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# Simultaneous Model Selection and Parameter Estimation in Heat Conduction

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**Abstract.** This paper deals with the solution of an inverse heat conduction problem by using Approximate Bayesian Computation (ABC). A Sequential Monte Carlo (SMC) method is applied for simultaneous model selection and model calibration (estimation of the model parameters) by using simulated transient measurements. Two competing models are considered in the analysis of a one-dimensional transient heat conduction problem. The results show that the ABC-SMC algorithm used in this work provides accurate results for the model selection and estimation of the model parameters.

## 1 INTRODUCTION

Despite the fact that many mathematical equations used to model physical phenomena are based on well-known conservation principles, in general more than one model can be proposed to represent the physics of a problem. Models can differ by the simplification hypotheses assumed for the conservation principles, their boundary and initial conditions, as well as for the required constitutive equations. Moreover, multiple scale phenomena might be taken into account or not in the formulation, depending on the sensitivity of the dependent variables of interest for the problem. Besides these situations where the models rely on conservation principles and constitutive equations, there are other situations that rely on models strongly based on the *a priori* information available about the phenomena. Such is specially the case when the models are stochastic, like in biology or economics, for example.

The main issue is thus the reliability and the realism of the computational results obtained with possible different models. As detailed phenomena is better comprehended, there is a clear trend to develop overly complex and detailed mathematical models, for which accurate predictions can only be obtained if the parameters appearing in the formulation are accurately known. Therefore, despite the detailed phenomena included in such models, their results might not be more accurate than simpler models that are better parameterized, based on the principle of parsimony (Beck and Arnold, 1977). Therefore, techniques for the selection of the most appropriate model to represent the phenomena of interest, as well as for the estimation of the parameters associated with this model, are of great interest for several nowadays practical applications.

Classical information criteria are available for model selection, such as the Akaike Information Criterion – AIC (Akaike, 1974) and the Bayesian Information Criterion – BIC (Schwarz, 1978). Similarly, many techniques have been developed in the past for the estimation of model parameters, from the measured and computational response of the system of interest, through inverse analyses (Beck and Arnold, 1977; Tikhonov, 1977; Sabatier, 1978; Dulikravich, 1984; Morozov, 1984; Beck, Blackwell and St. Clair, 1985; Dulikravich, 1987; Tarantola, 1987; Dulikravich,1991; Hensel, 1991; Dulikravich, 1992; Murio, 1993; Alifanov, 1994; Alifanov, Artyukhin and Rumyantsev, 1995; Dulikravich, 1995; Kurpisz and Nowak, 1995; Dulikravich, 1997; Trujillo and Busby, 1997; Bertero and Boccacci, 1998; Denisov, 1999; Yagola et al., 1999; Ozisik and Orlande, 2000; Woodbury, 2002; Kaipio and Somersalo, 2004; Colaço, Orlande and Dulikravich, 2006; Tan, Fox and Nicholls, 2006; Calvetti and Somersalo, 2007; Orlande et al., 2010). A recent article by Farrell, Oden and Faghihi (2015) presents a comprehensive approach for model selection, calibration and validation within the Bayesian framework. On the other hand, there are situations where the likelihood is not exactly known, analytically intractable or when the computational cost of the actual likelihood is prohibitive. For such cases, the so-called Approximate Bayesian Computation (ABC) has been developed, where the likelihood is not computed to quantify the mismatch between the computational and the experimental dependent variables (Del Moral, Doucet and Jasra, 2007; Sisson, Fan and Tanaka, 2007; Toni et al., 2009; Toni and Stumpf, 2010a; Toni and Stumpf; 2010b; Del Moral, Doucet and Jasra, 2012).

The Approximate Bayesian Computation algorithm of Toni et al. (2009) is used in this work for simultaneous model selection and model calibration (estimation of the model parameters) for an inverse heat conduction problem. A simple one-dimensional transient problem in a slab is analyzed. Two competing models are considered, namely: (i) a local formulation given in terms of the transient heat conduction equation; and (ii) a lumped formulation that neglects the temperature gradients inside the slab. In order to verify the Approximate Bayesian Computation algorithm of Toni et al (2009), temperature measurements at a specific position inside the slab were simulated with the local formulation, for a case involving a material with small thermal conductivity (where the lumped model is not appropriate), as well as for another case involving a material with large thermal conductivity (where the use of any of the two models can be justified).

## 2 PHYSICAL PROBLEM AND MATHEMATICAL FORMULATIONS

The physical problem considered here involves heat conduction in a slab with thickness $L$, initially at the uniform temperature $T_0$.The boundary at $x = 0$ is thermally insulated, while the boundary at $x = L$ exchanges heat by convection and linearized radiation with the surrounding environment at the temperature $T_\infty$, with a heat transfer coefficient $h$, as illustrated by figure 1. The physical properties are constant and there are no heat sources inside the slab.

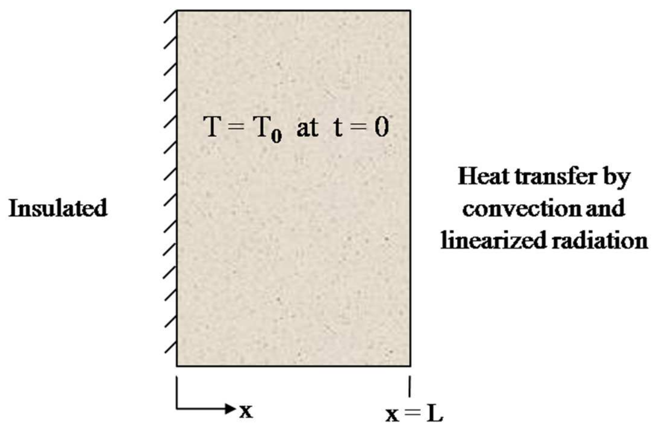


Figure 1: Physical problem.

The mathematical formulation for this physical problem, with multidimensional effects neglected, is thus given by:

$$C\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} \qquad 0 < x < L \text{ for } t > 0 \tag{1}$$

$$T = T_0 \qquad 0 < x < L \qquad t = 0 \tag{2}$$

$$\frac{\partial T}{\partial x} = 0 \qquad x = 0 \qquad t > 0 \tag{3}$$

$$-k\frac{\partial T}{\partial x} = h\left(T - T_\infty\right) \qquad x = L \qquad t > 0 \tag{4}$$

where $k$ is the thermal conductivity and $C$ is the volumetric heat capacity.

The analytical solution for this problem is obtained as (Özisik, 1993):

$$T\left(x,t\right) = T_\infty + \left(T_0 - T_\infty\right)\frac{\sin\left(\beta_m L\right)}{N(\beta_m)\beta_m}\sum_{m=0}^{L}\cos\left(\beta_m x\right)\exp\left(-\beta_m^2\frac{k}{C}t\right) \tag{5}$$

where the eigenvalues are the positive roots of the following transcendental equation:

$$\beta_m \tan\left(\beta_m L\right) = \frac{h}{k} \tag{6}$$

and the normalization integral is given by

$$N(\beta_m) = \frac{1}{2}\frac{L\left[\beta_m^{\ 2} + \left(\frac{h}{k}\right)^2\right] + \left(\frac{h}{k}\right)}{\beta_m^{\ 2} + \left(\frac{h}{k}\right)^2} \tag{7}$$

Temperature gradients within the slab can be neglected for cases involving slow processes and small Biot (*Bi*) numbers (Özisik, 1993), where

$$Bi = \frac{hL}{k} \tag{8}$$

Therefore, in such cases the temperature in the slab can be considered as uniform and the temperature becomes a function of time only. This lumped formulation is given by

$$CL\frac{dT}{dt} = h(T_\infty - T) \qquad t > 0 \tag{9}$$

$$T = T_0 \qquad t = 0 \tag{10}$$

The analytic solution of the problem given by equations (9) and (10) is given by:

$$T(t) = T_\infty + (T_0 - T_\infty)\exp\left(-\frac{h}{CL}t\right) \tag{11}$$

The mathematical formulations given, respectively, by equations (1) to (4) and equations (9) and (10), will be considered as the competing models to represent heat conduction in the slab. They are here after referred to as models 1 and 2, respectively.

## 3 MODEL SELECTION AND MODEL CALIBRATION

Approximate Bayesian Computation (ABC) is used in this work for simultaneous model selection and parameter estimation. Methods of this class can deal with experimental uncertainties that cannot be appropriately modeled in terms of analytical statistical distributions or the computation of the likelihood function is very time consuming (Beaumont et al., 2002, Marjoram et al., 2003, Toni et al., 2009, Toni and Stumpf 2010a, Wegmann et al., 2009).

The algorithm of Toni et al. (2009), which is an extension of the Sequential Monte Carlo algorithm of Sisson et al. (2007), is used for the model selection and for the estimation of the model parameters. Therefore, the objective is to obtain the combined posterior distribution (Toni et al. 2009):

$$\pi(\boldsymbol{\theta}, \mathbf{M} \mid \mathbf{z}) \tag{12}$$

where $\mathbf{M}$ is the vector that indexes the models that are considered in the analysis, $\boldsymbol{\theta}$ is the vector of model parameters and $\mathbf{z}$ is the vector of measurements. The ABC algorithm of Toni et al. (2009) is presented by Table 1.

**Table 1 -** ABC Algorithm of (Toni et al. 2009)

1. Define the tolerances $\varepsilon_1, \varepsilon_2, ..., \varepsilon_P$ for each of the iterations (populations) used for selecting the model and its parameters. Also, specify the distance function $d(\mathbf{z}, \mathbf{z}^*)$ that substitutes the likelihood function. Set the population indicator $p = 0$.
2. Set the particle indicator $i$ =1, where each particle represents, at each iteration, a model and its parameters.
3. Sample the model $M^*$ from the prior distribution for the models $\pi(\mathbf{M})$.

   If $p = 0$, sample the candidate parameters $\boldsymbol{\theta}^{**}$ from the prior distribution for the parameters of model $M^*$, that is, $\pi\left(\boldsymbol{\theta}(M^*)\right)$. Else, sample $\boldsymbol{\theta}^*$ from the previous population $\boldsymbol{\theta}(M^*)_{p-1}^i$ with weights $w(M^*)_{p-1}^i$ and perturb this particle to obtain $\boldsymbol{\theta}^{**} \approx K_p(\boldsymbol{\theta}^*, \boldsymbol{\theta}^{**})$, where $K_p$ is a perturbation kernel.
4. If $\pi\left(\boldsymbol{\theta}^{**}\right) = 0$, return to step 3. Else, simulate from the forward problem (operator $f$) a candidate set of observable variables with model $M^*$ and parameters $\boldsymbol{\theta}^{**}$, that is, $\mathbf{z}^* \approx f(\mathbf{z} \,|\, \boldsymbol{\theta}^{**}, M^*)$.
5. If $d(\mathbf{z}, \mathbf{z}^*) > \varepsilon_p$ return to step 3. Otherwise, set $M_p^i = M^*$, add $\boldsymbol{\theta}^{**}$ to the population of particles $\boldsymbol{\theta}(M^*)_p^i$ and calculate its weight as

$$w(M^*)_p^i = \begin{cases} 1 \quad , \quad \text{if } p = 0 \\ \dfrac{\pi\left(\boldsymbol{\theta}(M^*)_p^i\right)}{\sum_{j=1}^{N} w(M^*)_{p-1}^j K_p\left(\boldsymbol{\theta}(M^*)_{p-1}^j, \boldsymbol{\theta}(M^*)_p^i\right)} \quad , \quad \text{if } p > 0 \end{cases}$$

6. If $i<N$, where $N$ is the number of particles, set $i = i + 1$ and go to step 3.
7. Normalize the weights.
8. If $p < P$, where $P$ is the number of iterations (populations), set $p = p + 1$ and go to step 2. Otherwise, terminate the iterations.

## 4 RESULTS AND DISCUSSIONS

For the results presented below, simulated measurements were generated with the analytic solution of the local model, given by equation (5), by using a sufficient number of eigenvalues that assure convergence of the series solution. In order to avoid an inverse crime, the solution of the local model required for the implementation of the algorithm of Toni et al. (2009) was obtained with the finite volume method (Patankar, 1980, Ozisik et al, 2017). The distance function used in this work was the Euclidian distance between the vector of measurements, **z**, and the vector of estimated dependent variables, $\mathbf{z}^*$.

Two cases were examined here, involving different thermophysical properties of the slab material. For case 1, the slab was considered made of concrete ($C$= 2024 kJ/m$^3$K, $k$ = 1.4 W/m-K), while for case 2 the slab was considered made of aluminum ($C$ = 2439.9 kJ/m$^3$K, $k$ = 237 W/m-K). For both cases, the thickness of the slab was $L$ = 0.1 m, the heat transfer coefficient was $h$ = 10 W/m²K, the initial temperature was $T_0$ = 300 ºC and the surrounding temperature was $T_\infty$ = 400 ºC. The Biot numbers for cases 1 and 2 were 0.714 and 0.004, respectively. Therefore, the lumped model is not expected to provide an accurate representation of the problem for case 1. On the other hand, gradients can be fairly neglected for case 2, where both the local and the lumped models shall be appropriate for the problem.

The measurements were supposed to be taken at the surface x = L; they were simulated with a Gaussian distribution with zero mean and standard deviation of 0.5 ºC. Nine populations of the algorithm of Toni et al. (2009), with 1000 particles each, were used for the results presented below, where the local and the lumped models were considered as equally probable for the two cases examined. Uniform priors were used for the thermal conductivity and the volumetric heat capacity as $k$ ~ U(0,400) W/m-K and $C$ ~ U(1x10$^{+3}$, 4x10$^{+3}$) kJ/m$^3$-K, respectively. Although these distributions have finite variances, they can be considered as non-informative from the physical point of view, since they do not particularly represent any class of solid material. The perturbation kernels for these two parameters were also taken as uniform distributions, that is, $K_p = \sigma$U(-1,1). The maximum step in the perturbation kernel, $\sigma$, was 1x10$^{+3}$kJ/m$^3$K for the volumetric heat capacity, while for the thermal conductivity it was taken as 0.6 W/m-K for case 1 and 1.6 W/m-K for case 2. The vector of tolerances (see step 5 in table 1) was defined as $\boldsymbol{\varepsilon}$ = [46.5 , 23.25 , 12.4 , 9.3 , 6.2 , 4.65 , 3.1 , 2.325 , 1.86] °C, that is, they were gradually reduced as the populations advanced in order to gradually generate suitable posterior distributions for the parameters of the selected model. The minimum tolerance at the last population approximately corresponded to the distance function that resulted from Morozov´s discrepancy principle (Morozov, 1984).

Figure 2 presents the numbers of particles selected for each model as the populations generated with the algorithm of Toni et al. (2009) evolve. This figure shows that both models are equally selected up to the third population, since the tolerances are large. Afterwards, only model 1 was selected, but six generations were needed to improve the posterior distributions of the model parameters by reducing the tolerances for the distance function.The histograms of the estimated parameters estimated for the local model at population 9 are presented by figures 3 and 4. We note in these figures that the exact values of both parameters are in regions of high particle frequency. Moreover, the distributions of the particles show small variances, despite the large intervals assigned to the uniform priors of both parameters. Statistics (median and 95% credible intervals) of the distributions of the particles are presented by table 2.

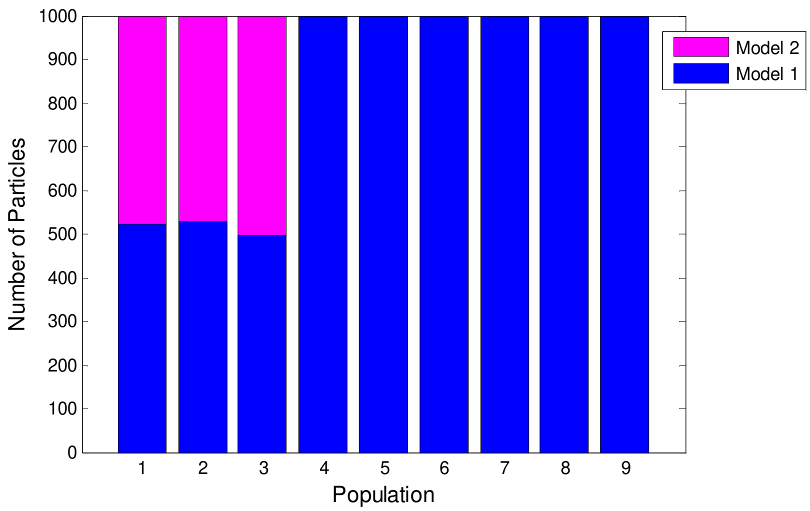


Figure 2: Numbers of accepted particles for the models in each population
(Model 1 = local model; Model 2 = lumped model).

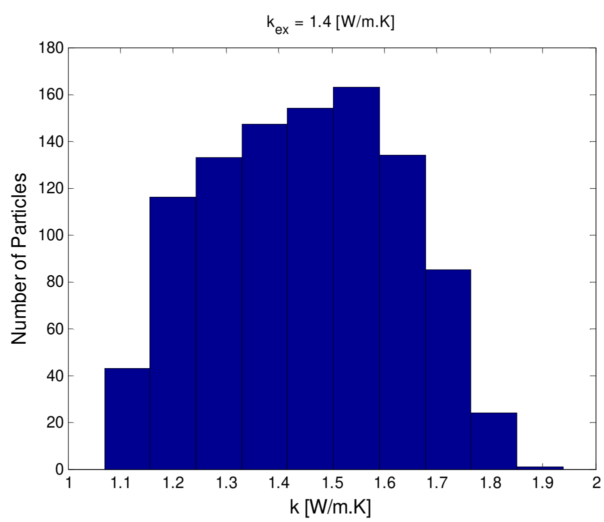


Figure 3: Histogram of the thermal conductivity estimated with Model 1 for case 1.

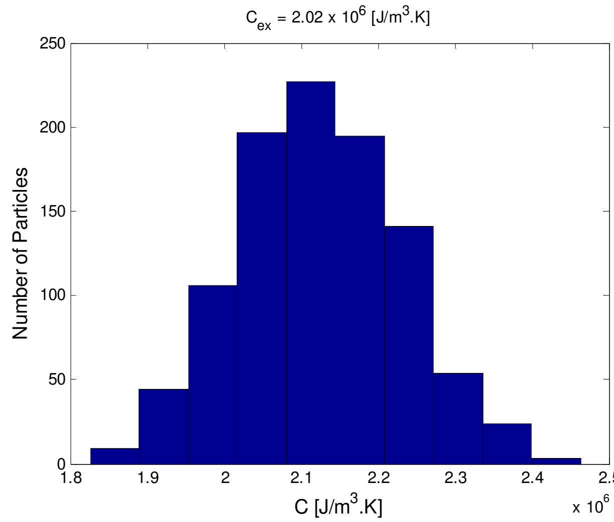


Figure 4: Histogram of the volumetric heat capacity estimated with Model 1 for case 1.

The simulated measurements and the estimated temperatures obtained with model 1 and the mean values of the parameters are presented by figure 5. Therefore, the algorithm of Toni et al. (2009) was capable of selecting the appropriate model to represent the simulated measurements, as well as estimatingposterior distributions for the model parameters with small variances, which contained the exact values in regions of high frequency with small variances.

**Table 2 –** Statistics of the estimated parameters for case 1

| Properties | Exact values | Median | Lower limit | Upper limit |
|---|---|---|---|---|
| *k* [W/m-K] | 1.4 | 1.4168 | 1.1844 | 1.6829 |
| *C* [J/m$^3$K] | 2.0240 x $10^6$ | 2.1205 x $10^6$ | 1.9300 x $10^6$ | 2.3321 x $10^6$ |

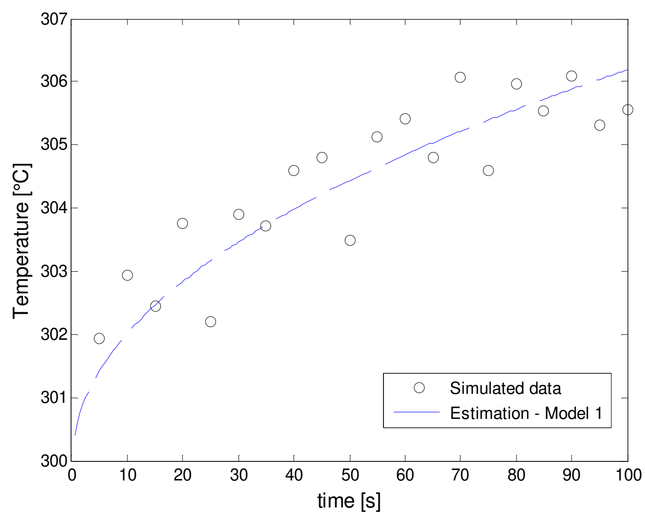


Figure 5: Estimation of the temperatures using Model 1 for case 1

The Biot number was quite small for the second case examined in this work. Therefore, it is expected that both models can appropriately represent the simulated measurements, although they were generated with the local model (model 1). The numbers of particles selected for each model as the populations evolve are presented by figure 6 for case 2. As expected, this figure shows that, despite the fact that the tolerances for the distance functions are reduced; the algorithm does not preferably select any of the two models for all populations. The acceptance ratio of each model is around 50% for all populations and none of the models can be statistically selected as the most accurate to represent at the simulated experimental data.

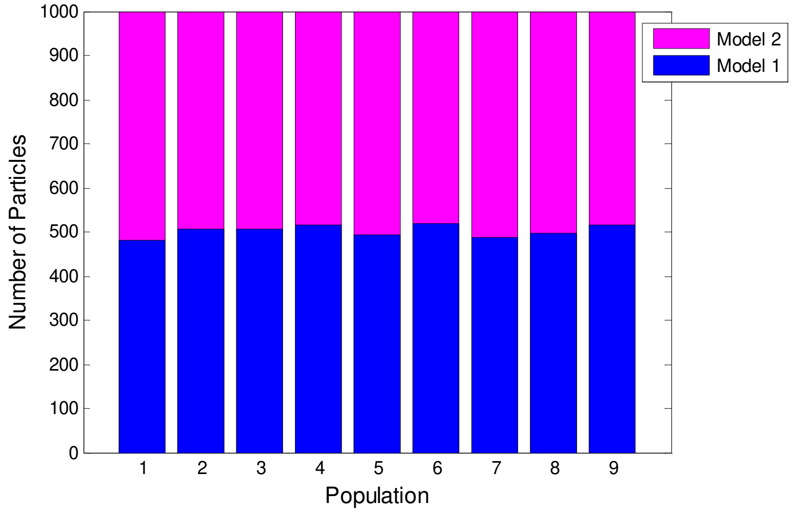


Figure 6: Numbers of accepted particles for the models in each population
(Model 1 = local model; Model 2 = lumped model) for case 2

The histograms of the particles selected for each parameter, for models 1 and 2 at the final population, are presented by figures 7 to 9. Figures 7 and 8 present the histograms for the thermal conductivity and volumetric heat capacity, respectively, obtained with model 1, while figure 9 presents the histogram for the volumetric heat capacity obtained with model 2. Note that the thermal conductivity is not a parameter for model 2 (lumped model), since the internal temperature gradients were neglected in this model. The median and the 95% credible intervals for the particle distributions are presented by table 3. Figures 7 to 9, as well as table 3, show that the estimated posterior distributions for the parameters are centered around their exact values and exhibit small variances. The temperatures estimated with the mean values of the parameters for each model are presented by figure 10. In fact, both models with their estimated parameters are appropriate to represent the experimental data for case 2.

**Table 3 –** Statistics of the estimated parameters for case 2

| Model | Properties | Exact values | Median | Lower limit | Upper limit |
|---|---|---|---|---|---|
| *1* | $k$ [W/(m-K)] | 237 | 227.0901 | 184.7962 | 274.8431 |
| | $C$ [J/(m$^3$-K)] | 2.4399 x 10$^6$ | 2.3056 x 10$^6$ | 1.8957 x 10$^6$ | 2.6871 x 10$^6$ |
| *2* | $C$ [J/(m$^3$-K)] | 2.4399 x 10$^6$ | 2.3238 x 10$^6$ | 1.9278 x 10$^6$ | 2.6959 x 10$^6$ |

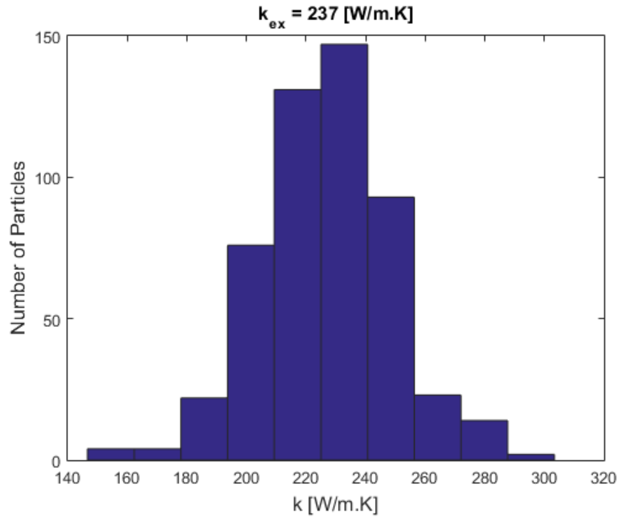


Figure 7: Histogram of the thermal conductivity estimated using Model 1 for case 2

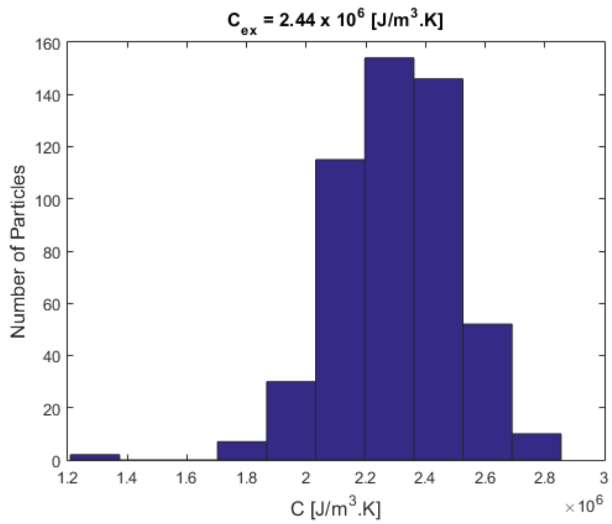


Figure 8: Histogram of the volumetric heat capacity estimated using Model 1 for case 2

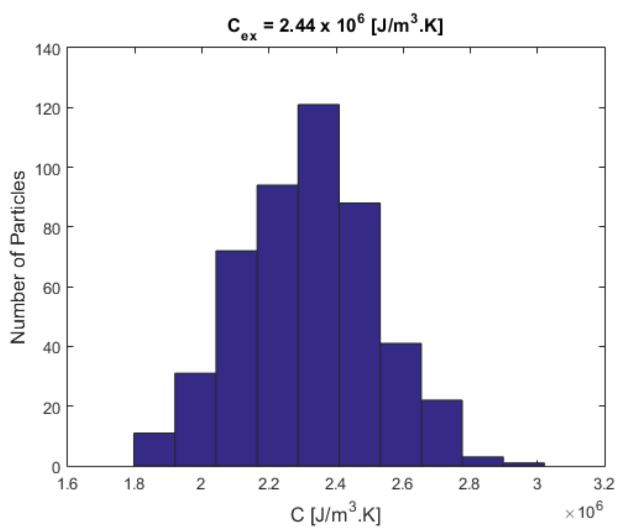


Figure 9: Histogram of the volumetric heat capacity estimated using Model 2 for case 2

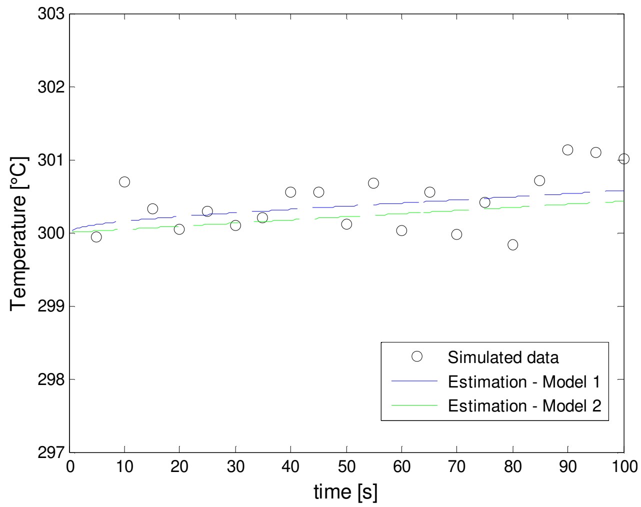


Figure 10: Estimation of the temperature using Models 1 and 2 for case 2

## 4 CONCLUSIONS

The Approximate Bayesian Computation (ABC) algorithm of Toni et al (2009) was used in this work for simultaneous model selection and model calibration in a heat conduction problem. Two test cases were examined, representing physical situations where only one of the models would suitably represent the physics of the problem, and another situation where both models would be suitable. Results obtained with a reduced number of simulated temperature measurements with large uncertainties show that this algorithm was capable of accurately selecting the most appropriate model for case 1 (the local model), as well as indicating that both models could be used for case 2. The histograms of the particles for the parameters of the selected models were centered around their exact values and exhibited variances much smaller than those of the uniform priors initially assigned. Therefore, the algorithm of Toni et al (2009) can accurate results for model selection and model calibration in heat transfer problems. As an ABC algorithm, it can be applied even for cases where the likelihood is not analytic or computationally expensive to compute.

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