Entropy-Based Uncertainty Quantification in Reaction-Diffusion Systems Using the Stochastic Finite Difference Method in Maple

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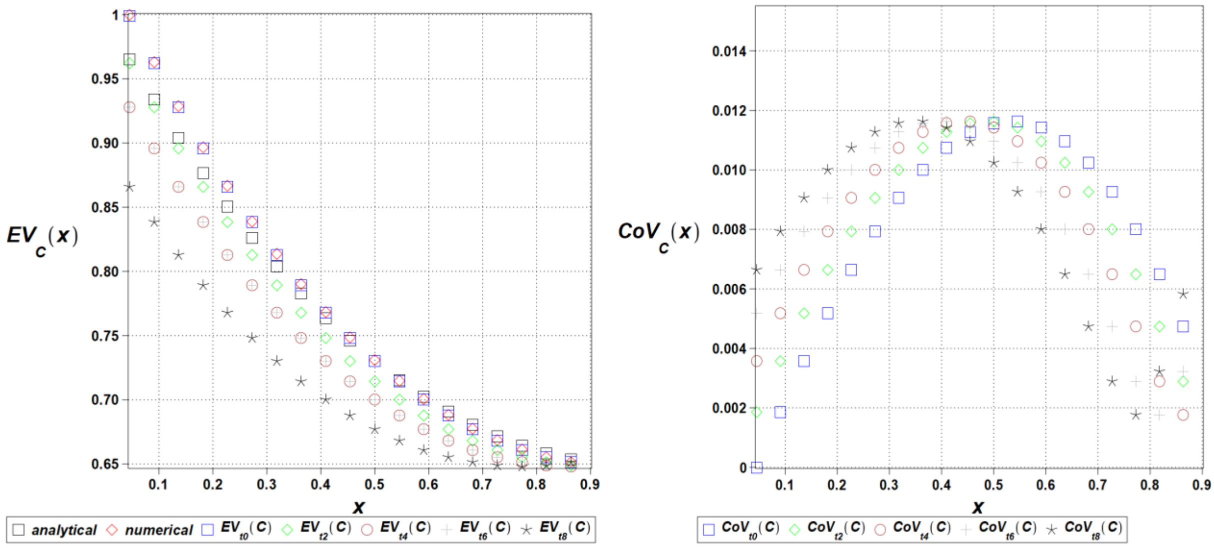
Abstract

Reaction-diffusion equations govern the interplay between molecular transport and chemical reactions, playing a central role in diverse areas such as physics, chemistry, and bioengineering [1,2]. In this contribution, we present a stochastic computational framework implemented in *Maple 2025* for analyzing uncertainty propagation in time-dependent reaction-diffusion systems. Our approach is based on the Stochastic Finite Difference Method (SFDM), enhanced with a generalized stochastic perturbation technique [3]. The implementation enables efficient computation of probabilistic moments up to fourth order, capturing dynamic variability in concentration fields over time and space.

A key innovation of our work is the integration of Shannon entropy as an information-theoretic measure of stochastic uncertainty [4]. Unlike standard metrics such as variance or coefficient of variation, the entropy-based indicator offers a global view of uncertainty by incorporating the full structure of evolving probability distributions. The analysis reveals that entropy dynamics highlight distinct phases of heightened uncertainty propagation that are not always captured by second-moment statistics.



a b

Figure 1. Expected Values (a) and Coefficients of Variation (b) of concentration in time-dependent 1D reaction-diffusion problem.

The stochastic model was developed and executed entirely in Maple 2025, leveraging its symbolic capabilities to represent time-dependent random processes as power series with Gaussian-distributed coefficients. Visualization and symbolic post-processing of entropy and probabilistic metrics were also conducted within Maple. The results demonstrate the value of entropy in complementing classical uncertainty quantification tools and provide a deeper understanding of information loss and variability in diffusive transport phenomena.

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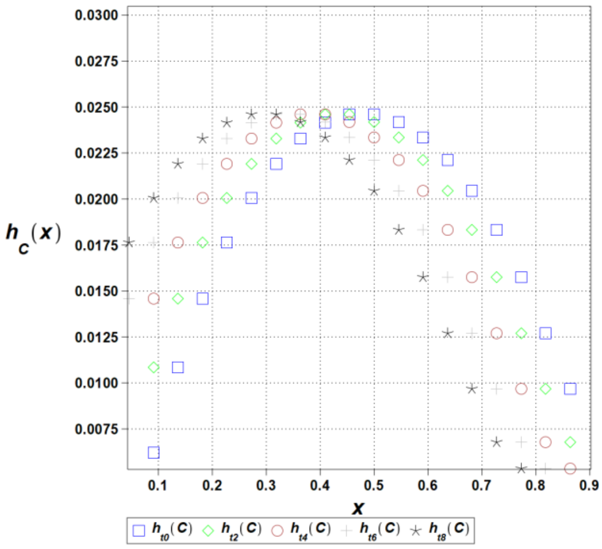

Figure 2. Shannon entropy of concentration in time-dependent 1D reaction-diffusion problem.

The observed entropy dynamics suggest that certain time intervals exhibit heightened uncertainty propagation, which may have implications for reliability analysis and predictive modeling in transport phenomena. A comparison between Fig. 1b and Fig. 2 reveals complementary insights: while the coefficient of variation directly quantifies relative dispersion in concentration profiles, Shannon entropy provides a more global measure of uncertainty by integrating information from the entire probability distribution. Notably, regions of high entropy do not always coincide with high variance, indicating that uncertainty propagation is influenced by both local fluctuations and broader stochastic dynamics.

This work showcases how Maple 2025 can be used as a comprehensive environment for symbolic–numerical modeling, uncertainty quantification, and information-theoretic analysis in time-dependent PDEs.

Keywords: Maple 2025, reaction-diffusion equation, stochastic finite difference method, Shannon entropy, uncertainty quantification, probabilistic modeling

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