0}^{t_{\mathrm{E}}} \boldsymbol{\lambda}^{\mathrm{T}}[t] \sin(\omega t) \mathrm{d}t \end{bmatrix}. \tag{33}
$$

Note that the adjoint variables μ_k, γ_k, and χ_k are required for each mode included in the reduced set of modes R. Moreover, we observe that the remaining time integrations are all forward in time, eliminating the backward integration. Also, all integration can be performed at once when the analytical system responses are determined. After calculation of the adjoint variables, the remaining terms are evaluated to obtain the complete sensitivity information:

$$\begin{aligned}\frac{\mathrm{d}r^\star}{\mathrm{d}s_i} = \int_{t_0}^{t_\mathrm{E}} & \frac{\partial \hat{P}}{\partial s_i} + \boldsymbol{\eta}^\mathrm{T}[t]\left[\frac{\mathrm{d}\boldsymbol{K}_\mathrm{u}}{\mathrm{d}s_i}\boldsymbol{u}[t] - \frac{\partial \boldsymbol{f}}{\partial s_i}[t] - \frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}s_i}\boldsymbol{\theta}[t]\right]\mathrm{d}t \\ & + \sum_{k=1}^{R}\mu_k\left[-\boldsymbol{\phi}_k^\mathrm{T}\left(\frac{\mathrm{d}\boldsymbol{C}_\mathrm{T}}{\mathrm{d}s_i}\left(\boldsymbol{\theta}^0 - \boldsymbol{a}\right) - \boldsymbol{C}_\mathrm{T}\frac{\partial \boldsymbol{\theta}^0}{\partial s_i}\right)\right] \\ & + \sum_{k=1}^{R}\gamma_k^\mathrm{T}\left[\left(\frac{\mathrm{d}\boldsymbol{K}_\mathrm{T}}{\mathrm{d}s_i} - \frac{1}{\tau_k}\frac{\mathrm{d}\boldsymbol{C}_\mathrm{T}}{\mathrm{d}s_i}\right)\boldsymbol{\phi}_k\right] \\ & + \sum_{k=1}^{R}\chi_k\left(-\frac{1}{2}\boldsymbol{\phi}_k^\mathrm{T}\frac{\mathrm{d}\boldsymbol{C}_\mathrm{T}}{\mathrm{d}s_i}\boldsymbol{\phi}_k\right) \\ & + \boldsymbol{\alpha}^\mathrm{T}\left(\frac{\mathrm{d}\boldsymbol{K}_\mathrm{T}}{\mathrm{d}s_i}\boldsymbol{a} + \omega\frac{\mathrm{d}\boldsymbol{C}_\mathrm{T}}{\mathrm{d}s_i}\boldsymbol{b}\right) + \boldsymbol{\beta}^\mathrm{T}\left(-\omega\frac{\mathrm{d}\boldsymbol{C}_\mathrm{T}}{\mathrm{d}s_i}\boldsymbol{a} + \frac{\mathrm{d}\boldsymbol{K}_\mathrm{T}}{\mathrm{d}s_i}\boldsymbol{b} - \frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}s_i}\right)\end{aligned} \quad (34)$$

The extension to include mode acceleration for the homogenous solution with the corresponding sensitivities is left as future work.

5 Discussion

In the presented method, we illustrate the possibility to combine exact particular solutions with truncated modal basis to effectively approximate the transient thermal response. However, it has to be noted that the presented method is particularly advantageous for cases with periodic and localized thermal loads. The introduced particular solution provides an enrichment to the modal basis. This is mainly of interest when excitations result in localized temperature distributions, that are typically hard to capture by a truncated modal basis, even with the introduction of mode acceleration. Moreover, the particular solution is especially effective for periodic excitations. If the temperature distribution as result of the applied loading is hard to describe by a reduced modal basis, the error will not decay from the solution. In these cases, the introduction of the particular solution provides an exact representation of the temperature distribution as a result of the applied forcing. The reduced homogenous solution has to capture only the response to the initial conditions and contributions of the particular solution at $t = 0$. The introduced approximations by the modal reductions are therefore only present in the homogenous solutions and will decay within a certain time span depending on the number of modes included in the reduction.

Furthermore, the applicability of the presented method is limited to linear, thermo-mechanical systems where the considered loading is accurately represented by harmonic, exponential or polynomial functions, of time. Load components that are not explicitly expressed by these functions, need to be approximated in order to find the corresponding particular solutions. The quality of this approximation will limit the potential improvements of the presented method compared to direct application of a modal reduction and mode acceleration. Alternatively, investigations into model order reduction using Ritz vectors might prove to be valuable extension for systems subjected to localized loads. The effects of the applied loading is included within the basis constructed by Ritz vectors. This might provide similar benefits as observed in this work as a result of the introduction of the particular solution as enrichment of the modal basis.

Besides, we would like to emphasize that the evaluation of the particular solution is not free of computational costs. Following the method of undetermined coefficients a system needs to be constructed and solved to obtain the exact particular solution. Detailed investigation is required to determine in which scenarios it is more effective to enlarge the truncated modal basis or to solve the set of equations related to the particular solution to improve the approximated response. Moreover, if the load contains multiple components, or if the loading is approximated by a summation of load components, multiple systems need to be constructed and solved to determine the corresponding particular solution of each component. Also, additional adjoint equations are introduced for each component in the sensitivity analysis. When considering multiple load components, it is not necessarily possible to reuse previously factorized systems, resulting in additional computational costs.

Finally, the proposed method is expected to be beneficial for application in topology optimization. The introduction of the modal basis and the exact particular solution provide an accurate response of the transient thermal behavior, with relatively limited computational costs. Moreover, the ability to eliminate the backward time integration during the sensitivity analysis overcomes storage issues and allows for efficient calculation of the sensitivities. Careful investigation is required to determine the quality of the obtained sensitivities, when considering different number of thermal modes in the reduction. Similar to previous work [10], the introduction of mode acceleration might prove to be critical to obtain accurate representation of the systems sensitivities.

6 Conclusions

This paper presents an extended method for modal reduction for transient thermo-mechanical topology optimizations, where only thermal loads are considered expressed by harmonic, exponential or polynomial functions of time. For these cases analytical solutions to the homogenous and particular solutions are determined. A truncated modal basis is introduced to represent the homogenous solution. The additional particular solution provides an exact representation of the response to the considered loads, significantly improving the obtained approximation. Moreover, this representation of the thermal response allows to eliminate backward time integration from the calculation of the adjoint sensitivities. The remaining time integrations are performed on decoupled systems, at relatively low computational costs. We expect this approach to enable topology optimization of certain large-scale transient linear thermo-mechanical problems with modest computational requirements.

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