Expectation-Maximization Algorithm for Identification of Mesh-Based Compartment Thermal Model of Power Modules

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ABSTRACT
Accurate prediction of temperatures in power modules is crucial for proper thermal management. Lumped parameter thermal models are preferred in this application for their low computational cost. The estimation procedure of the parameters of these models requires measurements of temperatures of all active elements. This requirement is relaxed in this contribution. Specifically, the previously used dark gray-box compartment model is replaced by a structured compartment model utilizing a mesh-based discretization of the physical layout of the module. Compartments are categorized into several types with common parameters for each type. The parameters are identified from the data of the measured elements using the Expectation-Maximization algorithm. The algorithm internally predicts the temperatures of the unmeasured elements. The sensitivity of the estimation to regularization of the process covariance matrix is also studied. The implied high-dimensionality of the state-space increases the computational cost of the conventional estimation procedure, therefore, a simplified procedure with a much lower computation cost is proposed. The performance of the proposed approach is tested on simulated data.

Introduction
Monitoring of temperature distribution and its accurate prediction in power semiconductor modules is fundamental for the proper thermal management that enables to operate the system at the physical limit and prevents device failures due to undesirable thermal stresses. Therefore, the integration of the precise thermal model into the thermal protection algorithm is essential, since the direct measurement of all temperature distribution is very often infeasible (e.g. due to the necessity for device encapsulating or low cost production claims). Therefore, we are interested in thermal models that can predict future temperatures at a low computational cost.

This requirement is in contrast with the popular class of models used for heat transfer simulations based on numerical discretization such as the Finite Difference Method (FDM), Finite Element Method (FEM), or Finite Volume Method (FVM) [1]. These methods yield very accurate results but at the expense of high computational requirements and thus they cannot be used in online prediction. Moreover, the design and especially validation of these models can be very time-consuming and without precise knowledge of the device’s physical structure difficultly realizable.

A more suitable class of models is based on Lumped Parameter Thermal Networks (LPTNs) using thermal resistors and thermal capacitors as an analogy to electrical circuits for modeling the heat transfer in the devices. Generally, LPTNs produce reasonably accurate results requiring much less computational time in comparison to models based on numerical discretization methods [2]. LPTNs can be classified into dark gray-box, light gray-box, or white-box models depending on the number of used equivalent resistor and capacitor (RC) elements [3]. Specifically, the dark gray-box LPTNs are typically input-output models with very few RC elements and their computational requirements are thus very low. However, this advantage is achieved at the cost of low generalization, where only selected points in the device can be monitored and several thermal phenomena (e.g. coupling effect or temperature distribution in the segment like...
a chip) are ignored. More complicated structures of LPTNs (light gray-box or white-box models) are becoming popular due to the increased computational performance of recent microcontrollers. These models use a higher number of RC elements in the LPTN that can lead to improved solution accuracy [2, 4] and finer details, for example, spatial temperature distribution, boundary conditions, or coupling effect [5, 6], can be considered in the model.

The key procedure in the development of these models is a proper estimation of their parameters. The parameters can be estimated directly from the

| Nomenclature | \( Q' \) | Covariance matrix of process noise in the \( r \)-th step of EM algorithm |
| --- | --- | --- |
| \( \mathbb{R}^* \) | The set of real numbers of the given dimension. |
| \( R \) | Covariance matrix of measurement noise |
| RC | Resistor and Capacitor |
| RTSS | Rauch Tung Striebel Smoother |
| \( S_i \) | Set of compartments indexes adjacent to the \( i \)th compartment |
| SS | State Space |
| \( T_i \) | Vector of compartment temperatures \( T_{i,t}, \; i \in 1:n \) |
| \( T \) | Temperature, [K], or temperature random variable |
| \( T_{i,t} \) | Temperature of the compartment \( i \) at the discrete time \( t \), [K] |
| \( w \) | Measurement noise |
| \( V_N^* \) | Covariance matrix of the smoothed posterior distribution |
| \( w_i \) | Process noise |
| \( x_{*}^t \) | Smoothed estimate of temperatures at the given time. |
| \( y_{*}^t \) | Measured temperatures, [K] |
| \( Y \) | Measured temperature, [K], or measured temperature random variable where it is meaningful |
| \( z \) | Vector of sorted parameters \( z_i \) |
| \( z_i \) | Estimated model parameter |

**Greek Symbols**

| \( \alpha \) | Parameter of a constrained covariance matrix estimation |
| \( \beta \) | Parameter of a constrained covariance matrix estimation |
| \( \theta \) | Model parameters |
| \( \theta' \) | Values of model parameters in the \( r \)-th step of EM algorithm |
| \( \Delta T_i \) | Temperature difference between one-time step (weighted by \( \Delta t \)) |
| \( \Delta t \) | Length of time step, [s] |
| \( \lambda \) | Thermal conductivity coefficient, [W/(m \cdot K)] |
| \( \Phi \) | An auxiliary/arbitrary distribution |
| \( \Phi' \) | Distribution of temperatures from RTSS in the \( r \)-th step of EM algorithm |
| \( \rho \) | Density of the material, [kg/m\(^3\)] |

**Subscripts**

| diag | Approximation using diagonal form of matrix |
| full | Using full form of matrix |
| \( i, j \) | Vector/matrix component |
| ss | Strongly shared parametrization |
| \( t \) | Time index |
| ws | Weakly shared parametrization |
| \( zLL' + \beta I \) | Approximation using the given form \((zLL' + \beta I)\) of matrix |

**Superscripts**

| \( r \) | \( r \)-th iteration of EM algorithm |
data, for example, in the case of dark-grey LPTNs. However, estimation of more complex models requires more data that are often not available. The lack of data can be overcome by simulating the required temperature profiles by a calibrated FEM model of the device. For example, transient (step) responses are simulated and the parameters are obtained by exponential fitting techniques applied to transient thermal impedance curves. An interesting approach how to create a light gray- or white-box RC model is to use a mesh-based LPTN [7, 8] that can be identified from a geometric and material description of the device. However, this standard identification procedure is strongly dependent on the quality of information about the physical structure of the device and still requires rich experience to obtain reasonable results [4]. We aim to decrease the need for this level of detail in the estimation procedure.

The problem of missing data may be addressed by the use of the Bayesian framework, which is well-known in this domain [9]. For example, Bayesian inference driven by the Monte Carlo method is used for estimation of the volumetric heat generation and heat transfer coefficient in [10], where a trained neural network is used as the forward model and only data from the steady states are considered. The need for transient temperature distribution estimates arises when temporal profiles are of concern [11, 12]. However, joint estimation of the model parameters from transients is challenging when the measurements are incomplete. Such a scenario can be covered by the Expectation-Maximization (EM) algorithm [13].

Recently, the authors of this contribution proposed the application of the EM algorithm to Linear Time Invariant (LTI) State Space (SS) compartment thermal model of semiconductor module with multiple heat sources [14]. This approach enables the identification of model parameters from incomplete temperature data and allows to combine sets of measurements using different sensors in each set. However, the model belongs to the category of dark gray-box model and requires measuring temperatures of all active elements at least in one set of measurements.

In this article, we aim to relax the need for the availability of measured temperatures of all elements of interest. Specifically, we propose to use a mesh-based structured compartment model with building blocks with shared parameters. The proposed mesh-based model falls into the class of white-box models since there is a much finer compartment structure based on discretization of the physical layout of the module. The implied dynamical model is once again an LTI SS model, however of a much larger state space of the temperatures than before. The state transition matrix is high-dimensional and estimation of all its parameters would require too much data. For that reason, the model complexity is reduced by sharing parameters of the compartments, so that they can be identified from the available data. We elaborate application of the EM algorithm to this model in this article and study its properties in detail.

### Mesh-based compartment structure

The proposed LTI SS thermal model is based on a compartment representation of the studied power semiconductor module. The compartment model may be understood as a coarsely discretized model in the sense of numerical methods. In other words, each compartment stands for a relatively spacious control volume of the area of interest. In comparison to the numerical discretization, the module is possible to be represented by only units of compartments, although a finer compartment representation can give better results. For that reason, the models based on mesh representation and comprising structured compartments (circa hundreds of compartments which is still much less than it is usual in numerical models) are objects of our interest.

The three-dimensional volume of the entire domain of the investigated power module is discretized into rectangular elements (cubes or cuboids) in a uniform Cartesian grid. We refer to these elements as to the compartments. Each basic-sized compartment can be further refined into four finer compartments in the X- and Y-axis in the quadtree sense in the case that the compartment contains more various components (e.g. a part of diode’s volume and a part of transistor’s volume are located in the same compartment).

A selection of the basic discretization level is a tradeoff between the growing number of compartments and the quality of the model. A layer arrangement in one axis (Z-axis in our case) is typical for a common power semiconductor module (Figure 1a), whereas a more complicated layout comprising diodes or transistors covers the surface (Figure 1b) in the remaining two axes (X- and Y-axis). For this reason, the suggested design of the discretization is divided into the selection of the number of compartment layers and the selection of the fineness of the power module surface grid.

The specific discretization levels used in this article for testing the proposed identification method are discussed in the verification section.
**Compartment state space model**

The governing equation for the LTI SS model is the well-known heat transfer equation

$$\nabla \cdot (\lambda \nabla T) + p = \rho c_p \frac{\partial T}{\partial t},$$  \hspace{1cm} (1)

where $T$ stands for the temperature, $p$ is the internal volumetric heat source (with base units $[\text{W/m}^3]$), $\lambda$ is the thermal conductivity coefficient, $\rho$ is the density of the material, and $c_p$ is the specific heat capacity at constant pressure. Under the assumption of uniform constant thermal properties of compartments, Eq. (1) can be discretized [15] using the fully explicit scheme in the form

$$T_{i,t+1} = T_{i,t} + \Delta t \sum_{j \in S_i} (k_{i,j}(T_{j,t} - T_{i,t}) + z_i P_{i,t}),$$ \hspace{1cm} (2)

where $T_{i,t}$ and $P_{i,t}$ are the temperature and the internal heat source (with base units $[\text{W}]$) inside the compartment $i$ at the discrete time $t$, $t \in \mathbb{Z}$. The time step is denoted by $\Delta t$ and $S_i$ is the set of indexes of the compartments adjacent to the $i$th compartment such that we assume thermal coupling with the $i$th compartment. Symbols $k_{i,j}$ and $z_i$ are unknown model parameters that have to be estimated from the measurements. More detail can be seen in ref. [14].

The proposed compartment model given by Eq. (2) can be viewed as a particular case of directed graphs. Using graph theory [16], the heat transfer between compartments given by Eq. (2) may be described by a directed graph with vertices $T_i$ and directed edges $k_{i,j}$. Coefficients $k_{i,j}$ can be arbitrarily sorted into a vector $k \in \mathbb{R}^m$, which corresponds to the ordering of edges in the graph. Then the directed graph can be represented by an *incidence matrix* $\mathcal{J}$. The incidence matrix is a sparse matrix of size $n \times m$ in general, where $n$ is the number of vertices (i.e. compartments) and $m$ is the number of edges (i.e. valid coefficients $k_{i,j}$). The element $j_{i,l}$ of the incidence matrix $\mathcal{J}$ is defined by the relation

$$j_{i,l} = \begin{cases} 
1 & \text{if } T_l \text{ is the tail of the } l\text{-th edge} \\
-1 & \text{if } T_l \text{ is the head of the } l\text{-th edge} \\
0 & \text{otherwise.}
\end{cases} \hspace{1cm} (3)$$

Introducing a temperature vector $T_t = [T_{1,t}, \ldots, T_{n,t}]'$, a vector of heat sources (power losses) $P_t = [P_{1,t}, \ldots, P_{n,t}]'$ and a parameter vector $z = [z_1, \ldots, z_n]'$, and employing the incidence matrix $\mathcal{J}$ and the parameter vector $k$, discrete thermal dynamic Eq. (2) can be written in the form using the parametrization by $k$ and $z$

$$T_{t+1} = T_t - \Delta t \mathcal{J} \text{diag}(Ck) T_t + \Delta t \text{diag}((Az)P_t),$$ \hspace{1cm} (4)

$$= T_t - \Delta t \mathcal{J} \text{diag}((\mathcal{J}'T_t)Ck) + \Delta t \text{diag}(P_t)Az,$$ \hspace{1cm} (5)

where matrix $\mathcal{J}$ is a matrix obtained from incidence matrix $\mathcal{J}$ by replacement $1 \rightarrow 0$. Matrices $A$, $B$ and $C$ in Eqs. (4) and (5) are auxiliary matrices of elementary vectors. If $A = I_n$, $B = I_n$, $C = I_m$, where $I_n$ is the identity matrix $n \times n$, Eqs. (4) and (5) exactly correspond to the Eq. (2).

In many cases, the power losses $P_t$ could be considered only for particular compartments (e.g. for compartments corresponding to transistors or diodes in the case of power module modeling). Furthermore, we wish to have the mesh-based compartment model described by shared parameters. It means that selected sets of coefficients $k_{i,j}$ and $z_i$ are required to be identical. These presumptions are very desirable for the following identification procedure since the dimension of the temperature vector in the proposed mesh-based model is relatively high.

In general, vectors $z = [z_1, \ldots, z_n]'$, $P_t = [P_{1,t}, \ldots, P_{n,t}]'$, and $k = [k_1, \ldots, k_m]'$ are of arbitrary lengths $n_z$, $n_p$, and $n_k$, respectively. Then $A$ is a matrix $n_p \times n_z$ of scaled elementary row vectors.
mapping vector $z$ to the corresponding heat sources, $B$ is a matrix $n \times n_p$ of scaled elementary row vectors mapping heat sources to the corresponding compartments, and $C$ is a matrix $m \times n_b$ of scaled elementary row vectors mapping vector $k$ to the corresponding edges of the graph representation (i.e. mapping vector $k$ to the corresponding differences $T_{j,t} - T_{i,t}$). The scale of each elementary vector corresponds to a certain weight of transfer coefficients among compartments in the case that only a fraction of compartment volume is occupied by the studied device, or in the case that compartment refining is utilized during designing of the mesh-based model. Then, these weights are dependent on the different volumes and outer surfaces of base-size compartments and refined compartments. In other cases, the default scale is set to one.

Further, Eqs. (4) and (5) can be rewritten in a more pleasant form. Establishing matrices $A$, $B$, and $M_t$:

$$A = I_n - \Delta \tau \text{diag}(Ck)J', \quad (6)$$
$$B = \Delta \tau \text{diag}(Az), \quad (7)$$
$$M_t = [-\Delta \tau \text{diag}(J'T_i)C, \ B \text{diag}(P_i)A] \quad (8)$$

and assuming an additional zero-mean Gaussian noise $w_t \in \mathbb{R}^n$ with a covariance matrix $Q$, $w_t \sim \mathcal{N}(w_t|0, Q)$, Eq. (4) can be put into the standard form of the explicit discrete LTI state equation

$$T_{t+1} = AT_t + BP_t + w_t \quad (9)$$
$$= T_0 + \Delta \tau M_t \theta + w_t, \quad (10)$$
$$\theta = [k', z']'. \quad (11)$$

with the state vector $T_0$ and the input vector $P_0$. Equation (10) is a notation enabling to use a least squares method for estimating unknown parameter vectors $k$ and $z$ of the proposed model.

For completeness of the model, we define the vector of measured temperatures as $y_t$ and the observation model (output equation)

$$y_t = CT_t + v_t, \quad (12)$$

where $C \in \mathbb{R}^h \times n_b$ is the matrix comprising elementary row vectors corresponding to the indices of $n_b$ measured (observed) compartment temperatures, and $v_t$ is a zero-mean Gaussian noise with a covariance matrix $R$, $v_t \sim \mathcal{N}(v_t|0, R)$. The length of the measurement vector is denoted by $N$, $t \in 1:N$. Then, Eqs (9) and (12) form a standard discrete LTI SS model with unknown parameters $\theta$.

**Expectation-maximization algorithm**

The EM algorithm [17] is a standard technique that allows to estimate model parameters from data sets with missing or hidden variables. Its application for the identification of the proposed model given by Eqs. (9)–(12) is now reviewed.

The objective of the EM algorithm is to maximize the log-likelihood of the measured data

$$\log f(Y|P, \theta) = \log \int_T f(T, Y|P, \theta)dT, \quad (13)$$

where $T = \{T_1, ..., T_N\}, P = \{P_1, ..., P_N\}, Y = \{y_1, ..., y_N\}$. In essence, the algorithm is proposed to approximate the correct marginal likelihood approach by iterative maximization of its lower bound. The lower bound $F(\Phi, \theta)$ is derived using any distribution of temperature random variable $\Phi(T)$ [13] as

$$\log \int_T f(T, Y|P, \theta)dT = \log \int_T \Phi(T) \frac{f(T, Y|P, \theta)}{\Phi(T)}dT =$$
$$= \log E_{\Phi(T)} \left[ \frac{f(T, Y|P, \theta)}{\Phi(T)} \right] \geq E_{\Phi(T)} \left[ \log \frac{f(T, Y|P, \theta)}{\Phi(T)} \right] =$$
$$= E_{\Phi(T)}[\log f(T, Y|P, \theta)] - E_{\Phi(T)}[\log \Phi(T)] = F(\Phi, \theta). \quad (14)$$

To find the maximum likelihood (ML) estimate of unknown parameters $\theta$, the EM algorithm seeks to maximize the lower bound $F(\Phi, \theta)$ of the observed data marginal likelihood by alternating so called Expectation step (E-step) and Maximization step (M-step). Intending to identify the proposed LTI SS model, we discuss these steps in the following text in more detail.

**Expectation step – Rauch Tung Striebel Smoother**

In the $r$-th E-step, the lower bound $F(\Phi, \theta^{-1})$ is maximized with respect to the distribution $\Phi$ holding fixed parameter vector $\theta^{-1}$. Assuming that we have some parameter values $\theta^{-1}$ available from the previous M-step, it is possible to show, that the desired distribution $\Phi(T)$ is exactly the conditional distribution of $T$ [13]

$$\Phi(T) = f(T|Y, P, \theta^{-1}). \quad (15)$$

Since for the known values of the parameter vector $\theta^{-1}$, that is, for known values of matrices $A$ and $B$ given by Eqs. (6) and (7), the system defined by Eqs. (9), (12) forms a state space model, the full distribution of all temperatures $\Phi(T)$ can be determined by Rauch Tung Striebel Smoother (RTSS) [18]. The RTSS
is a two-pass algorithm (Algorithm 1) for fixed interval smoothing, where the first pass is the regular forward Kalman filter and the second pass is the backward smoother.

The output of the RTSS is the smoothed posterior Gaussian distribution \( f(T_i | P, \theta^{t-1}, Q^{-1}, R) \). Moreover, the RTSS purveys the smoothed posterior joint distribution

\[
f\left( \begin{bmatrix} T_{t+1} \\ T_t \end{bmatrix} | P, \theta^{t-1}, Q^{-1}, R \right) = N \left( \begin{bmatrix} T_{t+1} \\ T_t \end{bmatrix} \left| \begin{bmatrix} x_{t+1}^N \\ x_t^N \end{bmatrix}, \left( V_{t+1}^N \right) , \left( V_t^N \right) \right) \right),
\]

(16)

where the notation from the Algorithm 1 is used. Note that the temperature random variable is marked by \( T_s \), whereas the smoothed estimate (or the expected value in other words) by \( x_t^N \).

As can be seen, the posterior distributions determined by RTSS are also conditioned by covariance matrices \( Q^{-1} \) and \( R \). These matrices can be either known in many cases and fixed by the user or they can be added to the identification process. In this article, we assume covariance matrix \( R \) of measurement noise to be known and we incorporate the identification of process noise covariance matrix \( Q \) into the estimation procedure. Therefore, \( Q^{-1} \) is available in the \( r \)-th E-step similarly to parameters vector \( \theta^{t-1} \). The estimation of \( Q^{-1} \) is the objective of the previous maximization step (discussed later in the maximization step section).

### Speeding up of E-step using steady-state covariances

The time and memory burdens of RTSS directly depend on the dimension of state space vector \( T_t \) (we assume the dimension of vector \( T_t \) much larger than dimensions of vectors \( P_t \) and \( y_t \)) and on the number of measurements \( N \). Since we are using the model with hundreds or even thousands of compartments (corresponding to the dimension of \( T_t \) and each dimension of covariance matrices \( V_{t+1}^* \)), especially the inversion \( (V_{t+1}^*)^{-1} \) (line 10 in Algorithm 1) in each for-cycle iteration of the backward pass is very time consuming apart from a large matrix multiplication in the remaining parts of RTSS. Besides, storing covariance matrices \( V_t^r \) and \( V_{t+1}^r \) in the forward pass (necessary for backward pass) is strongly memory-consuming as the number of observation \( N \) increases.

#### Algorithm 1. Original RTSS

1. **input** \( A, B, C, Q, R, x_1^t = T_1, P_t, y_t, N \)
2. **for** \( t = 1 : 1 : N - 1 \)
3. \( x_{t+1}^i = Ax_t^i + BP_t \)
4. \( V_t^r = AV_t^rA' + Q \)
5. \( K_t^r = V_t^rC(CV_{t+1}^rC' + R)^{-1} \)
6. \( V_{t+1}^r = V_{t+1}^r - K_t^rCV_{t+1}^r \)
7. \( x_{t+1}^i = x_{t+1}^i + K_t^r(y_{t+1} - Cx_{t+1}^i) \)
8. **end for**
9. **for** \( t = N - 1 : -1 : 1 \)
10. \( J_t = V_t^rA'(V_t^r)^{-1} \)
11. \( V_t^N = J_t + J_tV_{t+1}^rJ_t' \)
12. \( J_{t+1}^N = V_{t+1}^N J_t \)
13. \( x_t^N = x_t^i + J_t(x_{t+1}^N - Ax_t^i - BP_t) \)
14. **end for**

#### Algorithm 2. RTSS with steady covariances

1. **input** \( A, B, C, Q, R, x_1^t = T_1, P_t, y_t, N \)
2. compute Riccati equation for \( V_S^- \):
   \( V_S^- = AV_S^-A' - AV_S^-(CV_S^-C' + R)^{-1}CV_S^-A' + Q \)
3. \( K_S = V_S^-C(CV_S^-C' + R)^{-1} \)
4. \( V_S^- = (I_n - K Sv)C V_S^- \)
5. **for** \( t = 1 : 1 : N - 1 \)
6. \( x_{t+1}^i = Ax_t^i + BP_t \)
7. \( x_{t+1}^i = x_{t+1}^i + K_S(y_{t+1} - Cx_{t+1}^i) \)
8. **end for**
9. \( J_S = V_S^- A'(V_S^-)^{-1} \)
10. compute Lyapunov equation for \( V_S^- \):
    \( V_S^- = J_S V_S^- J_S' + (V_S^- - J_s V_S^- J_S') \)
11. **for** \( t = N - 1 : -1 : 1 \)
12. \( x_t^N = x_t^i + J_s(x_{t+1}^N - Ax_t^i - BP_t) \)
13. **end for**

For these reasons, we suggest to use steady covariance matrices in the RTSS which significantly reduces the computational requirements [19]. The implementation of the RTSS with steady covariances is shown in Algorithm 2.

Riccati equation on line 2 and Lyapunov equation on line 10 of Algorithm 2 can be evaluated by direct method or solvers (e.g. idare and dllyap Matlab's in-build function) or iteratively using e.g. Newton techniques. Specifically in our case, we employed the Modified Newton method for discrete-time algebraic Riccati equations [20] and Matlab’s function dllyap for solving discrete-time Lyapunov equations.

For an effective implementation, it is sufficient to collect only few statistics of relatively small size (square of
the number of compartments) for the following M-step. The necessary statistics utilized in the M-step and obtained from RTSS using steady covariance matrices (Algorithm 2) are

\[
\begin{align*}
XX' &\equiv (N - 1)V_N^X + \sum_{t=1}^{N-1} x_t^N (x^N_t)' \\
ZZ' &\equiv (N - 1)V_N^Z + \sum_{t=1}^{N-1} x_{t+1}^N (x^N_{t+1})' \\
XZ' &\equiv (N - 1)J_5(V_N^Z)' + \sum_{t=1}^{N-1} x_t^N (x_{t+1}^N)' \\
XU' &\equiv \sum_{t=1}^{N-1} x_t^N p_t' \\
ZU' &\equiv \sum_{t=1}^{N-1} x_{t+1}^N p_t' \\
UU' &\equiv \sum_{t=1}^{N-1} p_t p_t'
\end{align*}
\]  

(17)

For comparison, the form of statistics derived by the original full RTSS (Algorithm 1) and utilisable for the M-step can be found in [14].

**Maximization step – maximum likelihood estimate**

In the \( r \)-th M-step, the lower bound \( \mathcal{F}(\Phi', \theta) \) is maximized with respect to the unknown model parameters \( \theta \) and noise covariance matrix \( Q \) holding distribution \( \Phi'(T) \) fixed. The distribution \( \Phi'(T) \) is the smoothed posterior distribution given by Eq. (16) evaluated in the previous E-step of the EM algorithm. Then, the new updates of parameters \( \theta' \) and noise covariance matrix \( Q' \) are given by

\[
\begin{align*}
\theta', Q' = \arg \max_{\theta, Q} \sum_{t=1}^{N-1} E_{\Phi'(T)} \left\{ \ln |Q|^{-1} \right\} + \\
&\quad - \left( \Delta T_t - M_t \theta \right)' Q^{-1} (\Delta T_t - M_t \theta) + \\
&\quad - (y_t - C T_t)' R^{-1} (y_t - C T_t)
\end{align*}
\]

(18)

where \( \Delta T_t = T_{t+1} - T_t \), \( E_{\Phi'(T)} (\cdot) \) stands for the expected value with respect to the distribution \( \Phi'(T) \), and \( |\cdot| \) denotes the determinant of the particular matrix.

It is easy to show, that the ML estimator of the function given by Eq. (18) is of the form

\[
\begin{align*}
\theta' &= \left( \sum_{t=1}^{N-1} E_{\Phi'(T)} \left\{ M_t (Q')^{-1} M_t' \right\} \right)^{-1} \\
&\quad \left( \sum_{t=1}^{N-1} E_{\Phi'(T)} \left\{ M_t (Q')^{-1} \Delta T_t \right\} \right)^{-1}
\end{align*}
\]

(19)

\[
Q'_\text{full} = \frac{1}{N - 1} \sum_{t=1}^{N-1} E_{\Phi'(T)} \left\{ \Delta T_t \Delta T_t' - \Delta T_t (M_t \theta')' \right\} \\
&\quad - M_t \theta' (\Delta T_t)' + M_t \theta' (M_t \theta')
\]

(20)

where the individual expected terms can be expressed using only statistics obtained by RTSS in the previous \( r \)-th E-step and listed in Eq. (17). These terms are given in Appendix in detail.

The computational problem lies in the mutual cross dependency of \( \theta' \) on \( Q' \) and vice versa. This obstacle is connected with the structure of desired covariance matrix \( Q \) and may vanish in some particular cases. Moreover, the number of elements in the covariance matrix \( Q \) is much higher than the dimension of parameters vector \( \theta \) and thus a regularization of the problem (a shrinkage of covariance matrix estimation) is greatly desirable. Therefore, we investigate carefully the structure of the covariance matrix \( Q \) now and discuss possible solutions.

**Structure of process noise covariance matrix**

1. An easy approach is to assume the covariance matrix \( Q \) in the diagonal form with a constant on the diagonal, \( Q = q I_n \). In such case, Eq. (19) can be simplified, since the term \( (q I_n)^{-1} \) is possible to completely eliminate from the expression for \( \theta' \). Thus the evaluation of \( \theta' \) is not dependent on the constrained covariance matrix \( Q \) and can be directly executed. The formulation of the M-step is then similar to the ordinary least squares method but with proper consideration of expected values. The formula for computation of the covariance matrix \( q^2 I_n \), or scalar value \( q^2 \) actually, reads

\[
q^2 = \frac{1}{n} \text{Tr}(Q'_\text{full}).
\]

(21)

This case together with specific form of Eqs. (19) and (20) is described by authors in ref. [14].

2. There exist several other constraints on the covariance matrix \( Q \), where the direct derivation of the estimator is feasible. One representative of this group is non-homogeneous diagonal covariance matrix (compare with the weighted least squares method), \( Q = \text{diag}(q) \), where \( q = [q_1, ..., q_n]' \). In such case, the form of the ML estimators of \( \theta' \) and \( Q'_\text{diag} \) remain as in Eqs. (19) and (20), only with consideration that non-diagonal elements of \( Q' \) are zeros,

\[
q^2 = \text{diag}(Q'_\text{full}).
\]

(22)
The mutual cross dependency of $\theta^r$ and $Q^r_{\text{diag}}$ can be overcome by employing the previous estimation of the covariance matrix $Q^r_{\text{diag}}$ in Eq. (19) (i.e. utilizing the ML estimator of $Q$ from the $r-1$-th M-step of the EM algorithm for new update of $\theta^r$). Thereafter, the new update of $\theta^r$ can be used for evaluation of Eq. (20).

3. A constraint on the covariance matrix $Q$ can be formulated in the “infeasible” way, where the estimator $Q^r_{\text{LL}^{\prime}+\beta I}$ cannot be expressed analytically in the explicit form. The proper approach is to design an optimization task using, for example, method of Lagrange multipliers as the way how to cope with constraints on the covariance matrix [21]. The other approach is to use an approximate solution. We suggest to declare the nearest (in the sense of Frobenius norm) constrained covariance matrix to the full ML estimator given by Eq. (20) as the approximate constrained estimator

$$Q^r_{\text{LL}^{\prime}+\beta I} = \arg \min_{Q^r_{\text{LL}^{\prime}+\beta I}} \left\{ ||Q^r_{\text{full}} - Q^r_{\text{LL}^{\prime}+\beta I}||_F \right\}.$$  

(23)

The specific “infeasible” constraint on the covariance matrix, which we investigate in this
contribution, is of the form

\[ Q'_{sLL} + \beta I_n = x'LL + \beta' I_n, \]  \tag{24}

where \( x', \beta' > 0 \) are estimated optimal parameters and matrix \( L \in \mathbb{R}^{n \times n} \) is a predefined fixed constant matrix. The approximate solution given by Eq. (23) is then easy to write using the least squares method as

\[
\begin{bmatrix}
  x' \\
  \beta'
\end{bmatrix}
= \left( F_Q' F_Q \right)^{-1} F_Q' \text{vec}(Q'_\text{full}),
\]

where matrix \( F_Q = \left[ \text{vec}(LL') \quad \text{vec}(I_n) \right] \) and \( \text{vec}(\cdot) \) is operator of vectorization stacking the columns of the matrix on top of one another.

These three various structures of the covariance matrix, the convergence properties and their influence on the quality of results are analyzed in the following section in detail.

**Verification of the proposed method on synthetic data**

The performance of the proposed identification method of mesh-based compartment models is tested on generated data. For demonstration purposes, we use a mesh-based compartment model inspired by the physical properties of a real insulated-gate bipolar transistor (IGBT) three phase power module SK20 DGDL 065 ET (Figure 1b).

In a real experiment, this IGBT module is equipped by a negative temperature coefficient (NTC) thermistor, that gives information about a baseplate temperature. A direct measurement of temperatures of dies (transistors and diodes) is however difficulty realizable. The reason is that the module is encapsulated (which makes thermal camera impossible to use) and the switching frequency of the transistors can be too high (e.g. 10^4 Hz). To overcome these issues, a measurement of temperature sensitive electrical parameters can be used to obtain a data-set. For example, collector-emitter voltages of IGBTs have proven their applicability for this purpose [22]. The internal heat sources of dies (i.e. power losses \( P_i \) in IGBTs and diodes) can be determined by conduction losses and switching losses [22]. The ambient temperature around the device can be measured in any arbitrary way (e.g. using another external NTC thermistor).

**Discretization and parametrization of models**

Starting with the compartment model structure, the discretization level of the tested mesh-based model is selected as follows: four layers of compartments are used in the Z-axis (see a typical vertical sandwich structure of power module in Figure 2a) and the basic grid of 17 × 10 compartments is used for each layer in the X-Y plane. Using this level of discretization, the size of basic compartments corresponds to covering the surface of size cca 3 × 3 mm of the real power module. The total number of compartments of the model is 817, specifically the first upper layer contains 117 compartments (caused by neglecting of surface, where no transistor, diode, or rectifier exists, and on the contrary, refining some critical areas of the first layer – Figure 2b), the second layer contains 359 compartments (caused by refining), the third and the fourth 170 (only basic grid used) and the last remaining compartment is employed for the ambient temperature modeling. The dynamics of the last compartment (representing the ambient temperature) is dependent only on the previous value of the ambient temperature.

Such discretized compartment model is linked by two different parametrization specified in Table 1:

1. **Weakly shared parametrization** employing 12 parameters \( k_i \), that is, \( n_k = 12 \),
2. **Strongly shared parametrization** using only 5 parameters \( k_i \), that is, \( n_k = 5 \), for the description of state matrix \( A \).

In both case, there is another parameter connected with power losses \( P_{i,t} \) in compartments representing IGBTs of the real module \( (z \in \mathbb{R}^1) \) and parameters describing the estimator of state noise covariance matrix \( Q \).

For identification purposes, the values of temperatures in compartments corresponding to selected dies (IGBTs) in the real power module (specifically 40 compartments out of all 117 compartments in the first layer), the temperature of one selected compartment in layer 4 representing a temperature sensor in the real power module and the ambient temperature represented by the last compartment are observed according to observation model given by Eq. (12). The input vector \( P_{i,t} \) is also assumed to be known. The length of time-step \( \Delta t \) is assumed to be 0.01 s.

The applicability of the proposed method and described models is verified on two test cases.

**Test case 1: Convergence of parameters**

First we test convergence properties of the proposed method, that is, the ability of the simplified EM (with steady RTSS) to converge to the true parameters. In
In this test case, the forward model generating synthetic data is identical to the identified model. In other words, we know exactly the structure of the model (matrices $I$, $J$, $A$, $B$, $C$) and the true values of all parameters which we want to identify. Moreover, the process noise is neglected for better comparison.

The convergence of parameters $k$ during identification process is depicted in Figure 3. It can be seen that in the case of strongly shared parametrization, all parameters converge to their true values (marked by crosses in the graph). In the case of weakly shared parametrization, the EM algorithm converges as well, but not to all true values of parameters $k$. It can be caused by a lack of information about temperatures in unobserved compartments (e.g. compartments representing diodes or rectifiers in the real power module). Despite the EM algorithm not converging to the true parameters in the weakly shared parametric model, the trend of temperature predicted by the identified model stays valid in some cases as can be seen in Figure 4. Note that the temperature values are simulated using identified model from initial conditions ($t=0$) on a long horizon taking 18,000 time-steps, that is, 180 s, employing only information about power losses $P_i$. Nevertheless, measured temperatures are explained by the identified model still relatively correctly. This conclusion is probably valid if no specific temperature fluctuation exists in unobserved compartments connected with the remaining parts of the model with poorly identified connections (e.g. a connection between rectifiers and Cu layer or a connection between diodes and Cu layer).

The error in prediction of temperature depicted in Figure 4 is not greater than 0.33% (maximum error of 0.035°C for temperature trend, where the difference between ambient temperature and maximum temperature is more than 9°C) for the synthetic model on a long-term prediction. Note, that the same holds not only for the measured compartment but for all compartments in the model as well. The increased errors at the end of prediction ($t=180s$) are probably caused by a negligible underestimate of speed of module cooling.

Test case 2: Temperature prediction in dependency on covariance matrix structure

In this subsection, we investigate the convergence properties of the EM algorithm for the identification of the proposed mesh-based compartment thermal model in dependency on the structure’s constraint of the process noise covariance matrix $Q$.

For the analysis of covariance matrix estimation, the weakly shared parametrization of the model is employed to generate data (forward model), while during the identification process strongly shared...
parametrization is assumed. It means that the identified model is thus not identical to the ground truth. Although the structure (mesh-based discretization) of compartments is still the same, the parametrization of the forward model is much finer and therefore the forward model complexity is higher than the one of an identified model with strongly shared parametrization. In other words, using various parametrizations for generating data and for identifying model causes that we do not know the true form of auxiliary matrices $A$, $B$ and $C$ in Eqs. (6) and (7). Moreover, data are generated with process noise

$$w_t \sim \mathcal{N}(w_t|0, \sigma^2AA^T),$$

(26)

where $\sigma^2$ is set to value $10^{-4}$ and matrix $A$ is defined by Eq. (6).

We investigate three kinds of parametrization of the covariance matrix estimator similarly as it is introduced in the previous section. For covariance structure’s constraint $Q_{\alpha LL'} + \beta I = x'LL' + \beta'I_n$, elements $l_{ij}$ of matrix $L \in \mathbb{R}^{n \times n}$ are defined as

$$l_{ij} = \begin{cases} 1 & \text{if } (I_{\text{diag}}(C_0), I_{\text{diag}}(C_1))^T_{ij} \text{ is NOT 0 and } j < n \ i, j = 1 : n \\ 0 & \text{otherwise} \end{cases}$$

where $1$ is a vector of all ones with the same dimension as vector $k$ and where notation from Eq. (6) is used. For a better illustration, structures (i.e. non zero elements) of matrices $A$ and $LL'$ are depicted in Figure 5.

The convergence of parameters describing constrained covariance matrix $Q$ is depicted in Figure 6. The convergence of values of parameters vector $k$ dependent on the choice of regularization of process noise covariance estimator is depicted in Figure 7. It can be seen, that models using constraints on covariance matrix $Q$ in forms $Q = qI_n$ and $Q = \alpha LL' + \beta I_n$ give similar results and both of these forms are

![Figure 5](image_url)  
**Figure 5.** Illustration of matrix structure (the black color corresponds to not zero element, the white color corresponds to zero element).

![Figure 6](image_url)  
**Figure 6.** Convergence of process noise covariance matrix estimation.
sufficiently regularized. Moreover with knowledge of true covariance matrix defined by Eq. (26) and being aware of matrix \(A\) is diagonally dominant, we can claim, that these two approaches converge to the plausible values of covariance parameters. From this point of view, the constraint \(Q = \text{diag}(q)\) seems to be overparameterized, since the convergence of selected elements to the value \(10^{-2}\), that is, staying at the initial value, is not well-founded. Figure 8 can explain this phenomenon. Diagonal elements of covariance matrix taking higher values of variance \(10^{-2}\) are elements just corresponding to unobserved compartments. Elements converging to the true value of variance \(10^{-4}\) are elements corresponding to the observed compartments. Thus due to lack of information about unobserved compartments, we are not able to identify the variance correctly using constraint \(Q = \text{diag}(q)\).

The long-term predictions of 18,000 time steps, that is, till 180 s, using models identified with
constrained covariance estimators \( Q = qI_n \) and \( Q = \alpha LL' + \beta I_n \) respectively are depicted on the top rows of Figure 9. Similar to previous subsection, inputs of the prediction are the initial values of temperatures and vector \( P_{1:N} \) only. On the contrary, we do not know the true parameterization during the identification process (the parameterization used for identification is different from the one used for data generation). Nevertheless, the errors of prediction (bottom rows of Figure 9) are always smaller than 1 °C for temperature trends, where the difference between ambient temperature and maximum temperature is more than 10 °C. The majority of error magnitude is probably caused by additional dynamic white noise in synthetic data. The quality of temperature prediction is acceptable using both tested types of constrained covariance estimator \( (qI_n \text{ and } \alpha LL' + \beta I_n) \). The compartment model using strongly shared parametrization can explain and predict data generated by the model with weakly shared parameters.

**Conclusions**

Mesh-based compartment thermal model and its identification procedure using the Expectation-Maximization algorithm was studied. We proposed two extensions: (i) the use of the steady-state covariance matrix in the E-step of the EM algorithm yields significant speedup allowing to evaluate the algorithm even in the size of our problem, and (ii) estimation of the process noise covariance matrix with constrained structure.

Preliminary tests on synthetic data indicated the applicability of the proposed thermal model and the identification approach. The selection of parametrization of the compartments has a strong impact on the possibility to identify the model from incomplete temperature data. The model with coarse parametrization was able to predict data generated by a more detailed model. However, the validation of real measured data is needed and ought to be carried out by authors in the near future.

**Disclosure statement**

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Appendix. Expected terms for M-step

Expected terms necessary for evaluation of Eqs. (19) and (20) expressed using only statistics listed in Eq. (17):

\[
\sum_{i=1}^{N-1} E_{\Phi(T)} \{ \Delta T_i \Delta T'_i \} = \frac{1}{\Delta t^2} (XX' - XX'') - (XZ')' + ZZ'
\]

\[
\sum_{i=1}^{N-1} E_{\Phi(T)} \{ M'_i Q^{-1} M_i \} = \begin{bmatrix}
C'((J'Q^{-1}J)'(J'XX')(J'))C - C'((J'Q^{-1}B)'(J'XU'))A \\
-A'(B'Q^{-1}J)'((XU')'(J'))C \\
A'(B'Q^{-1}B'UU')A
\end{bmatrix}
\]

\[
\sum_{i=1}^{N-1} E_{\Phi(T)} \{ M'_i Q^{-1} \Delta T_i \} = \Delta t^{-1} \begin{bmatrix}
-C^T \text{diag}(J^T(XZ' - XX')(Q^{-1})') \\
A^T \text{diag}((ZU' - XU')(Q^{-1})')
\end{bmatrix}
\]

\[
\sum_{i=1}^{N-1} E_{\Phi(T)} \{ M_i \theta \theta'_i M'_i \} = \begin{bmatrix}
kk' \\
kz' \\
zk' \\
zz'
\end{bmatrix}
\]

where symbol \( \circ \) stands for Hadamard product, that is, element-wise multiplication, and operator \( \text{diag}(\cdot) \) applied on a vector creates diagonal matrix with the vector values on the main diagonal and operator \( \text{diag}(\cdot) \) applied on a matrix extracts the main diagonal and the rest of elements replaces with zeros.