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# Integration of multi-objective reliability-based design optimization into thermal energy management: Application on phase change material-based heat sinks

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#### 11 Abstract

Phase change material-based heat sinks are widely used in several industrial applications such as in the field of industrial automation and mechatronics. Nowadays, several researchers aim to obtain an optimal design of these systems in order to ameliorate its performances. Nevertheless, uncertainties are not considered for the majority of these studies. Furthermore, it has been confirmed that deterministic multi-objective optimization (DMOO) may lead to an unreliable design. In this study, a new methodology that leads to perform the Multi-Objective Reliability-Based Design Optimization (MORBDO) for thermal management of a passive cooling system is proposed. It consists in coupling the Finite Element Model (FEM), MORBDO procedures and surrogate approaches. Kriging predictor is used to construct metamodels and then validated using Cross-Validation (CV) and error predictions. A numerical investigation is carried out to study the different DMOO and MORBDO approaches. In this study, a 3D PCM-based round pin-fin heat sink is detailed. The aim of this problem is to minimize two objective functions: the cost (total volume V) and the final cooling time  $t_f$  by considering both thermal and physical constraints. For this purpose, geometrical uncertain parameters are considered such as length L, height Hand  $\phi$  pin diameter of the heat sink. This study leads to develop a well-distributed reliable Pareto solutions by combining the Robust Hybrid Method (RHM) and the Constrained Nondominated Sorting Genetic Algorithm (C-NSGA-II). Then, the efficiency of the proposed MORBDO-RHM approach for PCM-based heat sink is verified.

*Keywords:* Thermal energy management; PCM-based heat sinks; Kriging approach;
Pareto optimal front; C-NSGA-II; MORBDO-RHM.

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#### Nomenclature

- Abbreviations ANN Artificial neural networks Cov Covariance  $\mathrm{CV}$ Cross-validation DDO Deterministic design optimization DOE Design of experiments FES Finite element simulation HDS Hybrid design space Hybrid method HM HS Heat sink HSU Heat storage unit LHS Latin hypercube sampling MAE Maximum absolute error MCS Monte Carlo simulation MHM Modified hybrid method MSE Mean squares error PCM Phase change material QRS Quadratic response surface RHM Robust hybrid method RME Relative mean error RMSE Root mean squared error RSM Response surface methodology SPTs Set point temperatures
- TM Thermal management

#### Symbols

- $\hat{y}(\mathbf{x})$  The predictor of the model **F** Model matrix
- $\mathbf{f}(\mathbf{x})$  Vector of regression basis function
- **K** Matrix of correlation functions
- $\mathbf{r}(\mathbf{x})$  Vector of correlation functions
- **x** Design variables vector
- $\mathbf{x}_s$  Set of samples
- $\mathbf{y}_s$  Responses of the sample set
- $A_m$  Mushy region
- $C_p$  Specific heat of fusion
- f(x) Objective function
- g Gravitational acceleration
- $G_i(x, y)$  Performance functions
- H Height of heat sink
- H Total enthalpy of PCM
- $h_s$  Specific enthalpy
- $h_j(x)$  Deterministic constraints
- $h_{s,ref}$  Referential enthalpy
- L lenght of heat sink

- $L_f$  Laten heat of fusion
- *lb* Lower bound
- m Dimensional problem
- n Number of design points
- P Pressure
- *p* Number of kriging coefficients
- $P_i^T$  Target failure probability
- Pr[.] Probability operator
- S Source term
- $S_g$  Global safety factor
- $S_h$  Energy source term
- T Temperature
- t Time
- $T_l$  Liquid temperature
- $T_s$  Solid temperature
- $T_{amb}$  Ambient temperature
- $T_{max}$  Maximum temperature
- $T_{ref}$  Referential temperature
- RBDO Reliability-based design optimization u, v, w Velocity components in x, y and z RHM Robust hybrid method directions
  - ub Upper bound
  - V Volume
  - x Deterministic design variables
  - $x^*$  Optimal point
  - y Random variables
  - $y^*$  Failure point
  - $Z(\mathbf{x})$  Stochastic process

#### Greek symbols

- $\alpha_w$  Thermal expansion coefficient
- $\beta_t$  Target reliability level
- $\beta$  Vector of regression coefficients
- $oldsymbol{ heta}$  Vector of the correlation function parameters
- $\Delta H$  Latent heat
- $\lambda$  Thermal conductivity
- $\mu$  Dynamic viscosity
- $\phi$  Pin fin diameter
- $\rho$  Density
- $\sigma^2$  Variance of the stochastic model
- $\varepsilon$  Normal random error
- $\xi$  Liquid fraction of PCM
- $d_{\beta}(x,y)$  Distance between the optimal and design points
- $L(\boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta})$  Likelihood function

#### 14 1. Introduction

In recent years, thermal management in the field of mechatronics has become an important 15 factor for researchers in electronic packages design. In this context, electronic components 16 are getting ever-smaller with more design features in size due to the development of modern 17 technologies of electronic equipment. In fact, a high power and performance dissipated by the 18 electronic component can lead, not only to reduce their lifetime, but also to its immediate 19 failure. To this end, an efficient and novel cooling technology is needed to overcome the 20 overheating phenomenon and to avoid the deterioration of the device. Furthermore, the 21 choice of such a cooling system is based on many factors such as material cost, heat 22 dissipation rate, maintenance and space [1]. 23

In the literature, several technics of passive cooling are developed to ensure the smooth 25 operation of electronic devices using PCM-based heat sinks [2–4]. However, standard cooling 26 methods would not be sufficient. Therefore, to improve the performance of passive cooling 27 electronic device technologies, many studies are developed and some of them are based on 28 Phase Change Materials (PCM) [5, 6]. An experimental study is investigated in [7], to 29 improve and ensure the reliability and functionality of the installed features. A parametric 30 study leads to improve the thermal performance of PCM-based heat sinks by changing the 31 PCM volume fraction and pin thickness at various heat fluxes. A numerical and experimental 32 studies are presented by Thomas et al. [8] in order to evaluate the thermal performance 33 of a PCM-based heat sink using n-Eicosane at many constant input power levels. In this 34 study, the effect of natural convection has been discussed. Nowadays, PCM-based heat sink 35 optimization presents a huge challenge for developers. A numerical study is presented in 36 [9] which an optimal model is proposed in a passive cooling application using PCM-based 37 plate fin matrix for charging and discharging phases. The main purpose of this study is 38 to improve the thermal performance of the heat storage unit (HSU) by changing the input 39 power level, PCM material, PCM volume fraction and heat sink geometry. 40

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Integration of reliability methods in the optimization algorithm presents a new challenge 42 in mechatronics problem. The Reliability-Based Design Optimization (RBDO) aims then 43 to find the best compromise between cost and safety [10]. In this context, an efficient 44 RBDO study for PCM-based heat-sink is presented in [11, 12]. These studies lead to 45 determine an optimal and reliable design of a cooling system where two-dimensional Finite 46 Element Simulations (FES) are performed. These studies prove that, Deterministic Design 47 Optimization (DDO) approach leads to determine an optimal solution, but it represents a 48 missing level of confidence and a significant risk of failure, due to non-considering uncertainties. 49 Hence, to overcome this issue, it is recommended to integrate, during the optimization 50 process, the reliability analysis. Using the classical RBDO approach and, to obtain optimal 51 results, coupling of physical space and normalized space is needed. Which means a high 52 computation time for such an optimization problem [13-15]. In order to overcome this 53 issue, Kharmanda et al. [16] proposed a novel RBDO methodology called Hybrid reliability-54 optimization Method (HM) where its efficiency is presented and discussed. This method 55

efficiently reduces the computing time comparing with the classical approach. However, the 56 optimization problem becomes more complex and then it can lead to an infeasible solution. 57 In order to solve the difficulties of the classical one, Yaich et al. [17] proposed a novel 58 methodology called Robust Hybrid Method (RHM). The efficiency of this method has been 59 verified only on static and some specific nonlinear cases such as fatigue damage [17], coupled 60 acoustic-structural system [18, 19] and shape memory alloy micro-pump [20]. In addition, 61 in [21, 22], the authors aim to develop a new approach applied to an offshore wind turbine, 62 which it called Modified Hybrid Method (MHM) in order to avoid issues of other RBDO 63 methods. 64

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Otherwise, such an RBDO method needs a large number of evaluations. In the case 66 of PCM-based heat sink, a non-linear transient 3D model analysis is expensive in term of 67 computational time. To this end, surrogate models are then recommended as an alternative 68 to define original models' approximations. It consists in constructing mathematical models, 69 to determine the link between inputs and outputs of a specified system [23, 24]. Recent 70 approaches are developed in the field of design optimization [25] and probabilistic analysis 71 [26, 27], using surrogate models. Response Surface Methodology (RSM), Artificial Neural 72 Networks (ANN), Radial Basis Function (RBF) method and Kriging method are the most 73 popular surrogate modelling used recently. In [28], metamodels are applied in the field of 74 mechanical manufacturing for the purpose to enhance the computational efficiency. Also, 75 Fatma et al. [29] studied many metamodel techniques for a NiTi micro actuator. A Monte 76 Carlo Simulations (MCS) are then performed in order to prove its efficiency, using the 77 constructed metamodel. These studies demonstrate that kriging method presents more 78 efficiently and gives the best approximation of the original model. Recently, Dammak 79 and El Hami [30, 31] studied a numerical application of a cementless hip prosthesis and 80 a coupled acoustic-structural system. These studies are based on coupling multi-objective 81 optimization problem (MORBDO) with surrogate models. It has been demonstrated that 82 the studied problem using Kriging approach has the ability to generate a well-distributed 83 reliable Pareto solution. 84

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The aim of this paper is to propose a new methodology that leads to determine an 86 optimal design of a PCM-based round pin-fin heat sink with a required reliability level. Both 87 deterministic and multi-objective reliability optimization are presented. For this purpose, 88 the Constrained Non-dominated Sorting Genetic Algorithm (C-NSGA-II) is coupled with 89 HM and RHM approaches respectively. DMOO and MORBDO models are next coupled 90 with surrogate models which considerably reduced the computing time. To present the 91 advantages of the proposed method, a detailed numerical application of PCM-based round 92 pin-fin heat sink is investigated. Results show the improvement of the resulting optimal 93 solution using MORBDO-RHM coupled with Kriging surrogate model, and its capability to 94 develop a well-distributed reliable Pareto solutions with a required reliability level. 95

#### <sup>96</sup> 2. Heat transfer and PCM behavior: Mathematical model

The heat generated by the input power is transferred to all surfaces of heat sink by conduction. In fact, PCM allows energy to be absorbed by changing from the solid state to the liquid state. The dissipated energy by the PCM causes its transformation from liquid to solid state. It is supposed that thermo-physical properties of the PCM are independent of temperature and only the conduction equation is taken into consideration for the aluminum section as presented in equation (1):

#### • Energy conservation:

$$\rho C_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z}\right) = \lambda \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) + S_h \tag{1}$$

Where,  $\rho$ ,  $C_p$  and  $\lambda$  are respectively the density, specific heat of fusion and thermal conductivity of aluminum.

The latent heat storage is presented by the energy source term  $S_h$  due to melting and it is presented as follow:

$$S_h = -\frac{\partial}{\partial t} (\rho \Delta H) \tag{2}$$

The total enthalpy of PCM can be calculated as the sum of the latent heat  $\Delta H$  and the specific enthalpy  $h_s$ :

$$H = \Delta H + h_s \tag{3}$$

As mentioned in equation (3), the specific enthalpy  $h_s$  can be defined as follows:

$$h_s = \int_{T_{ref}}^T C_p \, dT + h_{s,ref} \tag{4}$$

Additionally, the latent heat  $\Delta H$  is calculated as follows:

$$\Delta H = \xi L_f \tag{5}$$

As mentioned in equation (5),  $L_f$  and  $\xi$  refer to latent heat of fusion and liquid fraction of PCM respectively. In fact, the parameter  $\xi$  presents the liquid quantity relative to the total volume of PCM and can be defined as below:

$$\xi = \begin{cases} 0 & \text{if } T \leq T_s \\ \frac{T - T_s}{T_l - T_s} & \text{if } T_s < T < T_l \\ 1 & \text{if } T \geq T_l \end{cases}$$
(6)

According to equations (3) to (5), the total enthalpy of PCM H can be calculated by:

$$H = \int_{T_{ref}}^{T} C_p \, dT + h_{s,ref} + \xi L_f \tag{7}$$

<sup>116</sup> The governing equations of mass and momentum conservation are defined as follow:

#### • Mass conservation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0$$
(8)

Note that u, v and w present velocity components in x, y and z directions, respectively. Furthermore, it is considered that the PCM in the liquid phase is an incompressible Newtonian fluid the fact that the density of the PCM is considered unchangeable for any fluid particle  $\left(\frac{\partial \rho}{\partial t}=0\right)$ . So, the previous equation is reduced to:

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$
(9)

#### • Momentum conservation:

$$\rho(\frac{\partial u}{\partial t} + \frac{\partial(u^2)}{\partial x} + \frac{\partial(uv)}{\partial y} + \frac{\partial(uw)}{\partial z}) = -\frac{\partial P}{\partial x} + \mu[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}] + S.u$$
(10)

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$$\rho(\frac{\partial v}{\partial t} + \frac{\partial(uv)}{\partial x} + \frac{\partial(v^2)}{\partial y} + \frac{\partial(vw)}{\partial z}) = -\frac{\partial P}{\partial y} + \mu[\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}] + S.v$$
(11)

$$\rho(\frac{\partial w}{\partial t} + \frac{\partial(uw)}{\partial x} + \frac{\partial(vw)}{\partial y} + \frac{\partial(w^2)}{\partial z}) = -\frac{\partial P}{\partial z} + \mu[\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}] - \rho g \alpha_w (T - T_s) + S.w$$
(12)

Where,  $\mu$  presents the dynamic viscosity,  $\alpha_w$  is the thermal expansion coefficient, P is the pressure and g is the gravitational acceleration. Due to the gravitational acceleration direction (negative z-direction), the Boussinesq approximation is determined by adding  $\rho g \alpha_w (T - T_s)$  term as presented in equation (12).

129 The following equation presents the source term S:

$$S = \frac{(1-\xi)^2}{(\xi^3 + \varepsilon)} A_m \tag{13}$$

To avoid division by zero in equation (13), a small positive parameter  $\varepsilon$  is used ( $\varepsilon = 10^{-10}$ ). The constant  $A_m$  presents the consecutive number in the mushy region and it is recommended to take  $A_m = 10^5$  in several studies [32–34].

Mathematical models in this study can be founded in Wang and Yang [32, 33], Shatikian et al. [34] and Nayak et al. [35]. They evaluated the performance of thermal management based on PCM in internal fins.

#### 136 3. Surrogate models

#### 137 3.1. Description of surrogate modeling process

Recently, metamodels are widely used in current engineering analysis in order to reduce the calculation cost. Surrogate models aim to construct the mathematical approximations to estimate system behaviour and to define the relationship between inputs and outputs of
the system [24]. The most used surrogate modelling methods are Radial Basis Function
(RBF) method, Response Surface Methodology (RSM), Artificial Neural Networks (ANN)
and Kriging method [23, 24]. Several researches [28-30] demonstrate that the Kriging
approach leads to a best approximation to a finite element analysis particularly for nonlinear problems. In this study, Kriging metamodel method is used to evaluate the outputs
of PCM-based heat sink in order to improve the computational efficiency.

#### 147

In the beginning, let us consider a *n*-dimensional problem. Table 1 presents the description of all parameters used in this problem.

Table 1:	Description	of all	used	parameters

Notation	Designation	Dimension	Vector
x	design variable vector	$1 \times n$	$x_1, x_2, \ldots, x_n$
$x_s$	set of samples	$n \times 1$	$x_s = \{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}^T$
$y_s$	outputs responses of the samples set	$n \times 1$	$y_s = \{y^{(1)}, y^{(2)}, \dots, y^{(n)}\}^T = \{y^{(1)}, y^{(2)}, \dots, y^{(n)}\}^T$

The sampled data set is indicated by the pair  $(x_s, y_s)$  in the vector space. The main aim of surrogate modeling is to build a meta-model in order to predict the output for any point x, thus, to estimate y(x) based on the pair  $(x_s, y_s)$ .



Figure 1: Surrogate modeling algorithm flowchart

The flowchart of the surrogate model process is presented in figure 1. Its implementation is a multi-step process. Forrester et al. [23] present some used techniques to solve this problem. First, Design Of Experiments (DOE) are applied by the surrogate modelling approach. Particulary, Latin Hypercube Sampling (LHS) [36] is used in order to repeat sampling in the design space. Kriging approach is then applied to represent the sampled data. Accordingly, surrogate model can replace the original analysis code during the RBDO procedure.

#### 160 3.2. Kriging approach

Nowadays, Kriging method is widely used as surrogate approach. In fact, it is characterized
by its high quality of approximation with a required robustness, compared to other methods.
Kriging method, also called Gaussian process modelling [37], consists of two nested functions:

a deterministic function K(x) and a Gaussian random function Z(x). 164

It can be written as follow: 165

$$y(x) = K(x) + Z(x) \tag{14}$$

K(x) is usually determined as : 166

$$K(x) = \sum_{i=1}^{p-1} \boldsymbol{\beta}_i \boldsymbol{f}_i(x) \tag{15}$$

Here,  $\boldsymbol{\beta} = [\beta_0, \beta_1, \dots, \beta_{p-1}]^T$  and  $f(x) = [f_0(x), f_1(x), \dots, f_{p-1}(x)]^T$  present the regression 167 coefficients vector and regression basis function vector respectively. 168

Z(x) is a zero-mean stochastic process with a non-zero covariance given by: 169

$$Cov(Z(\mathbf{x}) - Z(\mathbf{x}')) = \sigma^2 R(\mathbf{x}, \mathbf{x}')$$
(16)

We note that  $\sigma^2$  is the variance of Z(x), x and x' are the estimated sampling points in 170 the design space and  $R(\mathbf{x}, \mathbf{x}')$  is the correlation function. It is an *m*-dimensional correlation 171 functions constructed from *one*-dimensional correlation ones and obtained using a product 172 correlation rule. For m design variables, the correlation function is defined by: 173

$$R(\mathbf{x}, \mathbf{x}') = \prod_{i=1}^{m} R(x_i, x_i')$$
(17)

As mentioned in [38], exponential functions (equation (18)) and the Gaussian correlation 174 functions (equation (19)) are the commonly used functions: 175

$$R(\mathbf{x}, \mathbf{x}') = \exp\left[-\sum_{i=1}^{m} \theta_i |x_i - x'_i|\right]$$
(18)

176

$$R(\mathbf{x}, \mathbf{x}') = \exp\left[-\sum_{i=1}^{m} \theta_i |x_i - x'_i|^2\right]$$
(19)

With,  $\theta_i$  are the *m*-unknown parameters of  $R(\mathbf{x}, \mathbf{x}')$ . For any untried  $\mathbf{x}$ , the Kriging estimator 177 [39] can be written as: 178

$$\hat{y}(\mathbf{x}) = \mathbf{r}^{T}(\mathbf{x})\mathbf{R}^{-1}(\mathbf{y}_{S} - \mathbf{F}^{T}\boldsymbol{\beta}) + \mathbf{f}^{T}(\mathbf{x})\boldsymbol{\beta}$$
(20)

 $\hat{y}(\mathbf{x})$  is obtained by adding two functions. The first term consists in multiplying the untried 179 sites correlation functions vector  $\mathbf{r}(\mathbf{x}) = [R(\mathbf{x}, \mathbf{x}^{(1)}), R(\mathbf{x}, \mathbf{x}^{(2)}), \dots, R(\mathbf{x}, \mathbf{x}^{(n)})]^T$  by the inverse 180 of the correlation functions for the fitting sample matrix  $\mathbf{R}$  and the vector of residuals for 181 all fitting points  $(\mathbf{y}_S - \mathbf{F}^T \boldsymbol{\beta})$ . Here,  $\mathbf{y}_S$  is the observed responses vector in the fitting sample 182 and  $\mathbf{F}$  is the model matrix of variable parameters. It can be presented by: 183

$$\boldsymbol{F} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_m^{(1)} & x_1^{(1)} x_2^{(1)} & \dots & x_{m-1}^{(1)} x_m^{(1)} & (x_1^{(1)})^2 & \dots & (x_m^{(1)})^2 \\ 1 & x_1^{(2)} & \dots & x_m^{(2)} & x_1^{(2)} x_2^{(2)} & \dots & x_{m-1}^{(1)} x_m^{(2)} & (x_1^{(2)})^2 & \dots & (x_m^{(2)})^2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \dots & x_m^{(n)} & x_1^{(n)} x_2^{(n)} & \dots & x_{m-1}^{(1)} x_m^{(n)} & (x_1^{(n)})^2 & \dots & (x_m^{(n)})^2 \end{bmatrix}$$
(21)

The second term of (equation (20)) consists in multiplying the untired site regression basis function  $\mathbf{f}^T(\mathbf{x})$  by the estimated regression coefficients vector  $\boldsymbol{\beta}$ .

Furthermore, the unknown model parameters  $\beta$ ,  $\sigma^2$  and  $\theta$  presented in equations (15), (16), (18) and (19) respectively, needed to be determined to construct the Kriging predictor. To this end, a methodology based on the Gaussian process framework of Kriging approach is used. It consists in maximizing the likelihood function (equation (22)):

$$L(\boldsymbol{\beta}, \sigma^2, \boldsymbol{\theta}) = \frac{1}{\sqrt[n]{2\pi\sigma^2}\sqrt{|\mathbf{R}(\boldsymbol{\theta})|}} \exp\left[-\frac{(\mathbf{y}_S - \mathbf{F}^T \boldsymbol{\beta})^T \mathbf{R}^{-1}(\boldsymbol{\theta})(\mathbf{y}_S - \mathbf{F}^T \boldsymbol{\beta})}{2\sigma^2}\right]$$
(22)

<sup>190</sup> To simplify this function, the natural logarithm is then applied to the likelihood expression:

$$\ln(L) = -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln\left(\sigma^{2}\right) - \frac{1}{2}\ln(|\mathbf{R}(\boldsymbol{\theta})|) - \frac{(\mathbf{y}_{S} - \mathbf{F}^{T}\boldsymbol{\beta})^{T}\mathbf{R}^{-1}(\boldsymbol{\theta})(\mathbf{y}_{S} - \mathbf{F}^{T}\boldsymbol{\beta})}{2\sigma^{2}}$$
(23)

By canceling the derivative of equation (23) with respect to  $\sigma^2$  and  $\beta$  we obtain the Maximum Likelihood Estimates (MLEs)  $\hat{\beta}$  and  $\hat{\sigma}^2$ :

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F}\right)^{-1} \mathbf{F}^T \mathbf{R}^{-1} \mathbf{y}_S, \qquad (24)$$

193 and

$$\hat{\sigma}^2 = \frac{(\mathbf{y}_S - \mathbf{F}^T \boldsymbol{\beta})^T \mathbf{R}^{-1}(\boldsymbol{\theta})(\mathbf{y}_S - \mathbf{F}^T \boldsymbol{\beta})}{n}$$
(25)

<sup>194</sup> The estimator  $\hat{\theta}$  is obtained by solving the optimization problem of equation (26):

$$\max_{\theta} \quad L(\theta) = -\frac{1}{2} [n(\ln(2\pi) + \ln(\hat{\sigma}^2)) + \ln(|\mathbf{R}|)]$$
  
s.t.  $\theta_i > 0, \ i = 1, ..., m$  (26)

After determining the estimator  $\hat{\theta}$  by solving equation (26),  $\hat{\beta}$  and  $\hat{\sigma}^2$  can be defined using equations (24) and (25). Consequently, the prediction at any given point can be estimated by referring to equation (20).

#### 198 3.3. Metamodel validation

Referring to [40], the efficiency of the constructed surrogate model is influenced by the quantity and quality of the input dataset.

#### 201 3.3.1. Error measures

To examine the efficiency of the constructed metamodel, the most simple way is to verify its residual errors. It consists in determining the difference between predicted response  $\hat{y}^{(i)}$ and the original one  $y^{(i)}$ . Smaller residual error means grater estimator efficiency. The most used error indicators of such a surrogate model are:

206

<sup>207</sup> The Maximum Absolute Error (MAE):

$$MAE = \max \left| y^{(i)} - \hat{y}^{(i)} \right|, \quad i = 1, 2, ..., n_t$$
(27)

\*\* The Relative Mean Error (RME):

$$RME = \frac{1}{n_t} \sum_{i=1}^{n_t} \left| \frac{y^{(i)} - \hat{y}^{(i)}}{y^{(i)}} \right|$$
(28)

<sup>211</sup> \*\*\* The Root Mean Squared Error (RMSE):

$$RMSE = \sqrt{\frac{1}{n_t} \sum_{i=1}^{n_t} (y^{(i)} - \hat{y}^{(i)})^2}$$
(29)

where  $n_t$  is the sampling point number used to evaluate the error measures.

#### 214 3.3.2. Cross validation

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The Cross-Validation (CV) is another error indicator which we can verify the accuracy of a surrogate model [41]. In CV, we define two type of samples data: training points responses  $y^{(i)}$  and test points  $\hat{y}_{-i}^{(i)}$  used to check its performances. It presents the prediction at  $\mathbf{x}^{(i)}$ using the surrogate model constructed from all sampling points except  $(\mathbf{x}^{(i)}, y^{(i)})$  [42]. The Mean Squares Error (generalized error) for 'leave-one-out CV' can then be defined as:

$$MSE_{CV} = \frac{1}{n} \sum_{i=1}^{n} \left( y^{(i)} - \hat{y}^{(i)}_{-i} \right)^2$$
(30)

#### 220 4. Multi-objective optimization study

#### 221 4.1. Deterministic Multi-Objective Optimization problem (DMOO)

Let's consider M objective functions  $f_m(x)$  to minimize. A DMOO approach is then required to minimize these functions considering geometrical, physical and functional constraints. Equation (31) can be then written as follow:

$$\min_{x} f_{m}(x), \quad m = 1, ..., M$$
s.t.  $g_{k}(x) \leq 0, \quad k = 1, ..., K$   
 $h_{j}(x) = 0, \quad j = 1, ..., J$   
 $lb \leq x \leq ub$ 
(31)

Different from the mono-objective optimization, objective functions constitute a multidimensional space in the multi-objective optimization, called the *objective function space*, as well as the variable space used in all optimization problems. Figure 2 illustrates the transition from the design variable space to the objective function space. Furthermore, for each solution x, there is a point in the objective space, denoted by  $(f_1, f_2, ..., f_M)^T$ .



Figure 2: Transition from physical space (a) to objective space (b)

The DMOO approach aims to determine the optimal solution by choosing between a set of obtaining points on the Pareto front, using a higher-level qualitative considerations. Since, Evolutionary Multi-objective Optimization (EMO) approaches leads to find a set of non-dominated solutions by making each population of solutions in each iteration intuitive [43]. Figure 3 presents the EMO procedure for multi-objective optimization problems. It is based on two steps:

• Step1: consists in finding closest multiple non-dominated points to the Pareto-optimal front, with a wide trade-off among the objectives.

• Step2: consists in choosing the optimal point using higher-level information.



Figure 3: Flowchart of evolutionary multi-objective optimization procedure

#### 239 4.2. Multi-objective reliability based-design optimization (MORBDO)

Comparing with the DMOO, the MORBDO aims to find the best compromise between
cost and reliability, taking into account design uncertainties. It can be mathematically
presented by [44, 45]:

$$\min_{x} f_{m}(x), \quad m = 1, .., M$$
s.t.  $P_{r}[G_{k}(x, y) \leq 0] \leq P_{k}^{T}, \quad k = 1, .., K$ 
 $h_{j}(x) \leq 0, \quad j = 1, .., J$ 
(32)

x and y are deterministic and random variables respectively.  $P_r[.]$  presents the probability operator and  $P_i^T$  is the target failure probability.  $h_j(x)$  and  $G_i(x, y)$  are respectively the deterministic and the probabilistic constraints.

Dammak and El Hami [30] propose an efficient multi-objective optimization approach called MORBDO-HM. This method is based on the classical hybrid method proposed in [16, 17, 19]. The MORBDO-HM problem can be then described by:

$$\min_{\substack{x,y \\ x,y}} F_m(x,y) = f_m(x) \times d_\beta(x,y), \quad m = 1, .., M$$
s.t.  $G(x,y) \le 0$   
 $g_k(x,y) \le 0, \quad k = 1, .., K$   
 $d_\beta(x,y) \ge \beta_t$ 
(33)

It can be noted that  $d_{\beta}$  is the distance between the most probable failure point and the 250 optimal solution. It presents the reliability level and should be higher than the target 25 reliability level  $\beta_t$ . It has been proved in [30] that, MORBDO-HM has efficiently provided 252 an optimal solution where both physical and reliability constraints are respected. However, 253 the optimization problem becomes more complex and it may converge to a non-feasible 254 solution. To overcome this issue, an efficient method called MORBDO-RHM is proposed. 255 The basic idea of this method is based on adding a new constraint to the optimization 256 algorithm. The aim of this is to force the optimization problem to find the optimal point 257 where both physical and reliability constraints are respected. Mathematically, it is defined 258 as: 259

$$\min_{\substack{x,y \\ x,y}} F(x,y) = f_m(x) \times d_\beta(x,y) \quad m = 1, ..., M$$
s.t.  $G(x,y) \le 0$   
 $g_k(x) \le 0, \quad k = 1, ..., K$   
 $\beta(x,u) \ge \beta_t$   
 $lb \le x \le ub$   
 $f_m(x) \ge f_m(y)$ 
(34)

#### 260 5. Numerical analysis

#### 261 5.1. Description of the numerical model

Figure 4 presents a three-dimensional model of the studied cooling system. It is composed by an aluminum heat sink which contains a 11×12 round pin fin matrix. Note that aluminum presents a high thermal conductivity as well as a lower mass (lower density). The dimensional details of the heat sink design are shown in figure 4.

The choice of this numerical configuration is based on an experimental study presented in [7]. The aim of this study is to propose a new methodology that leads to determine numerically an optimal design. To this end, firstly, this configuration needs to be validated with experimental data. Recently, several studies have been reported using metal-fins and metal-foam [46, 47]. However, the use of these configurations is limited to some specific applications and they are proportionally more expensive than classical ones.



Figure 4: 3-D assembly of PCM-based heat sink

Experimentally, exterior walls of the heat sink are insulated with a rubber board, except the upper surface. The insulator presents a low thermal conductivity in order to minimize thermal losses and its properties are mentioned in table 2.



Figure 5: 2-D projections of 3mm round pin heat sink.

To control the liquid and solid fractions of PCM, the top surface is covered using silicon gasket and Perspex sheet. Note that these parts are not considered in the proposed numerical model.

The 3D numerical model is studied to compare the trends observed in the experimental results [7]. A uniform heat flux is supplied from the heat source to the bottom surface of the heat sink. It is transmitted then to the PCM, heat sink fins and finally to end walls. It can be considered that the model does not take into account marginal effects such as natural convection within melted PCM, and the volume changes in PCM after phase transition. All required material dimensions and thermo-physical properties of the studied system are available respectively in table 2 and table 3.

 Table 2: Dimensions of required materials

Material	Used materials	Dimensions
1	Perspex sheet	$115 \times 115 \times 5 \ mm^3$
2	Silicon rubber gasket	$115 \times 115 \times 5 \ mm^3$
		(with a cut out of $114 \times 114$ )
3	Rubber pad for heat sink	$220 \times 220 \times 25 \ mm^3$
		(with a cut out of $114 \times 114$ )
4	Rubber pad for heat sink bottom	$220 \times 220 \times 65 \ mm^3$
5	Plate heater	$101.6\times101.6\times2\ mm^3$

Material	Thermal conductivity	Specific heat	Latent heat	Solidification point	Melting point	Density
	(W/m.K)	(kJ/kgK)	(kJ/kg)	$(\ ^{\circ}C)$	$(\ ^{\circ}C)$	$(kg/m^3)$
Aluminum	201	0.9	-	-	606.4	2700
Paraffin Wax	0.212(s)	2.8(s)	173.6	56	58	880(s)
	0.167(l)					790(l)
Rubber Pad	0.043	1.23	-	-	-	2500

Table 3: Thermo-physical properties of each material

#### 285 5.2. Boundary conditions

A Finite Element (FE) computing software ANSYS Mechanical APDL is used to investigate the performance of the round pin fin heat sink filled with PCM.

A constant heat flux  $(Q=2800 W/m^2)$  is applied to mimic the heat source at the HS bottom (presented by the red plate in figure 4). The charging phase is established for 90min and it is performed at room temperature of 18°C.

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The "enthalpy-porosity" approach is adopted in the PCM-based heat sink to investigate the effect of the transition phase. In this numerical investigation, several hypotheses are considered:

• The HS material is homogeneous and isotropic .

- A local thermal equilibrium between fins and liquid PCM is considered.
- Whatever the phase and the temperature, the thermo-physical properties of PCM and fins are considered constant.
- The radiative heat transfer is also neglected.

Natural convection is applied on exterior areas of the insulator. To deal with governing equations, initial conditions as well as applied boundary conditions are:

- Initial conditions:
- 303  $t=0, T=T_{amb}=18^{\circ}C, \xi=0.$

Otherwise, at t=0, global model is maintained at room conditions and the proposed PCM is totally in the solid phase.

• Heat flux applied at the HS base:

307  $-\lambda \left| \frac{\partial T}{\partial x} \right|$ 

$$\begin{array}{ll} x = 6.2 \to 107.8 & = -\lambda \left. \frac{\partial T}{\partial y} \right|_{x} = 6.2 \to 107.8 & = Q \\ y = 6.2 \to 107.8 & y = 6.2 \to 107.8 \\ z = 2 & z = 2 \end{array}$$

#### 308 5.3. Preliminary results and discussion

Figure 6 shows the mesh of the global studied numerical design. It is divided into 39240 8-Node tetrahedral elements. Each element has eight nodes with a single degree of freedom, temperature, at each node. It can be noted that a mesh refining is applied on the contact surfaces of HS and PCM to give a better result.



Figure 6: Mesh of studied model

Five different mesh sizes are investigated. The total computing time and the maximum reached temperature  $T_{max}$  convergency are presented in table 4.

Table 4:	$\operatorname{Mesh}$	convergency	study
		() · ·	•/

Number of elements	36240	38001	39240	85756	141367
Simulation time $(min)$	11.55	12.7	12.87	27.5	85.15
$T_{max}(^{\circ}C)$	75.76	80.34	82.57	82.67	82.68

According to table 3, the mesh configuration with 39240 elements is chosen to compromise between cost and accuracy. In fact, the configuration with 141367 elements presents almost the same maximum reached temperature with a higher computing time comparing with 39240 elements configuration. Figure 7 presents the temperature-time profile at the HS base for 3 mm pin fin heat sink configuration. Note that blue and red curves correspond respectively to experimental and numerical results during the charging phase under Q= 2800 $W/m^2$ .

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For the heating phase, the temperature variation profile can be discretized into three different regions:

• Solid region:

Initially, the temperature increases in a linear way from the ambient temperature  $T_{amb}=18$  °C to the solidification temperature of PCM  $T_s=56$  °C.

• Liquid region:

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In this region, all the quantities of PCM inside enclosures will be totally melted. The temperature increases, until 90 min.

• Latent heating region:

It can be seen that, for both numerical and experimental simulations, the increase of the temperature has been significantly delayed due to the use of PCM. In fact, benefiting from PCM thermo-physical properties, the energy generated by the input source is stored by the PCM and causes its transition from the solid phase to liquid phase.



Figure 7: Temperature-time profile at the HS base under  $Q = 2800 W/m^2$ .

It can be observed that numerical data compare reasonably well with the experimental results found by Arshad et al. [7]. Hence, the coupled RBDO-metamodels problem can be then proceeded. The design parameters considered in this study are supposed a random probabilistic one which their characteristics are specified in table 5. We note that L and H are respectively the length and the height of the HS and  $\phi$  is the pin-fin diameter (see figure 5).

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In a mono-objective RBDO method, the aim is to minimize one objective function 344 subject to physical and reliability constraint. For a PCM-based cooling system problem, 345 the objective function is generally chosen as its total volume, considering the maximum 346 reached temperature  $T_{max}$ . However, obtained optimal design may present several issues 347 in term of heat dissipation for the discharging phase related to greater designs [11]. To 348 overcome this problem, minimizing cooling time must be considered. We note by  $t_f$  the 349 final time to reach 25°C for the discharging phase. Furthermore, a 3D PCM-based heat 350 sink model is expensive in term of computational time. Hence, the need to propose an 351 original methodology of multiobjective RBDO coupled with surrogate model. Therefore, 352 surrogate models are used to determine an approximation of  $T_{max}$  and  $t_f$  when changing 353 design variables. 354

Table 5: Random variables properties

Variables	Symbol	Distribution type	Cov	Mean value	Lower bound	Upper bound
					(lb)	(ub)
Length (mm)	L	Normal	0.1	114	110	125
Height $(mm)$	H	Normal	0.1	25	15	30
Pin fin diameter $(mm)$	$\phi$	Normal	0.1	3	2	4

355 5.4. Surrogate model results: Kriging approach accuracy

Meta-model approaches are applied to build estimations of the finite element simulation 356 and determine the link between input parameters and their responses. The maximum 357 reached temperature at the base of PCM-based round pin-fin heat sink is determined using 358 Kriging surrogate models (equation (14)). To develop the Kriging meta-model, the Matlab 359 toolbox package Design and Analysis of Computer Experiments (DACE) [48] is used. A 360 second order polynomial global trend function and exponential correlation function are 361 applied. Training data presented in (table 5) are then considered as the input of the FE 362 analysis. The efficiency of the Kriging surrogate model is validated using error measures 363 (equations (27) to (29)) as presented in table 6. 364

Table 6: Error measures of Kriging predictor

Error mossuros	20 LHS points		30 LHS <sub>I</sub>	$\mathbf{p}$ oints	50  LHS  I	50 LHS points	
	$T_{max}$	$t_f$	$T_{max}$	$t_{f}$	$T_{max}$	$t_{f}$	
MAE	1.354	2.054	1.216	2.1587	0.4353	1.3895	
RME	1.046e-03	0.0032	8.1313e-04	0.0027	3.5979e-04	0.0017	
RMSE	0.377	0.489	0.0905	0.7629	0.2531	0.3181	

Training points number with LHS comparison is presented via the CV in figures 8 to 10 for 20, 30 and 50 LHS points, respectively.

367 It can be concluded that the Kriging model obtained by 50 LHS points gives an estimation 368 of the original design with acceptable efficiency. In other words, the model validation using the Kriging approach with 50 LHS points is more accurate than other configurations to estimate the link between input variables and their responses.



Figure 8: Cross-validation using Kriging predictor with 20 LHS points for (a)  $T_{max}$  and (b)  $t_f$ 



Figure 9: Cross-validation using Kriging predictor with 30 LHS points for (a)  $T_{max}$  and (b)  $t_f$ 



Figure 10: Cross-validation using Kriging predictor with 50 LHS points for (a)  $T_{max}$  and (b)  $t_f$ 

In the next section, Kriging model will be coupled with MORBDO simulation to analyze optimization and reliability of the studied system.

#### 373 5.5. MORBDO for PCM-based heat sink

In [49], authors develop the constrained non-dominated sorting genetic algorithm (C-NSGA-II) to solve the optimization problem.

Pareto front using different populations sizes comparison is presented in figure 11. In this paper, a maximum of 500 generations and a population size of 200 are used. This configuration is used in order to determine if the spread in solutions is maintained.



Figure 11: A comparison between different populations sizes

The optimization problem is based on minimizing the cooling system volume as well as the final time  $(t_f)$  taken for the discharging phase subject to the maximum reached temperature  $(T_{max})$ . Note that the critical temperature for the charging phase is about  $T_{crit} = 70^{\circ}C$ . Generally, the target reliability level is supposed equal to:  $\beta_t=3$  which corresponds to a failure probability about  $10^{-3}$ .

#### 384 5.5.1. Results of DMOO

For the DMOO approach, the global safety factor  $S_g$  is chosen based on engineering experience. Consequently, the optimal design temperature should be lower than the critical values. Then, the DMOO problem is defined as:

$$\min_{x} \{f_{1}(x) = V, f_{2}(x) = t_{f}\}$$
s.t. 
$$T_{max}(x) \leq \frac{T_{crit}}{S_{g}}$$

$$lb < x < ub$$
(35)

Figure 12 presents the Pareto optimal front of DMOO. It provides, for design selection, decision-makers with a set of solutions over the Pareto space. To select the best optimum, called knee point [50], the Minimum Distance Selection Method (MDSM) [51] is considered here as shown in figure 12. In a Pareto front, the knee point provides a good trade-off between the objective functions. It presents the minimal distance from the utopia point.



Figure 12: DMOO Pareto front

Table 7 presents the deterministic MOO results. Referring to the baseline model, the DMOO approach presents an optimal design (the thermal constraint is verified), but its reliability level  $\beta$  is missing ( $\beta$ =1.85<3). Therefore, to solve this issue, MORBDO methods are extremely recommended.

Description		Design point	Optimal solution
		$y^*$	$x^*$
Design variables	L (mm)	125	125
	H~(mm)	23.78	28.64
	$\phi~(mm)$	4	3.72
Objective function	$V \ (mm^3)$	$3.51\mathrm{e}{+}05$	$4.268\mathrm{e}{+05}$
	$t_f (min)$	236.47	253.45
Thermal constraint	$T_{max}$ (°C)	70	63
Reliability value	$\beta$		1.85

Table 7: DMOO results

#### 397 5.5.2. Results of MORBDO

Equation (36) and equation (37) present respectively the MORBDO-HM and MORBDO-RHM optimization problem:

$$\min_{\substack{x,y \\ x,y}} F(x,y) = [V(x), t_f(x)] \times d_\beta(x,y)$$
s.t. 
$$T_{max}(y) \le 70^{\circ}C$$

$$lb \le x, y \le ub$$

$$d_\beta(x,y) \ge \beta_t$$
(36)

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$$\min_{\substack{x,y \\ x,y}} F(x,y) = [V(x), t_f(x)] \times d_\beta(x,y)$$
s.t. 
$$T_{max}(y) \leq 70^{\circ}C$$

$$lb \leq x, y \leq ub$$

$$d_\beta(x,y) \geq \beta_t$$

$$V(x) \geq V(y)$$

$$t_f(x) \geq t_f(y)$$
(37)

The corresponding Pareto front is illustrated in figure 13 for both MORBDO-HM and MORBDO-RHM. MORBDO results are presented in table 8. As well as DMOO, MORBDO results provide a set of optimal points over the Pareto space. Against DMOO, the reliability level with MORBDO is respected.



Figure 13: Pareto optimal front: (a) MORBDO-HM and (b) MORBDO-RHM

Table 8 illustrated that MORBDO-HM gives an optimal resulted point within the failure zone ( $T_{max} = 90.98^{\circ}C > 70^{\circ}C$ ). However, the MORBDO-RHM leads to obtain an optimal configuration with respect of reliability constraint as well as thermal constraint, comparing with DMOO and MORBDO-HM approaches.

Descrption		MOR	BDO-HM	MORI	MORBDO-RHM		
		Design point	Optimal solution	Design point	Optimal solution		
		$y^*$	$x^*$	$y^*$	$x^*$		
Design variables	L(mm)	124.67	110.81	122.62	121.96		
	H(mm)	24.04	18.89	26.82	30		
	$\phi(mm)$	4	4	2.82	3.92		
Objective functions	$V(mm^3)$	$3.53\mathrm{e}{+}05$	$2.11\mathrm{e}{+}05$	$3.8279\mathrm{e}{+}05$	$4.2558\mathrm{e}{+05}$		
	$t_f(min))$	237.43	216.56	254.8	257.42		
Thermal constraint	$T_{max}$ ° $C)$	70	90.98	69.86	64.61		
Reliability value	eta		3		3		

Table 8: MORBDO results

The temperature-time profile, measured at the HS base, is presented in figure 14, for baseline design (red curve) and MORBDO-RHM design (blue curve). In this figure, charging and discharging phases of cooling electronic devices are investigated.

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As presented in figure 14 and table 8, the optimal design obtained by the MORBDO-413 RHM approach verifies both thermal and reliability constraints. In fact, at t = 120min, the 414 maximum reached temperature  $T_{max}$  is lower than the critical temperature, which guarantees 415 a better performance of the electronic component. Moreover, reliability condition is verified 416 with this model. In fact, the reliability level of the optimal design is equal to the target 417 reliability level ( $\beta_{MORBDO-RHM} \geq \beta_t$ ). However, the baseline model does not respect this 418 condition and it may lead to an immediate failure of the electronic component. Furthermore, 419 for the optimal configuration, the latent heating phase period is more important than its 420 for baseline design throughout the charging phase. This can be explained by the fact that 421

the optimal configuration has the ability to store a large amount of thermal energy against the baseline design. On the other hand, for the discharging phase, optimal design has the ability to release the stored thermal energy in a minimal time compared with initial model. In fact, PCM takes about 40*min* to reach its solid states against over than 55*min* for the initial model.



Figure 14: Temperature profile for baseline design and optimal design: charging and discharging phases.

#### 427 6. Conclusion

This paper aims to propose an efficient method that leads to obtain an optimal configuration of thermal management systems based on PCM technology which ensure a recommended reliability level. In this work, a 3D transient numerical simulation of round pin-fin heat sink fully filled with PCM is studied to investigate the thermal management behaviours for passive cooling of electronic equipments.

Experimental results founded by Arshad et al. [7] are numerically validated for PCM embedded in 3mm round pin fin heat sink configuration subject to constant heat load (about 2800  $W/m^2$ ).

To determine the relationship between the input and output variables, Kriging approach is used in the construction of the surrogate model. The results of cross-validation and error measures show that Kriging estimator with 50 LHS points gives an approximation of the original design with great accuracy.

Although the DMOO approach is easy to apply and can ensure an optimum design, a reliability level of thermal constraint is missed. Therefore, and in order to overcome this issue, MORBDO methods are investigated for thermal management applications. MORBDORHM and MORBDO-HM approaches based on surrogate models are coupled with PCMbased heat sink design.

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The numerical study proves that the proposed MORBDO-RHM approach is more efficient 446 and reliable comparing with MORBDO-HM approach. We conclude that, for thermal 447 enhancer application using PCM-based HS, MORBDO-RHM approach leads to obtain an 448 optimal design, where both thermal and reliability constraints are verified. The proposed 449 methodology can be then applied to determine an optimal design of cooling systems that 450 guarantees a higher performance of electronic components. Furthermore, it gives a better 451 compromise between safety and cost, for both charging and discharging phases. An extension 452 to other heat sink configurations such as square and triangular pin-fin heat sink needs to be 453 studied and validated with experimental investigation. 454

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