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AN INVERSE PROBLEM OF TWO-DIMENSIONAL AND TIME DEPENDENT HEAT FLUX ESTIMATION VIA HAMILTONIAN MONTE CARLO METHOD

Gabriel Teixeira Soares das Neves
Fluminense Federal Institute of Education, Science and Technology, Cabo Frio, RJ, Brazil
gabriel.neves@iff.edu.br

Luiz Alberto da Silva Abreu
Diego Campos Knupp
Antônio J. Silva Neto
Polytechnic Institute, Rio de Janeiro State University - Nova Friburgo, RJ, Brazil
luiz.abreu@iprj.uerj.br, diegoknupp@iprj.uerj.br, ajsneto@iprj.uerj.br

Abstract. *This work addresses the problem of heat flux estimation with two-dimensional spatial and temporal variations. The inverse problem is conducted via a Hamiltonian Monte Carlo (a.k.a. Hybrid Monte Carlo) method, applied to a set of simulated experimental data. CPU time and regularization processes are taken into account in order to compare with the standard, Markov Chain Monte Carlo Method. As results, the HMC method proved able to reconstruct the heat flux much quicker than MCMC method. Furthermore, it dismiss the need of regularization processes, while the MCMC implementation uses a Total Variation prior for regularization.*

Keywords: *Heat Flux Estimate, Bayesian Inference, Inverse Problems, Hamiltonian Monte Carlo, Markov Chain Monte Carlo*

1. INTRODUCTION

A shift in the industrial production paradigm took place in recent decades, with the raise of wide social technological demand. This fact draw attention to the seek of solutions to a brand new set of problems, such as the miniaturization of electronic components. The treatment of heat fluxes and propagation of heat, witch includes solutions in detection and dissipation of theses fluxes, are now highly relevant.

Since the second half of twentieth century, academia has provided a rich literature on numerical methods for solving inverse problems within the heat transfer applications framework. Initially through a deterministic approach, such as the Alifanov's iterated regularization method (Silva Neto and Ozisik, 1993; Su and Silva Neto, 2001), among others.

More recently, the application of the Bayesian theory yield to the development of new methods (Kaipio and Somersalo, 2005) to reconstruct inverse problems solutions. This advance provided tools that enabled the approach of large and ill posed problems, in which the regularization process is a challenging, but hard task, therefore plays a central role in the theory.

As a Bayesian approach, the Monte Carlo Markov Chain (MCMC) method is a popular methodology, as it easily enables the implementation of regularization techniques. In previous works, the authors applied the MCMC method for the reconstruction of heat fluxes with different behaviors.

In Neves *et al.* (2017), a Bayesian methodology is applied in order to reconstruct a transient heat flux with two-dimensional variation applied to metal plates surfaces.

In Watanabe *et al.* (2018), it is used a Bayesian method with a TVD (Total Variation Denoising regularization method), originally developed for image processing, to estimate an one-dimensional varying heat flux applied to an aluminum plate.

In Neves *et al.* (2018), a Bayesian methodology is applied in order to reconstruct a transient bi-dimensional heat flux along with a hierarchic methodology able to auto tune a MCMC implementation.

The Bayensian methodology, with hierarchical algorithm, is implemented in order to estimate a two-dimensional and time dependent heat flux, in Neves *et al.* (2019), from infrared thermography images.

A problem relentlessly present in these works is the high CPU time typically required for the sampling methods, mainly when there is such a high amount of information about which is needed to infer. An approach that has been trending within the Bayesian framework is that of Hamiltonian Monte Carlo (HMC) family. Through calculating the gradient field of the parameters set along the domain, it aims at requiring less iterations in the sampling process once providing a preferential way for parameters to converge.

The LEMA laboratory (Patrícia Olivia Soares Laboratory for Experimentation and Numerical Simulation in Heat and Mass Transfer), in IPRJ/UERJ, has developed a number of works applying the HMC method for obtaining inverse problems solutions.

In Faria *et al.* (2017), the authors show success in calibrating non-local beam models via HMC.

Cordeiro *et al.* (2017) compare HMC and Markov Chain Monte Carlo (MCMC) methods in estimating viscoelastic parameters, with comparable results between the two methods.

In the present work, it is studied the application of a HMC method for the reconstruction of the functional dependence of a heat flux that varies over two spatial dimensions and over time. It constitutes a difficult regularization problem. The CPU time required and the regularization possibilities are discussed in comparison to previous works of the authors (Neves *et al.*, 2019), where the proposed problem is successfully solved via the MCMC method.

2. METHODOLOGY

2.1 Forward problem

Consider a two-dimensional transient heat conduction problem, generated by the application of a heat flux that varies in directions x and y, and over time (t), at the upper surface ($z = 0$) of a thermally thin plate initially at the ambient temperature (as shown in Fig. 1). The other surface ($z = L_z$) is subjected to the convective heat exchange with an ambient temperature T_∞, with heat transfer coefficient h. Its length, L_x, and width, L_y, are also represented in Fig. 1. The lateral boundaries at $x = 0$, $x = L_x$, $y = 0$ and $y = L_y$ are considered insulated. This may be a good assumption because the length and width dimensions are much larger than the thickness, L_z (Neves, 2019). Outside the area in which the heat flux is applied, at $z = 0$, the lower surface in Fig. 1 is considered insulated, i.e. with zero flux in the z direction.

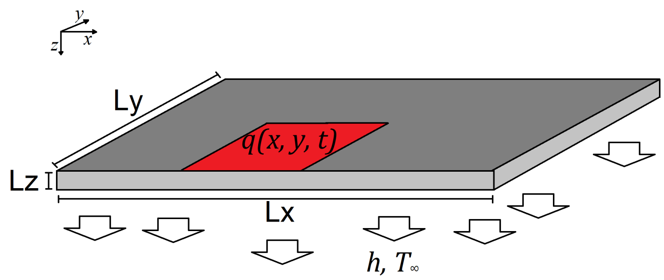

Figure 1. Schematic representation of the physical problem.

A lumped formulation is applied along the z direction, incorporating the corresponding boundary conditions. The phenomena, hence, can be described with Eq. (1) (Neves, 2019),

$$\rho c_p \frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + \frac{q}{L_z} + \frac{h}{L_z}(T - T_\infty) \tag{1}$$

with initial and boundary conditions

$$\frac{\partial T(\mathbf{x},t)}{\partial \mathbf{n}} = 0,\ x = 0,\ x = L_x,\ y = 0,\ y = L_y;\ T(\mathbf{x},0) = T_\infty \tag{2}$$

with $0 \le x \le L_x,\ 0 \le y \le L_y,\ 0 \le z \le L_z,\ t \ge 0$ and $\mathbf{x} = (x, y)$.

2.2 Inverse Problem

Consider a set of simulated experimental data organized in a series of vectors as expressed bellow, that includes a total of $N_x \times N_y \times N_t = D$ measurements, corresponding to $N_x \times N_y$ values and N_t time instants.

$$\mathbf{Y}^T = (Y_1, Y_2, \ldots, Y_D) \tag{3}$$

where Y_i, $i = 1, 2, \ldots, D$, corresponds to the measurement at each mesh position at a given instant in the time spam.

The estimates are organized in a computational mesh with $IP_x \times IP_y$ nodes and IP_t steps in time, where $IP_x \le N_x$, $IP_y \le N_y$ and $IP_t \le N_t$, leading to a total of $DP = IP_x \times IP_y \times IP_t$ used to estimate the heat flux $q(x, y, t)$. This data is organized in a vector described as

$$\mathbf{P}^T = (q_1, q_2, \ldots, q_{DP}) \tag{4}$$

For the inverse problem formulation, Bayesian theory is applied. One of the advantages of this choice is the possibility of naturally incorporating prior information in the calculation of the estimates by means of the Bayes' theorem,

$$\pi_{post}(\mathbf{P}) = \pi(\mathbf{P}|\mathbf{Y}) = \frac{\pi_{prior}(\mathbf{P})\pi(\mathbf{Y}|\mathbf{P})}{\pi(\mathbf{Y})} \tag{5}$$

where $\pi_{post}(\mathbf{P})$ represents the posterior probability distribution of the parameters $\mathbf{P}$, $\pi_{prior}(\mathbf{P})$ the probability distribution of prior data, $\pi(\mathbf{Y})$ the marginal distribution of probability of the experimental data $\mathbf{Y}$, which plays the role of a normalization constant, and $\pi(\mathbf{Y}|\mathbf{P})$, the likelihood function, expressed analytically in the form

$$\pi(\mathbf{Y}|\mathbf{P}) = (2\pi)^{-D/2}\mathbf{W}^{-1/2} \times \exp\left[-\frac{1}{2}[\mathbf{Y} - T(\mathbf{P})]^t\mathbf{W}^{-1}[\mathbf{Y} - T(\mathbf{P})]\right] \tag{6}$$

where $\mathbf{W}$ is the covariance matrix of the experimental errors, and $T(\mathbf{P})$ is the vector containing the solution of the direct problem given the values of $\mathbf{P}$, at the same position and instant in time in which the experimental measurements are obtained.

For the estimation of the heat flux, the Metropolis-Hastings algorithm, which is detailed by Kaipio and Somersalo (2005), is performed to sample candidates for posterior distribution required for the Markov Chain construction, that, under the proper circumstances, may converge to the inverse problem solution.

The Metropolis-Hastings criteria for sampling relies on the artificial Hamiltonian dynamics simulation over the estimation parameters. The joint target density (Eq. 6) can, hence, be rewritten as (Graham and Storkey, 2017)

$$H(\mathbf{P}, \rho) = -\log\pi(\mathbf{P}) + \frac{1}{2}\rho^T\mathbf{M}^{-1}\rho \tag{7}$$

where, ρ represents the momentum for each parameter in $\mathbf{P}$, taken as Gaussian, with zero mean and covariance $\mathbf{M}$. The Hamiltonian dynamics is described by equations

$$\frac{d\mathbf{P}}{dt} = \frac{\partial H}{\partial \rho}, \frac{d\rho}{dt} = -\frac{\partial H}{\partial \mathbf{P}} \tag{8}$$

and is implemented in terms of a Leapfrog formulation, described as Neal (2011):

$$\rho(t+\frac{\delta}{2}) = \rho(t) - \frac{\delta}{2}\frac{d(-\log\pi(\mathbf{P}))}{d\mathbf{P}} \quad \mathbf{P}(t+\delta) = \rho(t) + \delta\rho(t+\frac{\delta}{2}) \quad \rho(t+\delta) = \rho(t+\frac{\delta}{2}) - \frac{\delta}{2}\frac{d(-\log\pi(\mathbf{P}))}{d\mathbf{P}} \tag{9}$$

Starting with $(\mathbf{P}, \rho)$, the simulated Hamiltonian dynamics reaches a $(\mathbf{P}^*, \rho^*)$, witch is accepted as estimate if it passes the acceptance criteria given by

$$\beta = \min\{1, \exp(H(\mathbf{P}, \rho) - H(\mathbf{P}^*, \rho^*))\} \tag{10}$$

If the sample is accepted, the process restarts with $(\mathbf{P}, \rho) = (\mathbf{P}^*, \rho^*)$, otherwise, it is restarted with the same $(\mathbf{P}, \rho)$, creating, thus, a Markov Chain.

3. RESULTS AND DISCUSSION

The simulated experimental data is created by adding to the forward problem solution a Gaussian error with zero mean and standard deviation 0.06^oC, compatible with those observed in experiments (Neves *et al.*, 2019), over a mesh with $48 \times 24 \times 300 = 345,600$ nodes. Simulated properties are tuned as $\rho = 1,200\,kg/m^3$, $c_p = 800\,J/kg \cdot K$, $k = 0.2\,W/m \cdot K$, $h = 12\,W/m^2K$ and $T_\infty = 20\,^oC$.

The Leapfrog formulation used in reproducing Hamiltonian dynamics is discretized a in path of fictional size 65, with steps of 0.1 in length. HMC is tuned to perform 25 iterations over a mesh with $15 \times 15 \times 50 = 11,250$ nodes, with an acceptance rate of about 96%. Up to now, no regularization process was required.

In contrast, MCMC formulation used for comparison, as described in Neves (2019), is performed with 1,000,000 iterations along with Markov Random Fields prior for regularization, with an acceptance of around 25%.

As results, the HMC estimation was able to reconstruct information about the variation of the heat flux throughout the domain. Figures 2a-c show cuts in the x and y directions and along time.

The x and y cuts present good approximations of the exact solution. Meanwhile, in the t cut, the retrieved flux shows a more unstable behavior, although still carries general characteristics of the exact solution with relative precision.

Overall, the HMC method shows good results in regularizing the solution, without need of regularization processes, by hinting the better direction for sampling the aimed parameters. That configures as a great advance if compered to the MCMC. As shown in Neves (2019), this same problem solved via MCMC shows the necessity of a Markov Random Fields formulation used as prior information in order to regularize the solution. The regularization process is often the hardest and most time-consuming stage of reconstructing an inverse problem solution, so that represents a great feature.

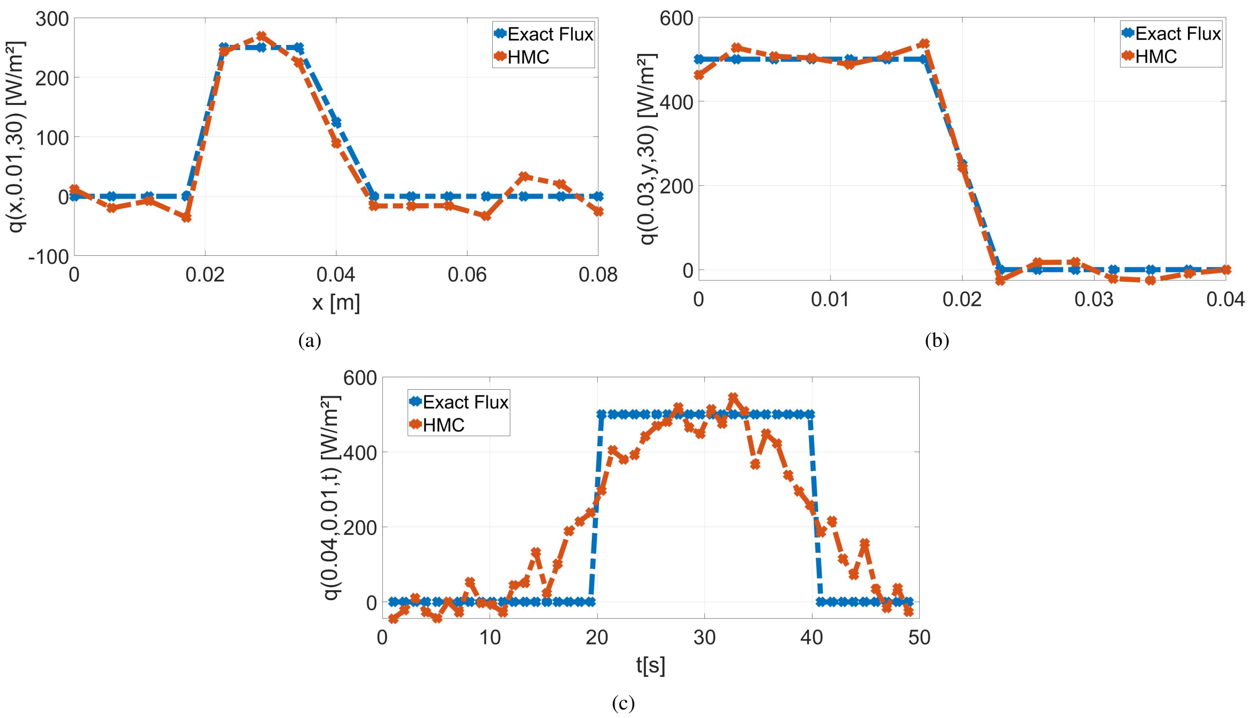

Figure 2. Comparison between estimated and exact flux in directions x, with $y = 0.01\,m$ and $t = 30\,s$ (a), y, with $x = 0.04\,m$ and $t = 30\,s$ (b), and time, with $x = 0.04\,m$ and $y = 0.01\,m$ (c).

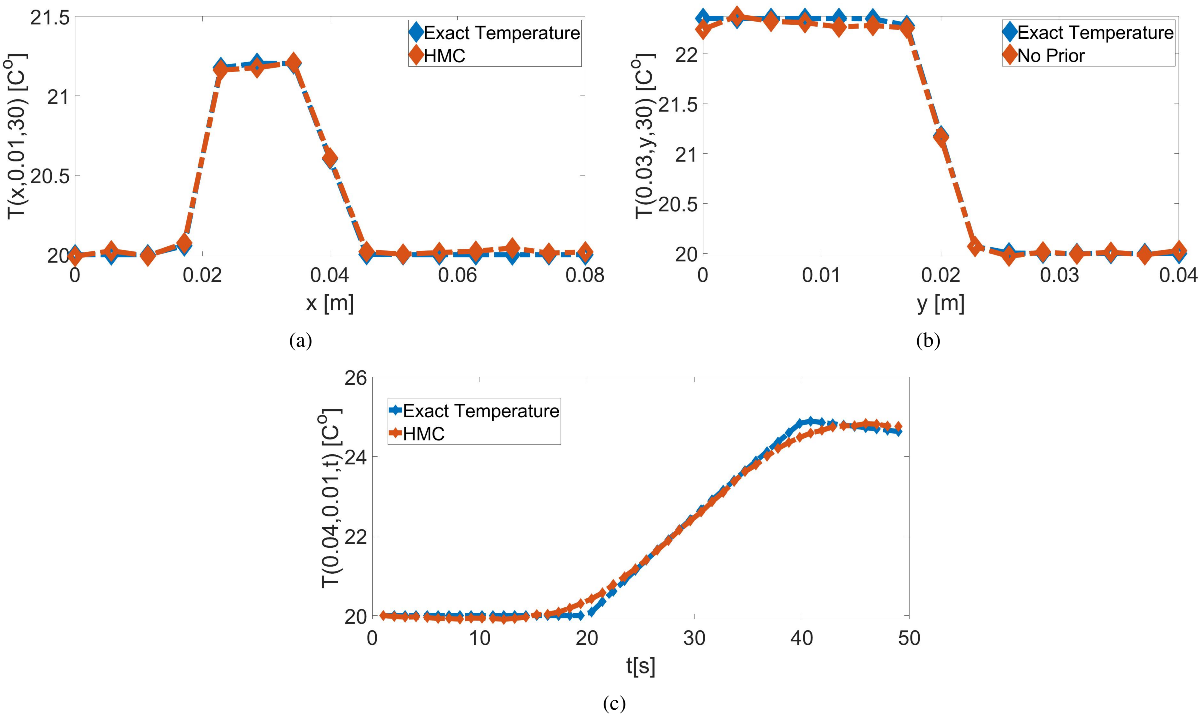

Figure 3. Comparison between estimated and exact temperature in directions x, with $y = 0.01\,m$ and $t = 30\,s$ (a), y, with $x = 0.04\,m$ and $t = 30\,s$ (b), and time, with $x = 0.04\,m$ and $y = 0.01\,m$ (c).

Retrieved temperature presents a good approximation of exact data as well. Figures 3a-c show a good approximation in both x and y directions as well as along the time span.

For means of comparison of both error and CPU time, Tab. 1 shows the error calculated via a RMS formulation, which is related to the mean of the relative error calculated in each nod of the mesh, both with HMC and MCMC.

The error produced by the HMC method holds close to that produced by the MCMC method. The high gain in CPU time, about 86% seems remarkable. It is import to highlight the fact that HMC needs no regularization processes, a great progress that makes the HMC results promising.

Table 1. Calculated error for values of estimated fluxes and calculated temperatures and spent CPU time.

Case	RMS_q $[W/m^2]$	RMS_T $[^oC]$	CPU Time [s]
HMC	7.8376	0.0089	$\approx$ 5,300
MCMC	7.1419	0.0051	$\approx$ 39,000

Onward, a better tuning along time in HMC is aimed, as well as approximation techniques, in order to optimize CPU time as close as possible to real time.

4. CONCLUSIONS

This work presented a novel application of the HMC model in the heat flux estimation problem framework. It compares HMC results with a more established approach, the MCMC. The error in the heat flux reconstruction is small and comparable to that produced by the MCMC method. Still, the CPU time gain is impressive, with a 86% reduction. Finally, no regularization method is necessary, which represents a theoretical and practical gain, also convertible in time.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE