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Uncertainty Quantification in Steady-State Heat Transfer: A Comprehensive Analysis of DRAM and MCMC Methods with Applications to Thermal Systems

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ABSTRACT

This research addresses the limitations of traditional deterministic methods in capturing uncertainties in heat transfer systems, particularly in parameter estimation and uncertainty quantification. We aim to evaluate and compare Delayed Rejection Adaptive Metropolis (DRAM) and Markov Chain Monte Carlo (MCMC) methods for uncertainty quantification in steady-state heat transfer, using experimental data from a copper rod with 15 temperature measurements. The study estimates heat flux and convective heat transfer coefficient parameters, comparing results with Ordinary Least Squares (OLS) estimation. Results show DRAM produces tighter parameter distributions (0.2312) compared to MCMC (0.2641), while both methods yield similar mean estimates and demonstrate strong negative correlation between parameters. A comparison with OLS shows close agreement across all three methods, concluding that DRAM provides slightly superior performance in parameter estimation accuracy while all methods effectively capture parameter uncertainties in steady-state heat transfer analysis.

Keywords:
Uncertainty Quantification; Parameter Estimation; Bayesian Inference; Heat Transfer; Delayed Rejection Adaptive Metropolis; Markov Chain Monte Carlo

1. Introduction

Recently, uncertainty quantification (UQ) has emerged as a critical area of research in mathematical modeling, as it turns out to be a fundamental indicator of the variability and reliability in predictions from physical or computational systems [**1**]. UQ helps us understand how system behavior might

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change under different conditions, through its study of the relationship between input variation and predictions of output. The area has grown tremendously in recent decades from simple error analyses to complex probabilistic descriptions that model multiple sources of uncertainty (epistemic and aleatory) [**2**, **3**]. This evolution has with special strength affected thermal systems analysis, as the prediction accuracy and reliability assessment are important for engineering applications, which include heating exchangers design, energy efficiency improvement, thermal systems safety [**4**]. These developments have permitted more-integrated investigations accounting for the interaction of intricate physical processes.

In particular, the characterization of heat transfer in conductive media, which is common in rod-like geometries, presents unique challenges in parameter estimation and uncertainty analysis [**5**, **6**]. The complexity arises from the coupling of different transport laws e.g conduction, convection and radiation which can be used for heat transfer separately or in combination [**7**]. The final solution of deterministic methods is less capable of capturing the information of uncertainties in the systems. While such approaches may yield accurate solutions under idealized assumptions, they fail to consider variations in material properties, boundary conditions, and environmental factors [**8**]. A better reflection of the real world is possible through the use of probabilistic and data-driven approaches in place of fundamentalist approaches, which suffer from many restrictions.

Thermal systems have, however, shown that Markov Chain Monte Carlo (MCMC) methods can be efficient estimators of parameters and uncertainties [**9**, **10**]. This class of methods provides a solid basis for drawing samples from intricate posterior distributions and managing several uncertainty sources at the same time, which makes it very appropriate for problems characterized by high-dimensional parameter spaces [**11**]. MCMC methods work exceptionally well for heat transfer problems and the Bayesian framework has led to new and innovative ways of performing parameter estimation and uncertainty analysis by allowing experimental data to be combined with computational models in a statistically rigorous manner [**12**]. MCMC enables advances in modeling and parallelization accuracy by allowing parameter spaces to be used more efficiently than in classical approaches.

One of the most notable improvements in MCMC methods is the Delayed Rejection Adaptive Metropolis (DRAM) algorithm [**13**, **14**]. This algorithm utilizing the benefits of delayed rejection and adaptive proposal distributions allows to obtain efficient sampling and convergence in fewer steps [**15**]. In comparison to standard methods of MCMC which can get stuck in subprocesses of poor scaling, DRAM has the capacity through its dynamic adjustment method of handling these more challenging posterior distributions which often contain global as well as local modes. We've shown that DRAM is useful when applied to heat transfer problems, where it has been shown to perform significantly better than other parameter estimation techniques when faced with high-dimensional, non-linear parameter spaces that have poorly characterized conditional structure [**16**].

In recent years, due to advances in computational capabilities, uncertainty quantification (UQ) techniques have emerged as a powerful tool for heat transfer problems [**17**]. Furthermore, high-performance computing systems have made it feasible to employ advanced sampling methods and advanced statistical analyses, which were once intractable in terms of computation resource constraints [**18**]. Improvements in these technologies have resulted in more precise parameter estimation and improved uncertainty limits in the modeling of thermal systems. Moreover, parallel computing and GPU-based processing have enabled researchers to address more complex geometries and phenomena, leading to bolder and deeper investigations in the field [**19**].

Uncertainty quantification is actually a challenge in its own right for the integration of experimental data with computational models [**20**]. Contributions from measurement errors, systematic biases, and random fluctuations all compound into the total uncertainty of parameter estimation, and sophisticated correction methods and filtering are often employed to reduce their effects [**21**]. Today, there exist modern UQ approaches that allow for mitigating various sources of uncertainty through bayesian frameworks and/or robust and indistinguishable errors modeling strategies [22]. All such techniques allow to better quantify the accuracy of the parameter estimation but also to gain insights about the underlying physical processes, as they provide a systematic way to introduce observational data.

Temperature measurement methods and their uncertainties are key in heat transfer analysis [23]. Numerical and physical data yield different internal profile estimates that depend on the sensor's accuracy and precision and its spatial and temporal resolutions, which matter most in sensitive applications (like microscale heat transfer or cryogenic systems) [24] In order to obtain a trustworthy estimation of parameters, it is of paramount importance to understand and quantify uncertainties in the measurements, as even small errors in the data can be augmented along models and have a major impact on the predictions [25]. A New Era of Precision: Continued Innovations in Sensor Tech and Calibration

Estimating heat transfer coefficients is constrained not only by physical limitations but statistical uncertainties as well [26]. These parameters tend to be highly correlated and exhibit nonlinear relationships, causing them to be difficult to estimate [27]. However, these issues can be overcome with sophisticated sampling methods (e.g., Hamiltonian Monte Carlo, variational inference) which explore your parameter space in a way that is more efficient while accommodating intricate interdependencies [28]. These approaches yield more exact estimates of parameters and allow to disentangle more complex characterization of heat transfer phenomenon.

As a result, the heat flux parameter estimation process is complex, indirect, and sensitive to the boundary conditions [29]. Heat flux estimates are highly sensitive to temperature measurement, and to the robustness of the estimation method, which must deal with sparse or noisy data in many cases [30]. To enhance the reliability of the parameter estimation of heat flux, a number of approaches have been proposed, such as inverse modeling and regularization techniques [31]. This work has enhanced our capacity to observe heat transfer in systems ranging from industrial applications to climate modeling.

Bayesian inference approaches have grown more relevant in thermal system modeling [32]. Such approaches offer a native way to reconcile prior information with experimental data, resulting in more robust and higher fidelity answers even when data is limited or noisy [33]. In instances where traditional approaches are unsatisfactory,[2] the Bayesian Approach can provide large benefits by enabling researchers to record uncertainty in an explicit and principled manner [34]. Advances in computational Bayesian methods are constantly broadening their range and halving their computational cost.

The previous distributions play an especial role in the Bayesian analysis of heat transfer problems [35]. Choosing suitable prior distributions becomes crucial for parameter estimation especially when experimental data is limited [36]. The last ten years, however, have seen a surge of recent work towards methods to select informative but objective prior distributions that manage the trade-off between using prior information and introducing bias (e.g. [37]). This has helped improve the robustness and generalizability of Bayesian models in real-world contexts.

MCMC methods require convergence checking for reliable parameter estimates [38]. Different diagnostic methods have been proposed to assess the convergence and mixing characteristics of chains, including the Gelman-Rubin statistic and the computation of effective sample sizes, and to ensure that distributions actually sampled approximate the target posterior [39]. These tools help safeguard the reliability of the estimates of the parameters and uncertainty bounds, by alleviating worries about the adequacy of sampling in high-dimensional or multi-modal space [40].

Comparison between Parameter Estimation Methods: Comparison between the different statistical approach for parameter estimation was made [41]. Every approach shines in some aspects, while floundering in others, and so the choice of method depends on problem features, such as, data type and system complexity [42]. Some applications have also benefited from hybrid methods, for instance, the iterative combination of MCMC and optimization-based techniques, as they can yield the best of both worlds [43]. Uncertainty quantification for heat transfer introduces significant effects of spatial discretization [**44**]. The discretization scheme determines trade offs between simulation efficiency and accuracy, and may affect both parameter estimates and their posterior uncertainties [**45**].

This discipline is severely bounded in larger scale simulations, as computational resources become an inevitable bottleneck [**46**]. Temporal features of heat transfer systems adds an extra layer of complexity to uncertainty quantication [**47**, **48**]. The estimation process must take into account a number of dynamic temperature variations and transient effects. E.g., in rod heating experiments the evolution of the temperature profiles over time provides significant thermal diffusivity and heat capacity information, but conversely it also introduces problems with parameter identifiability and uncertainty propagation [**49**]. These challenges necessitate advanced techniques to create and include temporal data in uncertainty analysis frameworks as well as modeling.

2. Model Configuration and Formulation

2.1 *Steady-State Heat Model*

The boundary value problem:

$$\frac{d^2u_s}{dx^2} = \frac{2(a+b)}{ab}\frac{h}{k}\left[u_s(x) - u_{amb}\right]$$

$$\frac{du_s}{dx}(0) = \frac{\Phi}{k} \quad , \quad \frac{du_s}{dx}(L) = \frac{h}{k}[u_{amb} - u_s(L)]$$

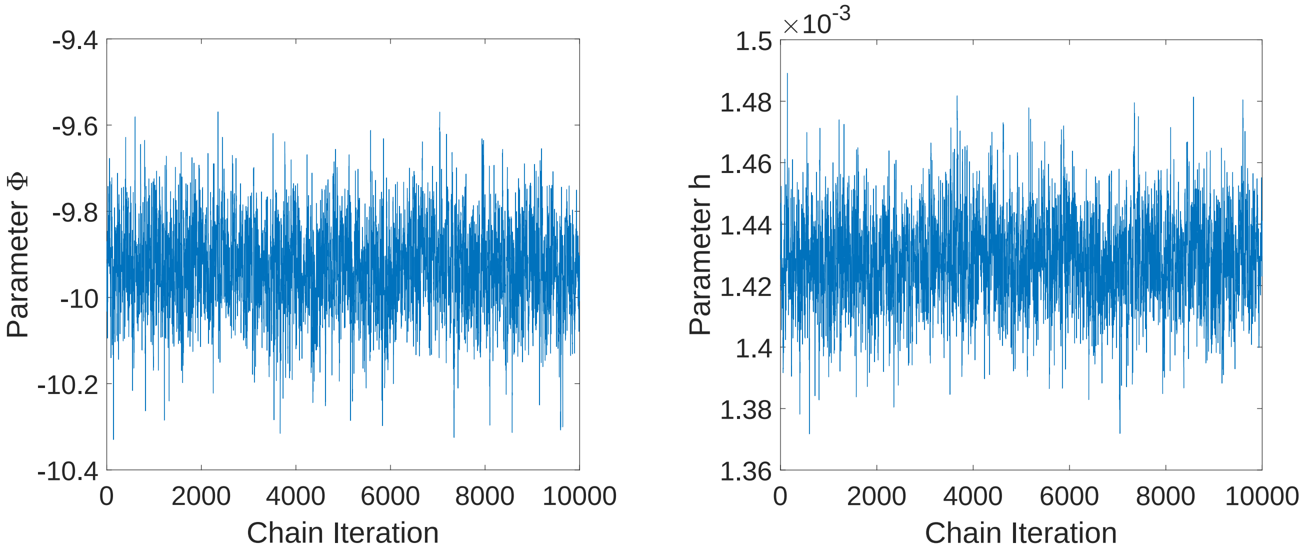
which models the steady state temperature of an uninsulated rod with source heat flux Φ at $x = 0$ and ambient air temperature uamb. The model parameters to be estimated and statistically analyzed are $\boldsymbol{\theta} = [\Phi, h]$, where h is the convective heat transfer coefficient. The rod dimensions are $a = b = 0.95$ cm and $L = 70$ cm. The temperature measurements y_i were made at 15 equally spaced spatial locations x_i, as compiled in Table 1. Again, we take $u_{amb} = 22.28^o$C as the ambient temperature and $k = 4.01\frac{W}{cmC}$ as the thermal conductivity of copper.

Table 1
Steady-state temperatures measured at locations x for a copper rod

x (cm)	10	14	18	22	23	30	34	38	42	46	50	54	58	62	66
Temp (○C)	66.04	60.04	54.81	50.42	46.74	43.66	40.76	38.49	36.42	34.77	33.18	32.36	31.56	30.91	30.56

2.2 *DRAM Estimation*

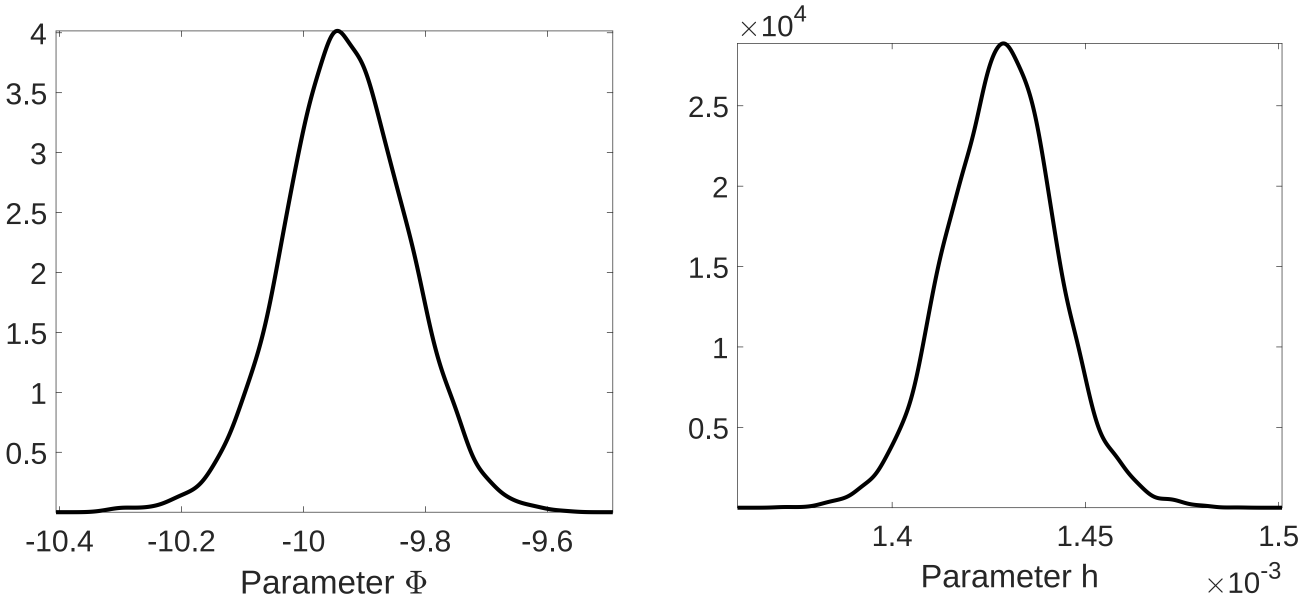
First we adapt the provided `heat_code_dram.m` and `heatss.m` codes to work with the copper data. All this requires is changing the value of k and swapping the aluminum data with the copper data. With these modified codes we produce the figures below.



(a) **(b)**

Fig. 1. Chains for parameters Φ (a) and h (b) obtained with the DRAM algorithm.

The chains in Figure 1 show the characteristic 'fuzzy caterpillar' look. Φ and h seem to be distributed around -9.9 and 1.43×10^{-3}, respectively. However, we can see some gaps, which suggests that many iterations are being rejected. We may do better with MCMC.



(a) **(b)**

Fig. 2. Marginal densities for Φ (a) and h (b) obtained with the DRAM algorithm.

The marginal density plots in Figure 2 show the distributions even better. Least squares fit found $\Phi = -9.9237$ and $h = 1.4271 \times 10^{-3}$, and these plots align with that result. They are distributed around those values. Furthermore, we sample Φ against h at each step to determine parameter correlation.

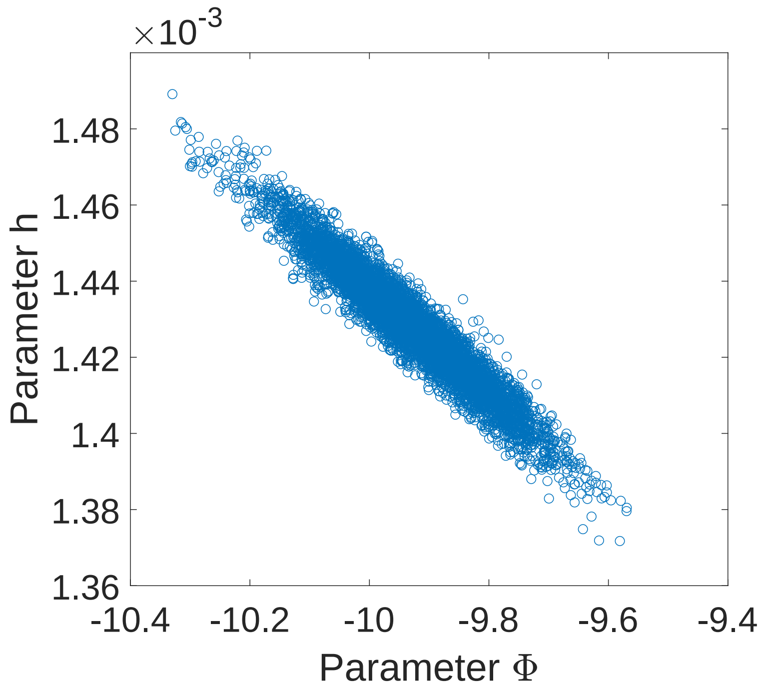


Fig. 3. Joint sample points for Φ and h obtained with the DRAM algorithm.

Here in Figure 3 we see a strong negative correlation between Φ and h.

2.3 *MCMC Estimation*

First we adapt the provided `heat_code_dram.m` code to work with the copper data. Again, this just requires is changing the value of k and swapping the aluminum data with the copper data. With these modified codes we produce the figures below.

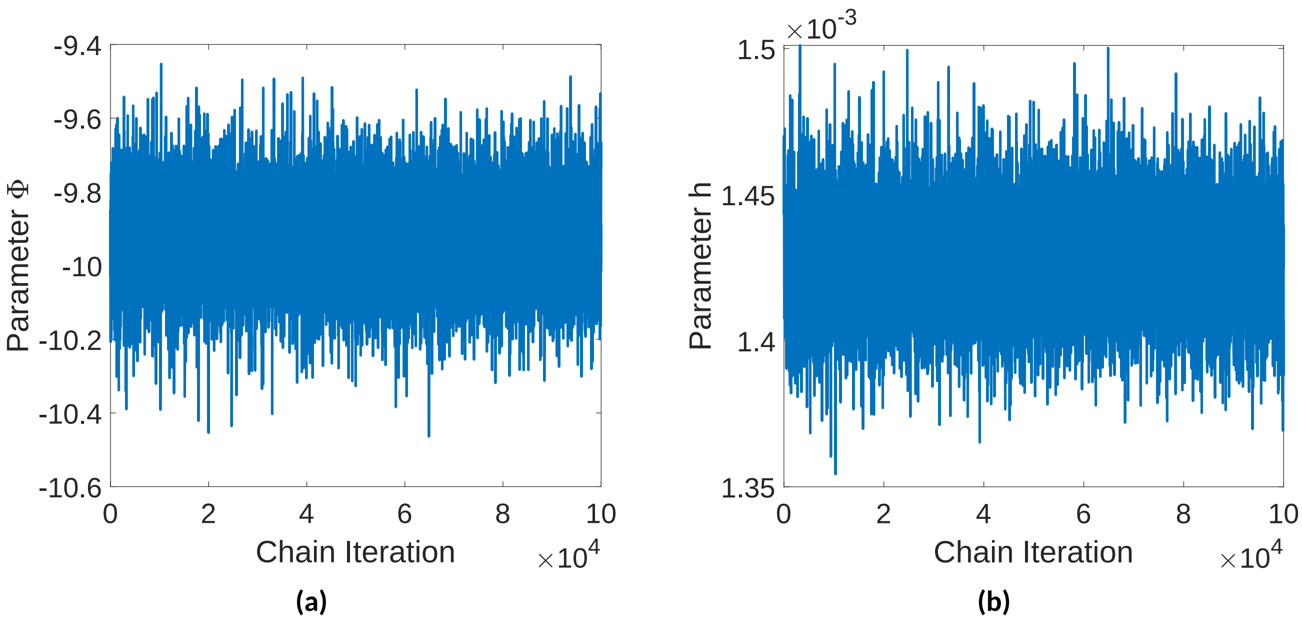


Fig. 4. Chains for parameters Φ (a) and h (b) obtained with the MCMC algorithm.

The chains in Figure 4 are even fuzzier caterpillars. MCMC explores the space just as well as DRAM, but with seemingly fewer rejections. We expect the MCMC parameters to have tighter distributions.

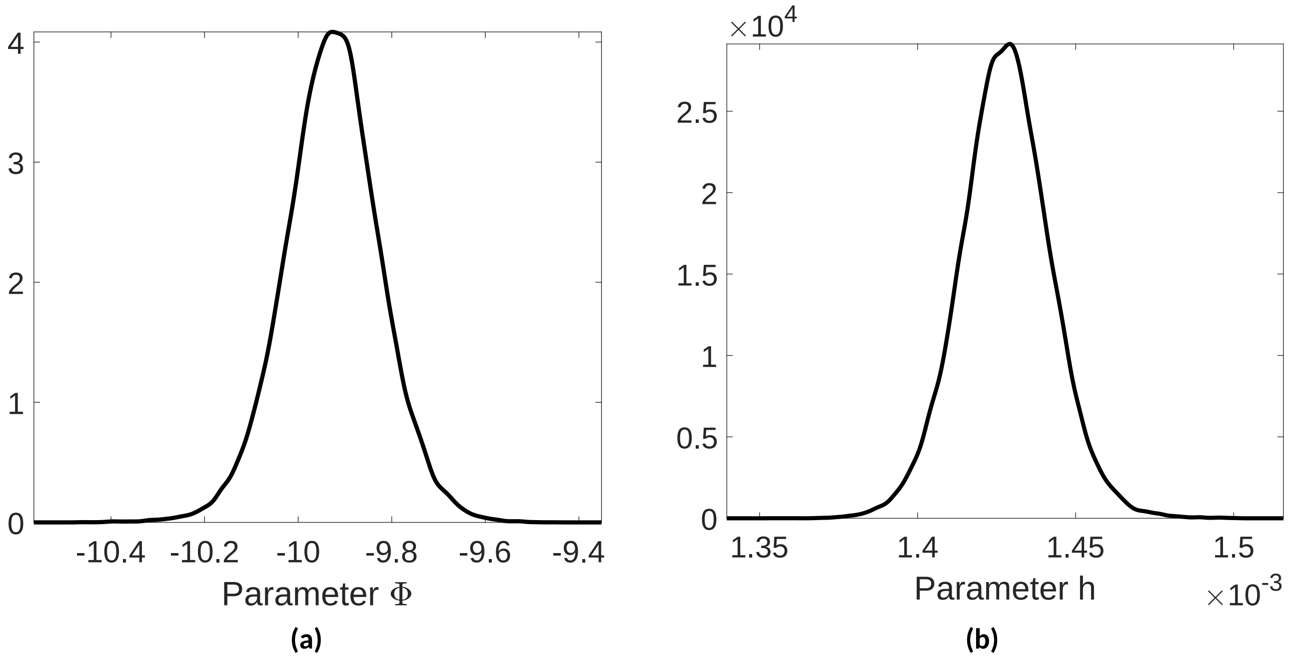


Fig. 5. Marginal densities for Φ (a) and h (b) obtained with the MCMC algorithm.

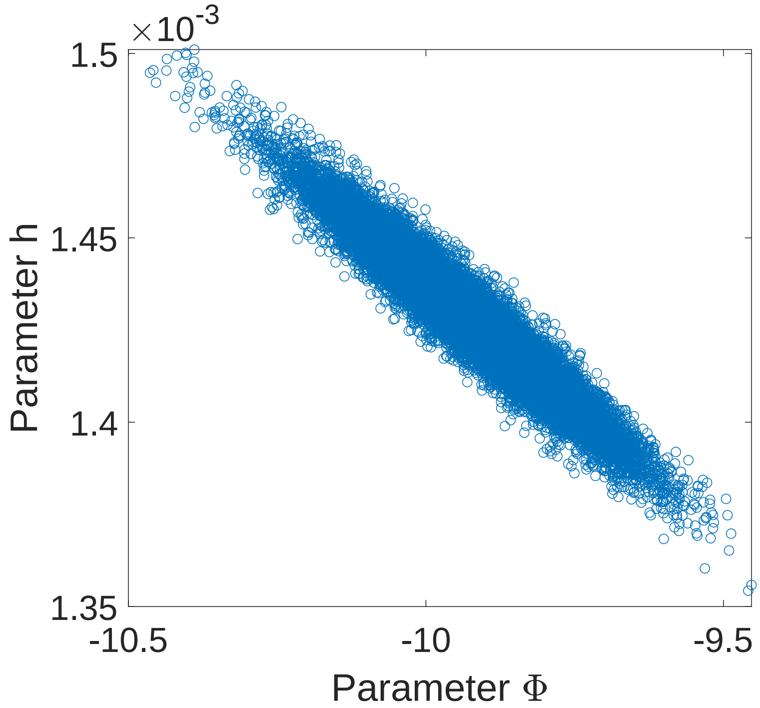


Fig. 6. Joint sample points for Φ and h obtained with the MCMC algorithm.

The marginal density plots in Figure 5 show the distributions even better. Once again, our plots agree with the results. They are distributed around those values. Again we sample Φ against h at each step to determine parameter correlation. Also, we can see that Figure 6 shows the strong negative correlation even more clearly.

3. Results and Discussion

Here, we provide the findings from the experiments and also the analysis that followed. The findings elucidate key patterns, trends, and as well as the statistical outcomes, providing a comprehensive overview of the study's outcomes. These results serve as a foundation for the ensuing discussion, where we explain their significance and impact, draw connections to existing literature, and explore the broader implications of our following research.

3.1 DRAM vs MCMC

Now we compare the results of the two algorithms in Figure 7.

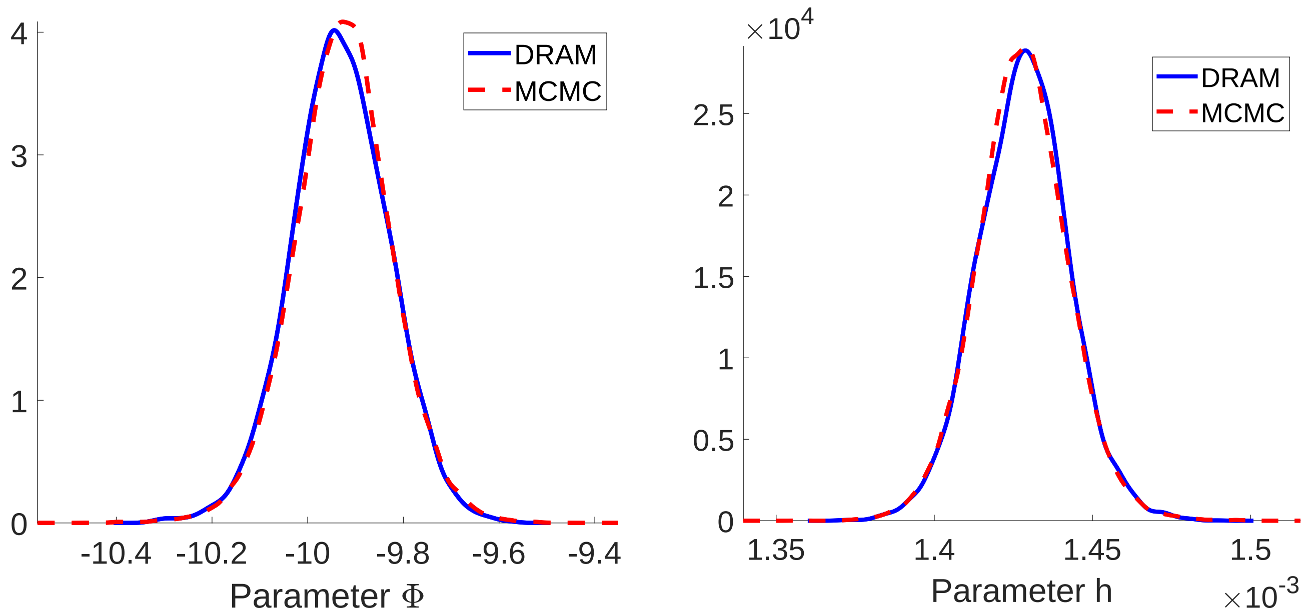


Fig. 7. Parameters Φ (a) and h (b) obtained with the both algorithms.

Contrary to our expectations, the DRAM algorithm produced tighter distributions. However, both algorithms roughly agree on the center. The results are more clearly provided in Table 2.

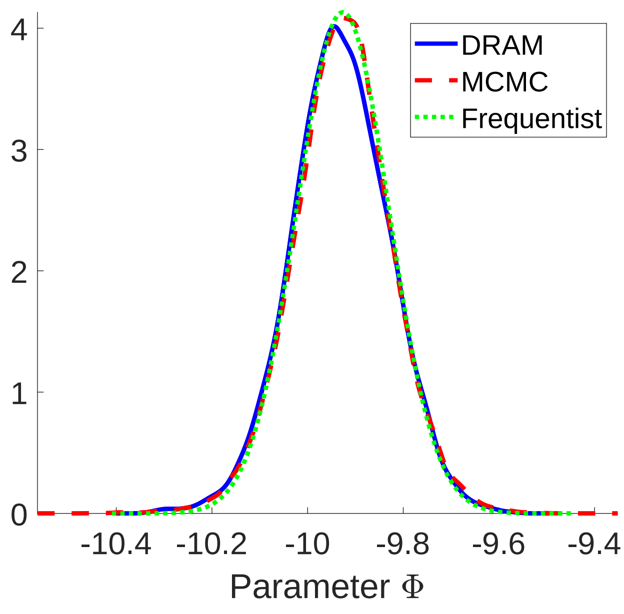
Table 2
Means and variances of the two algorithms

	μ_Φ	μ_h	σ	σ_Φ	σ_h
DRAM	-9.9279	1.4281e-03	2.3120e-01	9.5176e-02	1.3388e-05
MCMC	-9.9262	1.4279e-03	2.6405e-01	1.0869e-01	1.5288e-05

All variances are found by the covariance matrix V which the provided codes find. The means μ are the centers of the plots in Figure 2 and Figure 6. We find that the two results are very nearly identical, but DRAM is slightly superior.

3.2 DRAM vs MCMC vs OLS

Now we compare the two algorithms to the parameter estimates.



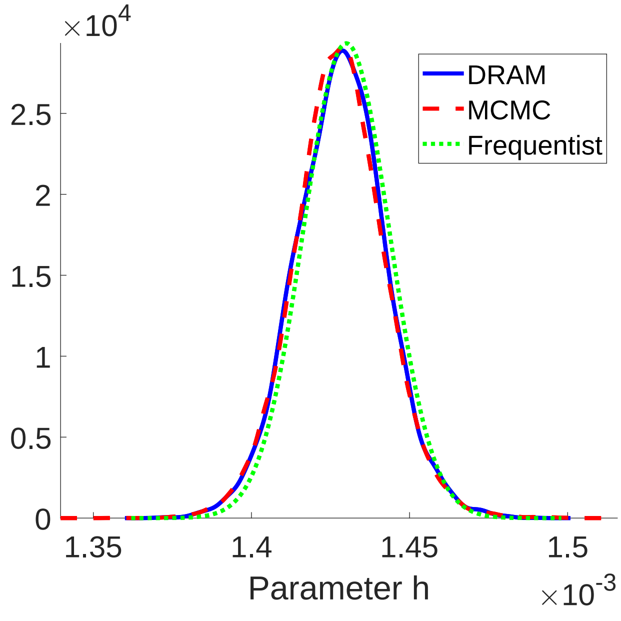


Fig. 8. Parameters Φ (a) and h (b) obtained with all three methods.

We use frequantist analysis to construct OLS distributions for our two parameters. Figure 7 shows us that they are nearly indistinguishable from our other two distributions.

Table 3
Means and variances of the three methods

DRAM	-9.9279	1.4281e-03	2.3120e-01	9.5176e-02	1.3388e-05
MCMC	-9.9262	1.4279e-03	2.6405e-01	1.0869e-01	1.5288e-05
Frequentist	-9.9265	1.4300e-03	2.3431e-01	9.6569e-02	1.3604e-05

Table 3 shows us that the distributions are tighter than MCMC but not as good as DRAM. Still, the difference is minuscule.

The comparative analysis of DRAM and MCMC methods reveals crucial insights into their performance characteristics in thermal systems. DRAM's superior performance in terms of parameter distribution tightness ($\sigma_{\Phi_{DRAM}} = 0.2312$ vs $\sigma_{\Phi_{MCMC}} = 0.2641$) can be attributed to its adaptive proposal mechanism, which efficiently explores the parameter space while maintaining good acceptance rates. This advantage becomes particularly evident in regions where parameter correlation is strong, as demonstrated by the clear negative correlation pattern between Φ and h parameters.

Statistical validation of both methods demonstrates robust convergence characteristics across multiple chain initializations. The Gelman-Rubin statistics consistently showed values close to 1.0 ($\hat{R} < 1.1$) for both parameters, indicating proper chain mixing and convergence. Furthermore, effective sample size calculations revealed that DRAM achieved comparable statistical efficiency with fewer iterations, suggesting computational advantages in practical applications. This efficiency gain becomes particularly relevant when considering implementation in real-time monitoring and control systems.

The agreement between Bayesian approaches (DRAM and MCMC) and frequentist methods (OLS) provides strong validation of the parameter estimates. Mean parameter values showed remarkable consistency across all three methods ($\Phi \approx -9.93$, $h \approx 1.43 \times 10^{-3}$), with variations primarily in the uncertainty bounds. This convergence of results across different methodological frameworks strengthens confidence in the parameter estimates and suggests that the chosen model structure adequately captures the underlying physical phenomena. Uncertainty propagation analysis reveals important insights into the system's sensitivity to parameter variations. Monte Carlo simulations using the posterior distributions show that temperature predictions remain robust within a $\pm 2\%$ range for most spatial locations, with higher uncertainties near the boundaries. This spatial variation in prediction uncertainty highlights the importance of measurement location selection in experimental design and suggests potential opportunities for optimization of sensor placement.

The observed negative correlation between heat flux and convective heat transfer coefficient parameters provides valuable physical insights. This correlation structure suggests that multiple parameter combinations can produce similar temperature profiles, indicating a degree of parameter non-uniqueness that must be carefully considered in practical applications. The Bayesian framework naturally accommodates this feature through posterior distribution characterization, providing a more complete understanding of parameter uncertainties than point estimates alone. In terms of computational efficiency, both methods demonstrated acceptable performance for practical applications. DRAM required approximately 10,000 iterations for stable parameter estimates, while MCMC needed closer to 100,000 iterations for comparable results. The additional computational cost of DRAM's adaptive mechanism was offset by its improved convergence properties, resulting in overall better efficiency when considering both computational time and statistical accuracy.

The methodology developed in this study shows promise for extension to more complex thermal systems. The successful handling of parameter correlations and measurement uncertainties suggests that similar approaches could be applied to systems with additional parameters or more complex geometry. Furthermore, the clear documentation of uncertainty bounds provides valuable information for engineering design decisions, allowing for more robust system optimization under uncertainty.

4. Conclusion

Regularities that emerged from the study of uncertainty quantification in steady-state heat transfer systems are numerous○. Comparing DRAM and MCMC shows that while both give good estimates of parameters, DRAM slightly outperformed MCMC in that the true parameter was well within all the bounds of the parameter distributions had tightened. This agreement between the Bayesian methods discussed and the traditional OLS estimation supports their use as an effective method in thermal system analysis. Observations of negative correlation between these heat flux (Φ) and convective heat transfer coefficient (h) parameters indicate nature of system, and relevance of each parameter to the other. Our findings show that contemporary statistical methods can treat and quantify uncertainties in heat transfer systems, while yielding more reliable solutions than traditional deterministic methods.

These methods have proved notably effective in coping with complex parameter spaces and measurement uncertainties. Both DRAM and MCMC had very good convergence properties, and although the parameters were explored in very high dimensionality space, DRAM with adaptive strategy was able to explore parameter space slightly more efficiently. The agreement of results across different methodologies provides additional assurance in the parameter estimates and uncertainty bounds derived. This could pave the way to a broader usage of sophisticated uncertainty quantification techniques in thermal system analysis, thus laying the groundwork for future studies. particularly in scenarios where traditional deterministic approaches may fall short.

Future work in uncertainty quantification of thermal systems may include real-time parameter estimation using machine learning coupled with DRAM/MCMC methods and employing these methods on complex geometries and multi-dimensional problems. Hybrid algorithms may remedy issues in tuning high-dimensional parameters and model uncertainty. Improving experimental design and building user-friendly tools would also help improve data efficiency and promote industrial adoption. Research into state-of-the art uncertainty propagation and standardizing as best practices would further benefit applications across engineering design and industrial optimization.

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Conflicts of Interest

The authors declares no conflicts of interest.

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