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RECONSTRUCTION OF SPACEWISE VARYING BOUNDARY HEAT FLUX EMPLOYING A COMBINATION OF EXPLICIT ESTIMATION WITH MARKOV CHAIN MONTE CARLO METHOD

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Abstract. *The main objective of the present work is the validation of a new hybrid inverse methodology based on the Markov Chain Monte Carlo method (MCMC) and an explicit method, applying it to estimate a boundary heat flux. The idea is to first solve an inverse heat conduction problem using the explicit method, with the truncated eigenfunction expansions to regularize the measured temperatures. Posteriorly, the obtained estimates are used as the initial candidate for the first Markov Chain's state of the MCMC iterative procedure, which are sampled adopting the Total Variation (TV) technique as a priori information. Besides that, this second approach use the regularized temperature obtained with the explicit methodology as the input data for the inverse problem. This proposed procedure can possibly reduce the computational time of the MCMC method, since the initial state of the Markov Chain will be more similar to the final estimate, accelerating the convergence of the method and improving the final results. As a case study, it is chosen a steady state heat conduction problem with spatial variation along two directions of a thermally thin sample, with a two-dimensional heat flux applied on the boundary. For this purpose, the measured temperature is simulated with the addition of experimental noise on the direct problem solution, representing synthetic data acquired through infrared thermography.*

Keywords: *Heat Conduction, Inverse Problem, Regularization Techniques, Explicit Formulation, Bayesian Inference.*

1. INTRODUCTION

The increasing coupling of multiple components in primary devices and the continuous reduction of their dimensions has generated not only the associated advantages but also a greater complexity with regard to the correct functioning of these structures. Among the recurring factors, the thermal behavior of systems and processes exerts a great influence on the performance of these equipments and their knowledge has become increasingly crucial for many objectives (Bojić and Loveday, 1997; Botte et al., 1999; Rocha et al., 2006; Eberhart and Shitzer, 2012; Liang et al., 2015; Ghasemi et al., 2017).

In particular, the study and determination of the magnitude, profile and location of heat fluxes and sources is extremely important for the solution of industrial, medical and scientific problems (Marinetti et al., 2002; Agnelli et al., 2011; Wrobel et al., 2015).

Allied to these phenomena and their respective models of heat transfer, the principles of inverse problems play a fundamental role in the mathematical-computational formulation and resolution of several thermal problems (Jarny et al., 1991; Huang and Chin, 2000; Fudym et al., 2008; Singh et al., 2017).

Due to the complexity associated with the ill-posed behavior of the inverse problems (Kirsh, 2011), numerous solution techniques are developed within the scope of inverse problems, aiming at better results with the lowest mathematical-computational cost possible (Orlande, 2010; Alifanov, 2012; Özişik, 2018).

In many cases, a hybrid approach is used to take advantage of different methods and thus to improve the solution of the studied problem (Huang and Özişik, 1992; Mota et al., 2004; Molavi et al., 2010; Mohasseb et al., 2017). However, most of the developed methods address the inverse problem solution in an implicit way, combined with regularization

techniques, using iterative methods, such as MCMC (Wang and Zabarar, 2004; Orlande et al., 2014; Watanabe et al., 2018).

In order to combine the speed of non-iterative methods and the robustness of the Bayesian approach, this work basically deals with the application of the explicit method, with regularization by eigenfunction truncation (Knupp and Abreu, 2016; Sanches et al., 2018a), together with the Markov Chain Monte Carlo method (MCMC), with regularization via *Total Variation (TV)* in *a priori* information (Sanches et al., 2018b).

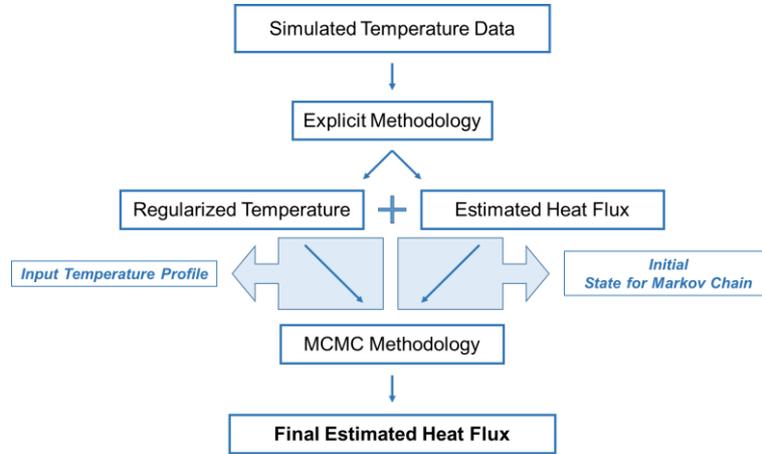


Figure 1. Hybrid methodology summary flowchart.

This hybrid methodology is here applied for the estimation of a two-dimensional boundary heat flux in steady state, using synthetic experimental data.

2. DEVELOPMENT AND MATHEMATICAL FORMULATION

2.1 Direct Problem

Consider a thin plate whose surface at $z = 0$ receives a two-dimensional heat flux, i.e. $q(x, y)$, while the opposite face, at $z = L_z$, just like the other four boundaries, is exposed to the environment at the temperature T_∞ , exchanging heat by convection, under natural and homogeneous conditions, with a constant heat transfer coefficient h , as illustrated by Figures 2 and 3.

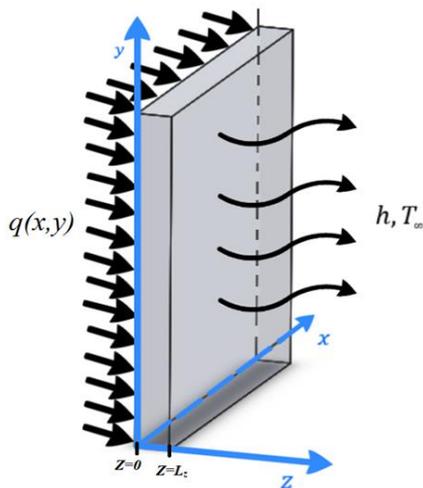


Figure 2. Schematic representation of the physical problem.

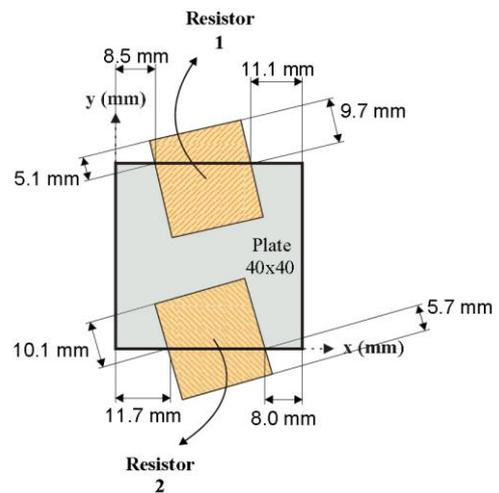


Figure 3. Spatial representation of the exact applied heat flux $q(x, y)$.

In general, the addressed problem can be initially modeled by the equation of the thermal diffusion in Cartesian coordinates, with variable thermal properties and internal energy (Bergman et al., 2011), given by:

$$\rho(\mathbf{x}, t, T(\mathbf{x}, t)) c_p(\mathbf{x}, t, T(\mathbf{x}, t)) \frac{\partial T(\mathbf{x}, t)}{\partial t} = \nabla \cdot [k(\mathbf{x}, t, T(\mathbf{x}, t)) \nabla \cdot T(\mathbf{x}, t)] + \dot{g}(\mathbf{x}, t, T(\mathbf{x}, t)) \quad (1)$$

where $\rho(\mathbf{x}, t, T(\mathbf{x}, t))$ is the material specific mass in terms of space, time and temperature itself $T(\mathbf{x}, t)$, $c_p(\mathbf{x}, t, T(\mathbf{x}, t))$ the specific heat function, $k(\mathbf{x}, t, T(\mathbf{x}, t))$ the thermal conductivity function and $\dot{g}(\mathbf{x}, t, T(\mathbf{x}, t))$ the term referring to the internal energy generation. In addition to the heat equation, the problem as proposed above requires six boundary conditions and one initial condition.

Considering a linear steady state problem in a thermally thin plate, with an exclusively two-dimensional imposed heat flux, i.e. $q(x, y)$, without internal heat sources and using the *Lumped Analysis* method at z -direction, we have the following simplified final model, with the governing equation, Eq. (2.a), and the four boundary conditions, Eqs. (2.b-c).

$$k \left(\frac{\partial^2 T_m(x, y)}{\partial x^2} + \frac{\partial^2 T_m(x, y)}{\partial y^2} \right) + \frac{1}{L_z} [q(x, y) - h(T_m(x, y) - T_\infty)] = 0 \quad (2.a)$$

$$k \frac{\partial T_m(x, y)}{\partial x} \Big|_{x=0} = h(T_m(0, y) - T_\infty); \quad -k \frac{\partial T_m(x, y)}{\partial x} \Big|_{x=L_x} = h(T_m(L_x, y) - T_\infty) \quad (2.b)$$

$$k \frac{\partial T_m(x, y)}{\partial y} \Big|_{y=0} = h(T_m(x, 0) - T_\infty); \quad -k \frac{\partial T_m(x, y)}{\partial y} \Big|_{y=L_y} = h(T_m(x, L_y) - T_\infty) \quad (2.c)$$

The solution of the proposed problem, represented by Eqs. (2.a-c), is numerically obtained via Finite Difference Method (FDM) and computationally solved using the pre-implemented function *LinearSolve* of the software *Wolfram Mathematica*. The second-order spatial derivatives in Eq. (2.a) are substituted by three-point centered final approximations, while the first-order spatial derivatives in Eqs. (2.b-c) are substituted by three-point forward and backward final approximations (depending on the boundary).

2.2 Inverse Problem and Regularization

The solution of the inverse problem associated with the direct model previously presented consists on the two-dimensional heat flux (cause) determination using the simulated experimental temperatures (effect). For the computational solution of this problem, two different methods will be used together, being one of them the explicit method, recently developed (Knupp and Abreu, 2016), and the other the classic iterative MCMC method.

Firstly, the function $q(x, y)$ is estimated using the explicit method, whose final discrete equation is represented by:

$$q_{i,j} = h(T_{i,j}^{Reg} - T_\infty) - kL_z \left(\frac{T_{i-1,j}^{Reg} - 2T_{i,j}^{Reg} + T_{i+1,j}^{Reg}}{\Delta x^2} + \frac{T_{i,j-1}^{Reg} - 2T_{i,j}^{Reg} + T_{i,j+1}^{Reg}}{\Delta y^2} \right) \quad (3)$$

where $T_{i,j}^{Reg}$ is the regularized value of the simulated temperature at the node (i, j) of the 2D discretized mesh. This regularization procedure basically consists on the expansion of the thermal data in terms of eigenfunction $\psi(x, y)$ in order to minimize the amplification of the errors contained in the synthetic temperature data, i.e.:

$$T_{Reg}(x, y) = \sum_{m=1}^{N_m} \frac{\bar{T}_{sim_m} \psi_m(x, y)}{N_m}, \quad \text{with} \quad \begin{cases} N_m = \int_0^{L_x} \int_0^{L_y} [\psi_m(x, y)]^2 dx dy \\ \bar{T}_{sim_m} = \int_0^{L_x} \int_0^{L_y} \psi_m(x, y) T_{sim}(x, y) dx dy \end{cases} \quad (4)$$

where N_m is the truncation order, \bar{T}_{sim_m} is the expansion coefficients (transformed potential) and $T_{sim}(x, y)$ is the function obtained through the linear interpolation of the synthetic temperature data.

Now, in a Bayesian approach, the previous estimated heat flux q_{est} can be used to compose the parameter vector \mathbf{Z} of the initial Markov Chain's state, and then start the iterative process with the *Metropolis-Hastings* algorithm. This

parameter vector \mathbf{Z} is composed by $Nq_x \times Nq_y$ discrete values of the function $q(x, y)$, being Nq_x and Nq_y the number of discrete points in each direction, and by the unique value of h .

Another crucial factor of the methodology used with MCMC is that the likelihood function $\pi(\mathbf{T}_{reg} | \mathbf{Z})$ (present on the Bayes' theorem) is calculated, at every step, using the regularized temperature obtained by the process presented in Eq. (4).

The *Metropolis-Hastings* algorithm, for this case, can be summarized with the following steps:

- 1) Start the iterative counter at 0 and use the estimated heat flux \mathbf{q}_{est} as the initial candidate \mathbf{Z}^0 ;
- 2) Generate a candidate \mathbf{Z}^* from the current chain state and the auxiliary transition distribution $p[\mathbf{Z}^* | \mathbf{Z}^t]$;
- 3) Calculate the acceptance factor β_h (Hastings' ratio)

$$\beta_h = \min \left[1, \frac{\pi_{pos}(\mathbf{Z}^*) p(\mathbf{Z}^* | \mathbf{Z}^t)}{\pi_{pos}(\mathbf{Z}^t) p(\mathbf{Z}^t | \mathbf{Z}^*)} \right] = \min \left[1, \frac{\pi_{pr}(\mathbf{Z}^*) \cdot \pi(\mathbf{T}_{reg} | \mathbf{Z}^*) p(\mathbf{Z}^* | \mathbf{Z}^t)}{\pi_{pr}(\mathbf{Z}^t) \cdot \pi(\mathbf{T}_{reg} | \mathbf{Z}^t) p(\mathbf{Z}^t | \mathbf{Z}^*)} \right] \quad (5)$$

- 4) Generate a random number r from an auxiliary uniform distribution delimited between 0 and 1, i.e. $r \sim U(1, 0)$;
- 5) If $\beta_h \geq r$, the new candidate is accept in the chain ($\mathbf{Z}^{t+1} = \mathbf{Z}^*$). Otherwise, it is rejected and the previous state is repeated ($\mathbf{Z}^{t+1} = \mathbf{Z}^t$);
- 6) Increase a unit in the iterative counter and return to the Step 2.

In Bayes' theorem, it is also included *a priori* information, as can be seen in Eq. (5) by the probability distribution $\pi_{pr}(\mathbf{Z})$. This prior distribution is formulated by the *TV* regularization technique, which is applied on the parameter vector and no longer at the simulated temperatures.

$$\pi_{pr}(\mathbf{Z}) \propto \exp[-0,5\gamma TV(\mathbf{Z})] \quad (6)$$

where γ is the regularization parameter and $TV(\mathbf{Z})$ is represented by:

$$TV(\mathbf{Z}) = \sum_{u=2}^{Nq_x-1} \sum_{v=2}^{Nq_y-1} (\Delta x_z [|q_{u+1,v} - q_{u,v}| + |q_{u,v} - q_{u-1,v}|] + \Delta y_z [|q_{u,v+1} - q_{u,v}| + |q_{u,v} - q_{u,v-1}|]) \quad (7)$$

with Δx_z and Δy_z being the spatial gap between each one of the discrete parameters of the vector \mathbf{Z} along the x-direction and y-direction, respectively.

3. RESULTS AND DISCUSSION

With the direct and inverse methodologies formulated, they can now be applied to the computational solution of the addressed problem, using codes developed in the symbolic computing software *Wolfram Mathematica 11*. The main goal is to compare the results using each of the separate methods with the results obtained with the proposed hybrid method.

For all results, the properties of the common glass were used, specifically $k = 1.2 \text{ W/mK}$, considering a pair of thin square plates $40 \times 40 \times 2 \text{ mm}$ in size. Besides these data, it were considered $h = 20.64 \text{ W/m}^2\text{K}$, $T_\infty = 19.96 \text{ }^\circ\text{C}$ and a standard deviation $\sigma_{sim} = 0.5 \text{ }^\circ\text{C}$ for the simulation of the synthetic measured temperatures, all based on real experiments previously performed.

The simulated data were obtained with the addition of experimental noise to the exact solution of the direct problem in Eqs. (2.a-c), using random values drawn from a normal distribution N with zero mean and standard deviation σ_{sim} , as represented by the following equation:

$$T_{sim}(x, y) = T(x, y) + \eta, \quad \eta \sim N(0, \sigma_{sim}) \quad (8)$$

For this simulation procedure, it was chosen a specific case of study regarding to the applied heat flux on the boundary, as previously shown in Figure 3, considering abrupt variations along both spatial directions and an inclination related to

positioning of the fictitious resistor. Figure 4 presents the three-dimensional graphic of the imposed heat flux function, with a non-zero mean value of 2475 W/m^2 , for the chosen case and Figure 5 shows the resulting simulated temperatures.

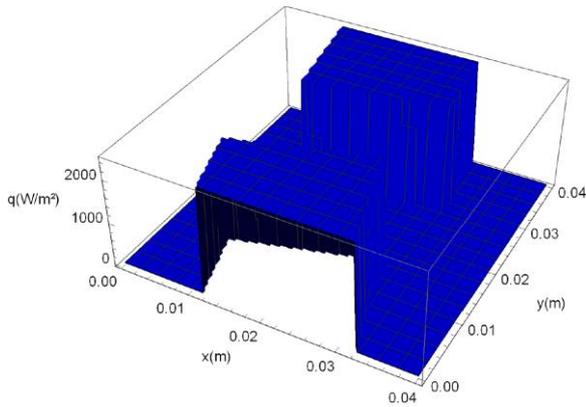


Figure 4. Three-dimensional graphic for $q(x, y)$.

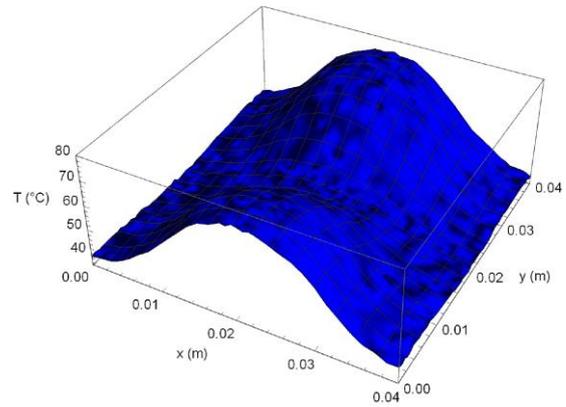


Figure 5. Synthetic temperature data with $\sigma_{sim} = 0.5^{\circ}\text{C}$.

Adopting the synthetic temperature as the input data for the explicit methodology, it is first necessary to choose the truncation order to correctly apply the regularization procedure, specified by Eq. (4). For this purpose, it is used the Morozov's discrepancy principle, which basically compares the variance of the simulated data, σ_{sim}^2 , and the variance of the regularized data regarding to the simulated ones, σ_{reg}^2 , as shown in Figure 6.

According to the analysis of the plotted curves in Figure 6, a truncation order of $N_{tr} = 200$ is the optimal order for the evaluated case, being able to smooth the oscillations caused by the added synthetic noise, as can be seen in Figure 7.

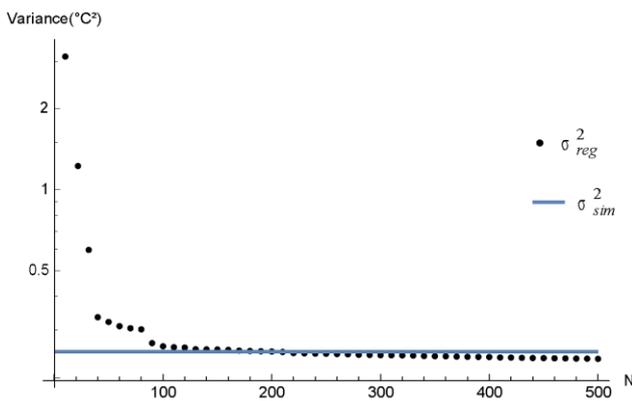


Figure 6. Discrepancy principle.

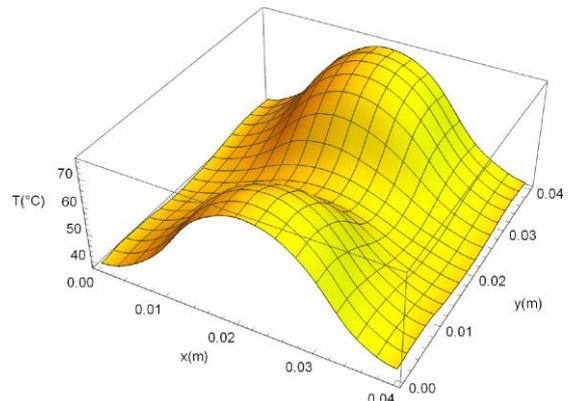


Figure 7. Regularized temperature using $N_{tr} = 200$.

After applying the inverse explicit method with the regularized data, the estimated heat flux is obtained, as shown in Figures 8 and 9 below.

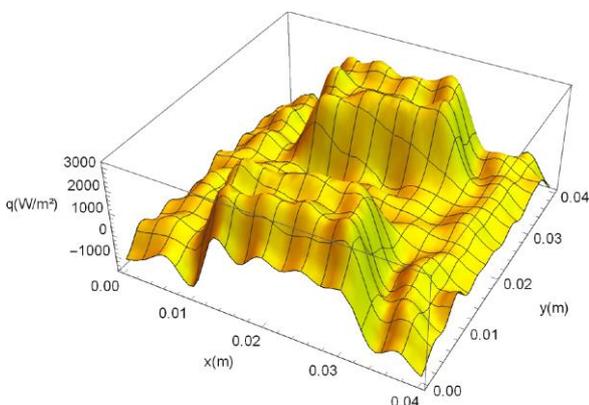


Figure 8. 3D plot of the estimated heat flux using only the explicit method with $N_{tr} = 200$.

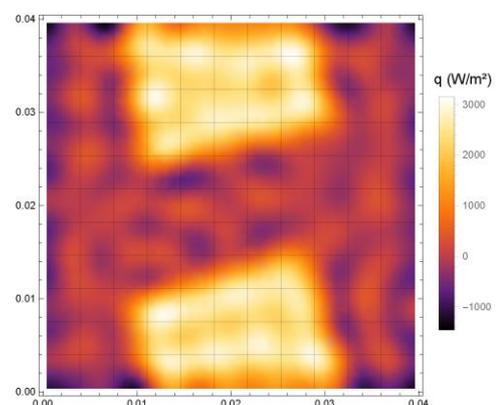


Figure 9. Contour plot of the estimated heat flux using only the explicit method with $N_{tr} = 200$.

The estimated heat flux presents a well-defined profile, with the regions and the associated values correctly delimited comparing to the reference flux shown in Figure 4. Despite the general estimate's behavior, there are oscillations due to the mathematical base of the used regularization procedure, which, for this reason, is normal and expected.

An important factor favoring the use of the explicit method is the associated low computational cost and the ease of implementation, as it does not require the solution of an optimization problem, either by deterministic or stochastic approaches.

Now, it is analyzed the results for the same case obtained with the use of the Bayesian approach via MCMC. Figures 10 and 11 show the heat flux estimated only with MCMC, using $\gamma = 75$ as the TV regularization parameter, 250000 states for the Markov chains, being the initial state the null vector, and a total of 961 discrete parameters of the vector \mathbf{Z} that represents the heat flux function (31x31 mesh).

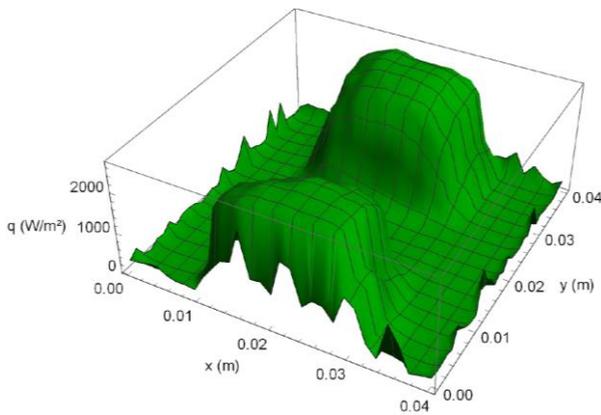


Figure 10. 3D plot of the estimated heat flux using only MCMC with 250000 states and $\gamma = 75$.

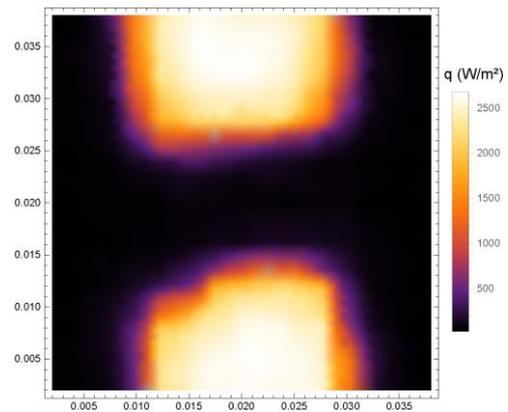


Figure 11. Contour plot of the estimated heat flux using only MCMC with 250000 states and $\gamma = 75$.

The obtained results were fairly similar to those shown by Figures 8 and 9. However, the estimates via MCMC have a smoother profile and present more accurate results when compared to those obtained by the explicit method. In addition, since the iterative procedure prevents the generation of candidates with associated negative values, which is physically more correct, the estimated heat flux using MCMC are even more similar to the reference function.

Despite the accuracy, the computational cost of MCMC to solve the addressed problem is the main negative factor. Figure 12 shows the Markov chains for two out of 961 estimated parameters of the heat flux function, using 250000 states to ensure the convergence. Both parameters refer to a central region of the spatial domain along the x-direction, contemplating a position with heat flux and one without heat flux as well.

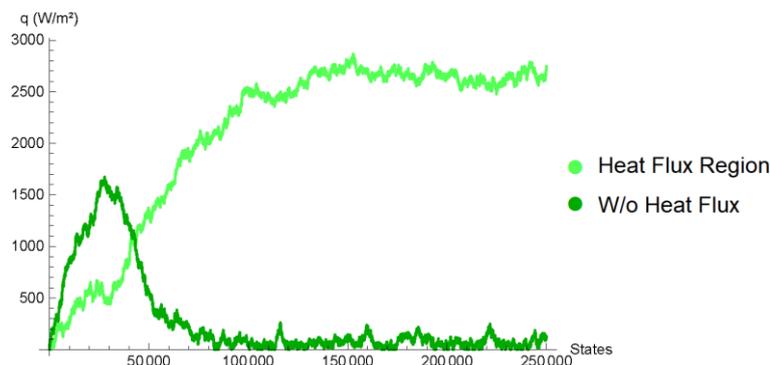


Figure 12. Markov chains for two estimated parameters in different regions of the spatial domain, using only MCMC with 250000 states and $\gamma = 75$.

All the obtained Markov chains have presented a good convergence, following the profile exemplified with the curves in Figure 12, achieving stability with about 150000 states. The *Metropolis-Hastings* algorithm had an acceptance rate of approximately 51.4%, having taken about 2 hours and 45 minutes to complete all the iterations of the 250000 states.

Another procedure to verify the convergence of the Markov chain was performed with the obtained results. After eliminating the first 150000 states (burn-in states), it was calculated the slope of the lines that best fit the remaining states for all estimated parameters of the heat flux function. In general, the slope associated with all the Markov chains was considerably small, being numerically represented by an average value of 0.002° .

As well as done for the explicit method, other tests were performed with respect to the parameter associated with the regularization technique. Besides that, the parameter related to the generation of the candidates with the auxiliary transition distribution $p[\mathbf{Z}^* | \mathbf{Z}']$, which dimension the size of the region, around the current state, within which test candidate is generated, was also varied.

Lastly, the results using the hybrid methodology (explicit method + MCMC) are presented. Figures 13 and 14 show the heat flux estimated with this methodology, using once again $\gamma = 75$ as the TV regularization parameter and a total of 961 discrete parameters of the vector \mathbf{Z} that represents the heat flux's function (31x31 mesh).

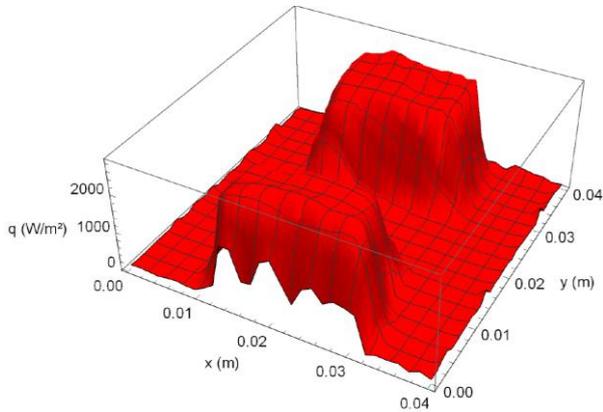


Figure 13. 3D plot of the estimated heat flux using the hybrid methodology with 50000 states and $\gamma = 75$.

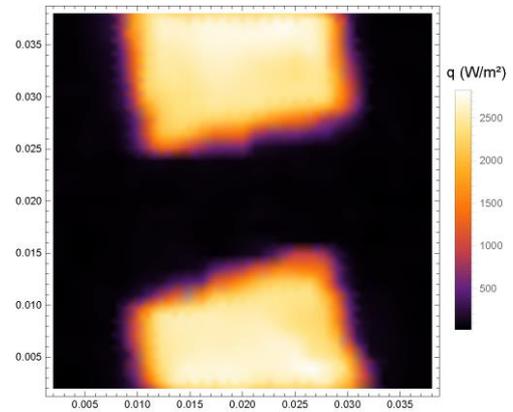


Figure 14. Contour plot of the estimated heat flux using the hybrid methodology with 50000 states and $\gamma = 75$.

The big difference now is that it was considered just 50000 states for the Markov chains, due to the fact of adopting the regularized temperature shown in Figure 7 as the input data and the estimated heat flux shown in Figures 8 and 9 as the initial state for the iterative algorithm.

Comparing with the previous estimates, either using the explicit method or MCMC, the results for the hybrid methodology show the best recovery of the imposed heat flux function, as can be seen in the graphs above and in the Figure 15 below.

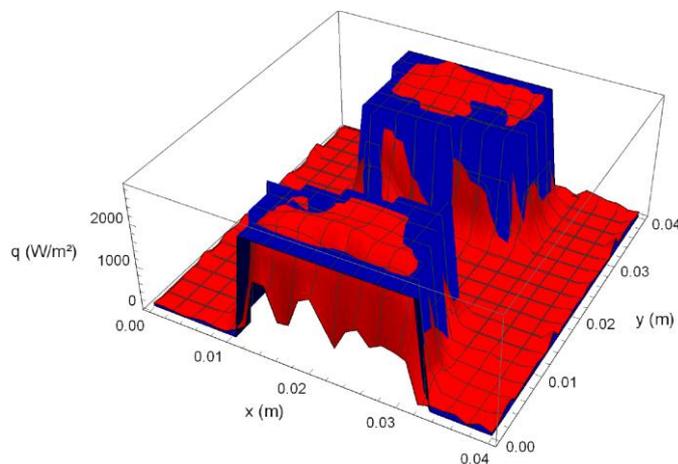


Figure 15. Comparison between the reference and the estimated heat flux using the hybrid methodology with 50000 states and $\gamma = 75$.

The three-dimensional profile is noticeably less noisy, especially in the boundary and abrupt variation regions. The fact of using a regularized temperature in the iterative procedure decreased noise amplification at each iteration, granting smoothness to the estimated function.

Also, the technique of applying the explicit estimate for the initial state of the Markov chain played an important role in directing the algorithm to a previously verified and possibly generally correct region in general, limiting the space of candidates' generation around that region and thus increasing the convergence.

Figure 16 shows the Markov chains for two out of 961 estimated parameters of the heat flux function, using 50000 states to ensure the convergence. The chosen parameters refer exactly to the same position as those shown in Figure 12, contemplating both a region with and without heat flux.

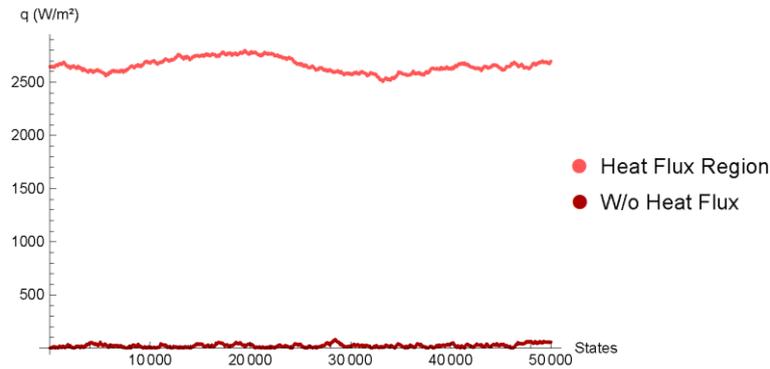


Figure 16. Markov chains for two estimated parameters in different regions of the spatial domain, using the hybrid methodology with 50000 states and $\gamma = 75$.

The Markov chains obtained with the hybrid methodology have presented an excellent convergence, since these already start close to expected value. Once more, all the others obtained Markov chains had a similar behavior, following the profile exemplified with the curves in Figure 16, exhibiting an average stability around the estimated value from the beginning.

The *Metropolis-Hastings* algorithm had an acceptance rate of approximately 51.2%, having taken just about 30 minutes to complete all the iterations of the 50000 states. Considering 20000 as burn-in states, the average slope of the lines that best fit the remaining states for all estimated parameters of the heat flux function was calculated, being numerically represented by a value of approximately 0.008° .

Figure 17 and 18 present the same Markov chains as Figures 12 and 16, but with the abscissa of the chart limited in 50000 states in order to allow the comparison between the convergence of both methodology and thus highlight the efficiency of the hybrid approach for the studied case.

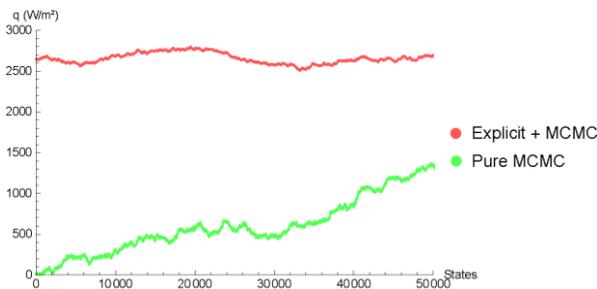


Figure 17. Comparison between the Markov chains obtained using only the MCMC and the hybrid methodology in a region with non-zero value for q .

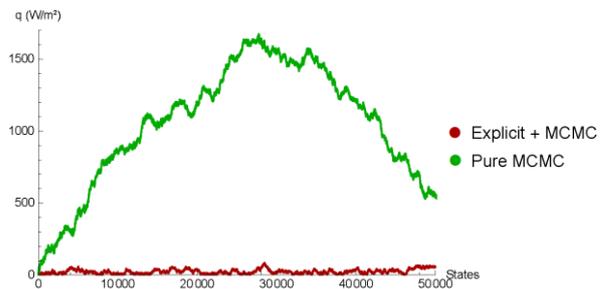


Figure 18. Comparison between the Markov chains obtained using only the MCMC and the hybrid methodology in a region with zero value for q .

4. CONCLUSION

The obtained results indicate a promising and effective application of the hybrid approach, using both the explicit and MCMC methods, in the inverse solution of the addressed physico-mathematical model, and of other possible related models, being capable to reconstruct a two-dimensional simulated heat flux with abrupt discontinuities along the spatial domain. The methods applied alone were also able to provide reasonable estimates, but with specific caveats.

According to the presented results, it is clear that the estimate using the explicit method is the noisiest, as shown in Figures 8 and 9, even if it correctly represents the geometry and the values of the heat flux function. These oscillations occur because of the sinusoidal behavior of the eigenfunctions in the regularization procedure. As a primary result, it is completely acceptable, mainly due to its excellent computational cost, presenting an average time of approximately 3 minutes.

On the other hand, the results obtained from the MCMC method have a more regular profile, as shown in Figures 10 and 11, besides restricting the estimates to positive values. However, this method alone needs many states for the Markov Chain's convergence to be achieved (about 150000 in this case), considering that the initial candidate was set to zero. Thus, the associated computational cost is very high, presenting an average time of approximately 2 hour and 45 minutes.

Lastly, the results combining both methods showed the best profile (Figures 13-15), with the lowest oscillations and error when compared to the reference heat flux. While presenting the best results, the hybrid method was able to considerably reduce the associated computational cost, taking only about 30 minutes to achieve to sample the 50000 Markov Chain's states with a good acceptance rate of the algorithm.

The procedure was able to considerably reduce the computational time associated with the MCMC method, since the initial state is similar to the final estimate and, thus, the convergence is accelerated and even guaranteed, depending on the case studied.

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