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Stochastic Diffusion Problems: Comparison Between Euler-Maruyama and Runge-Kutta Schemes

M. ZAHRI

Department of Computer Science and Mathematics, Johann Wolfganng Goethe-University, Frankfurt am Main, Germany, E-mail: zahri@math.uni-frankfurt.de

Abstract. *Using a class of stochastic Euler and Runge-Kutta methods, we numerically solve a reaction-diffusion equation with additive random excitation. By discretizing the space and the associated stochastic differential system, we present a comparison of the diffusibility behaviors between the schemes above. The model presented here consists of reaction-diffusion equations describing the evolution of the concentration of a population, which we numerically solve using the method of lines. Numerical experiments and Results are given in a two dimensional space.*

Key words: Reaction-diffusion, Stochastic Partial Differential Equations, Method of Lines, Euler-Maruyama, Stochastic Runge-Kutta.

AMS Subject Classifications : 35R60, 60H15, 65L06, 35K57

1. Introduction

Many reaction-diffusion problems in systems biology, chemistry and ecology are modeled either by partial differential equations (PDEs) or by agents based models. These problems have been extensively studied in literature and their numerical solution can be accurately computed provided the diffusion coefficients, reaction excitations and initial data, and boundary conditions. However, modeling real-life reaction-diffusion systems is complicated by indeterminacy and high heterogeneity of the diffusion process, combined with insufficient information characterizing the reactions or the causes. An example concerns the spatio-temporal pattern formation in cell metabolism where the intact living cell is based on a highly complex spatial organization of its constituents. The reactants mediating, and processed by the chemical pathways of cell are heterogeneously distributed through the cytoplasm and cell membranes. The diffusion of reactant species among localized reaction regions within the cell is therefore a central feature of biochemistry.

A number of numerical methods have been developed to analyze self-organizing groups

models. In [11] we have analyzed and simulated a rule model based on a local energy. In the present work, we propose another approach to approximate numerical solutions of stochastic reaction-problems, which can be applied to agents based model. The central idea is to discretize the spatial variable and keep the time continuous in the considered problem. This results in a semi-discrete system of Itô stochastic differential equations, which are solved using numerical techniques developed and used in literature. The proposed approach, known as method of lines, has been widely used to solve deterministic boundary-value problems. For example we refer to [5,9,10]. The spatial discretization in this method can be carried out using finite difference, finite element, or finite volume methods. The dimension of the derived stochastic differential systems depends on the number of gridpoints used in the spatial discretization. We formulate our approach for a second-order finite volume method which incorporates slope limiters in its reconstruction to preserve monotonicity in the computed solutions. We consider a class of stochastic Euler-Maruyama (EM) and Runge-Kutta (RK) methods studied in [12,6,7] for the time integration of stochastic differential equations. The emphasis is given to a second-order explicit RK method with two stages easy to implement and linearly stable, provided the condition for linear stability for diffusion as well as for the Courant-Friderichs-Lewy (CFL) condition are both satisfied.

This paper is structured as follows. Preliminaries on stochastic reaction-diffusion problems are stated in section 2. In section 3, we formulate the stochastic integration schemes. This section includes a passage from partial differential equation to stochastic Runge-Kutta scheme for time integration. Numerical results are presented in section 4 while section 5 contains concluding remarks.

2. Stochastic Reaction-Diffusion Problem

Let $(\Omega, \mathcal{F}, P)$ be a probability space, where Ω is the space of basic outcomes, $\mathcal{F}$ is the σ-algebra associated with Ω, and P is the (probability) measure on $\mathcal{F}$. This σ-algebra can be interpreted as a collection of all possible events that could be derived from the basic outcomes in Ω, and that have a probability that is well defined with respect to P. A random variable X is a mapping $X : \Omega \rightarrow \mathbb{R}$. The L^p-norm of a random variable can be defined as $\|X\|_p = \langle |X|^p \rangle$, for $0 < p < \infty$, where $\langle \cdot \rangle$ denotes the operation of mathematical expectation.
Equipped with this norm, the space L^p is a Banach space of all random variables X defined on $(\Omega, \mathcal{F}, P)$ and having a finite norm.

Our concern in the current work is on developing a novel numerical method for solving a reaction-diffusion problem of with a right side stochastic excitation of the following form

$$\partial_t u(t,x) - (D\, \partial^2_{xx} u(t,x)) = F(t,x)\zeta(t,x), \qquad (t,x) \in (0,T] \times \mathcal{D}, \tag{1}$$

where t is the time variable, x the space coordinate, ∂_t and ∂_x denote derivatives with respect to t and x, respectively. The function $u(t,x)$ represents for example, the concentration of a self-organizing homogenous population, and $F(t,x)$ is a linear flux function. Here, $\zeta(t,x)$ is a random noise assumed to be either time-dependent or space-dependent with amplitude σ. In practice, the random process $\zeta(t,x)$ is Gaussian with zero mean and statistically homogeneous with covariance

$$\langle \zeta(t,x)\zeta(s,x') \rangle = 2B(x - x')\delta(t - s),$$

where $B(x)$ is a smooth function and δ is the Dirac function. In (1), D is the diffusion coefficient assumed to be a nonnegative constant. Note that the flux function F may depend on space x, while the coefficient σ can depend on the time t and the solution u as well.
The equation (1) is solved in a bounded spatial domain $\mathcal{D}$ with smooth boundary, for a time interval $(0, T]$, and equipped with the initial condition

$$u(0,x) = u_0(x), \qquad x \in \mathcal{D}, \tag{2}$$

where u_0 is a given initial data. In order to formulate a well-posed mathematical problem, boundary conditions are required for the equation (1). These conditions are problem dependent and their discussion is postponed for section 4 where numerical examples are discussed.
For two-dimensional reaction-diffusion problems, the equation (1) can be formulated in analogous form as

$$\partial_t\, u - (\partial^2_{xx} u + \partial^2_{yy} u) = F(t,x,y)\zeta(t,x,y), \tag{3}$$

Notice that, the considered boundary-value equations have been widely used to model practical problems from engineering and industrial applications. For instance, stochastic advection-diffusion equations, stochastic Burgers equation, and stochastic Navier-Stokes equations [1] are among others.

The reaction-diffusion equation as a stochastic differential equations is interpreted as following

$$du = (\mathrm{D}\partial^2_{xx} u)dt + \sigma(x)dW(t,x), \tag{4}$$

where $dW(t,x)$ is a white noise process satisfying

$$dW(t,x)\; dW(t,x') = 2B(x - x')dt.$$

It is important to note that in our numerical simulations, we have used only an additive white noise as stochastic excitations. The case of multiplicative noise is more difficult to handle and is not with the scope of the present work.

3. Stochastic Schemes for Time Integration

The passage from a system of equation carried out from the discretization of the reaction-diffusion equation to a stochastic differential equation is subject of this section, we use the method of lines proposed to solve the equations (1)-(2) and already tested by [9,10]. Notice that the space and time are treated separately, and a class of stochastic Euler and Runge-Kutta schemes is used to solve the resulted system of differential equations, For more details about these stochastic methods we refer to [6,7,12]. For convenience, we formulate our method for the two-dimensional reaction-diffusion problem (1)-(2) using a finite volume method. The spatial discretization of the equations (1)-(2) can be carried out using the finite difference, finite element, or finite volume methods. In the current work, we adapt a second-order finite volume method for the spatial discretization of (1)-(2). Hence, the spatial domain $\mathcal{D}$ is discretizated into control volumes $[x_{i-1/2}, x_{i+1/2}]$ with uniform dimension $\Delta x = x_{i+1/2} - x_{i-1/2}$. Integrating (1) with respect to x over the control volume and keeping the time t continuous we obtain the following semi-discrete system

$$\frac{dU_{i,j}}{dt} - D\frac{U_{i+1,j} - 2U_{ij} + U_{i-1,j}}{(\Delta x)^2} - D\frac{U_{i,j+1} - 2U_{ij} + U_{i,j-1}}{(\Delta y)^2} = \sigma_i \zeta(t, x_i, y_j) \tag{5}$$

where $U_{i,j}$ is the space average of a generic solution u in the cell $[x_{i-1/2}, x_{i+1/2}] \times [y_{i-1/2}, y_{i+1/2}]$ at time t,

$$U_{i,j}(t) = \frac{1}{\Delta x \Delta y} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{i-1/2}}^{y_{i+1/2}} u(t,x,y)\ dydx.$$

The system (5) can be written as

$$dU_{i,j} = \left(D\frac{U_{i+1,j} - 2U_{ij} + U_{i-1,j}}{(\Delta x)^2} + D\frac{U_{i,j+1} - 2U_{ij} + U_{i,j-1}}{(\Delta y)^2} \right) dt + (\sigma_i \zeta(t, x_i, y_j))dt \tag{6}$$

Notice that the semi-discrete equations (6) can be formulated as a system of Itô stochastic differential equations (SDEs) rewritten in a compact form as

$$d\mathbf{X}_t = \mathbf{F}(t, \mathbf{X}_t)dt + \mathbf{G}(t, \mathbf{X}_t)d\mathbf{W}_t, \tag{7}$$

where $\mathbf{X}_t$ contains the unknown semi-discretized solution, $\mathbf{F}(t, \mathbf{X}_t)$ and $\mathbf{G}(t, \mathbf{X}_t)$ represent respectively, the semi-discrete form of the deterministic differential operator and the stochastic part in (5). If the spatial domain is discretized in M control volumes then, $\mathbf{X}_t$, $\mathbf{W}_t$ and $\mathbf{F}$ are M-valued vectors with entries

$$U_{i,j},\ W_{i,j,t},\ D\frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{(\Delta x)^2} \quad \text{and} \quad D\frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{(\Delta y)^2}$$

respectively. The second term $\mathbf{G}$ in the right-hand side of (7) is an $M \times M$ diagonal matrix with entry σ_i. In what follows we denote by $\mathbf{G}^k$, $k = 1, \ldots, M$ the kth column of the matrix $\mathbf{G}$. Note that, in the case of additive noise, $\mathbf{G}$ depends only of time variable *i.e.*, $\mathbf{G}(t, \mathbf{X}_t) = \mathbf{G}(t)$. It should be stressed that the stochastic differential equation (7) can be obtained by directly discretizing the space in the partial differential equation (4). For more details, we refer to [9,10].

Let the time interval $[0, T]$ be divided into N subintervals $[t_n, t_{n+1}]$ of length Δt such that $t_n = n\Delta T$ and $T = N\Delta t$. We also use the notation $\mathbf{Y}_n = \mathbf{Y}(t_n)$. Applied to the equation (7), the canonical Euler-Maruyama method results

$$\mathbf{Y}_0 = \mathbf{X}_{t_0},$$

$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + \mathbf{F}(t_n, \mathbf{Y}_n)\Delta t + \mathbf{G}^k(t_n)\Delta \mathbf{W}, \qquad n = 0, 1, \ldots, N-1, \tag{8}$$

where the Brownian increment $\Delta \mathbf{W}$ is $N(0, \sqrt{\Delta t}\,)$. It is well-known that the Euler-Maruyama method (8) is only $\mathcal{O}((\Delta t)^{0.5})$ accurate. As described in the previous section, the spatial discretization is $\mathcal{O}((\Delta x)^2)$ accurate. Therefore, in order to preserve an overall second-order accuracy in the presented method, it is necessary that the time integration of the stochastic differential equations (8) should be at least $\mathcal{O}((\Delta t)^2)$ accurate.

Actually, we apply a class of stochastic Runge-Kutta (SRK) methods studied in [6] for the numerical solution of systems of stochastic differential equations. The methods exhibit a weak convergence with second order in the case of additive noise. Thus, the considered error of the SRK approximation $\mathbf{Y}$ is bounded as

$$|\langle\psi(\mathbf{X}_t)\rangle - \langle\psi(\mathbf{Y}(t))\rangle| \le C_\psi\,(\Delta t)^2,$$

with some constant $C_\psi > 0$ for all functionals $\psi \in C_P^6(\mathbb{R}^M, \mathbb{R})$ with polynomial growth and sufficient small time step Δt. The s-stage SRK method applied to the SDE (7) is given by

$$\mathbf{Y}_0 = \mathbf{X}_{t_0},$$

$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + \sum_{i=1}^{s} \alpha_i\,\mathbf{F}(t_n + c_i\,\Delta t, \mathbf{H}_i)\,\Delta t + \sum_{k=1}^{M}\sum_{i=1}^{s} \beta_i\,\mathbf{G}^k(t_n)\,\hat{I}_{(k)}, \tag{9}$$

where the SRK stages are defined for $i = 1, \ldots, s$ as

$$\mathbf{H}_i = \mathbf{Y}_n + \sum_{j=1}^{s} A_{ij}\,\mathbf{F}(t_n + c_j\,\Delta t, \mathbf{H}_j)\,\Delta t + \sum_{l=1}^{M}\sum_{j=1}^{s} B_{ij}\,\mathbf{G}^l(t_n)\,\hat{I}_{(l)}. \tag{10}$$

The random variables $\hat{I}_{(k)}$ used by the SRK method are, for example, independent identically $N(0, \Delta t)$ distributed or simply independent identically distributed with probabilities

$$\mathrm{P}\left(\hat{I}_{(k)} = \pm\sqrt{3\Delta t}\,\right) = \frac{1}{6}, \qquad \text{and} \qquad \mathrm{P}\left(\hat{I}_{(k)} = 0\right) = \frac{2}{3}, \qquad k = 1, \ldots, M.$$

The coefficients appeared in the SRK method (9)-(10) are usually given by the following extended Butcher tableau

$$\begin{array}{c|ccc|ccc} c_1 & A_{11} & \cdots & A_{1s} & B_{11} & \cdots & B_{1s} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c_s & A_{s1} & \cdots & A_{ss} & B_{s1} & \cdots & B_{ss} \\ \hline & \alpha_1 & \cdots & \alpha_s & \beta_1 & \cdots & \beta_s \end{array}$$

Note that the considered SRK method (9) is a simplified version of the more general second-order SRK methods introduced in [6,7]. Since only additive noise is considered, many order conditions turn out to be automatically fulfilled. In the simulations presented in section 4, we have implemented an explicit SRK method with the number of stages $s = 2$. Its associated extended Butcher tableau is

$$\begin{array}{c|cc|cc} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} & 1 & 0 \end{array} \tag{11}$$

It is evident that, due to the stochasticity in the SDE system (7), the SRK method (9)-(11) is used to generate a number N_R of realizations. Thus, a Monte Carlo simulation is performed for the solution samples $\mathbf{Y}_N^{(m)}$ for $m = 1, \ldots, N_R$, and we estimate the expectation of the solution $\mathbf{Y}_N$ at final time T by

$$\langle\psi(\mathbf{Y}_N)\rangle \approx \frac{1}{N_R}\sum_{m=1}^{N_R} \psi\left(\mathbf{Y}_N^{(m)}\right).$$

Note that other SRK methods as those studied in [7] can also be applied for solving the SDE system (7). Their implementation for solving the considered stochastic boundary-value problem (1) can be carried out using the same formalism as described above.

4. Numerical Results

We examine the performance of the proposed method of lines for the stochastic Euler and Runge-Kutta schemes for a class of stochastic reaction-diffusion problems in two dimension space. For each test example and for each scheme we perform $N_R = 10^3$ realizations and statistical moments such as mean and standard deviation are computed. In all our simulations we use variable time steps Δt adjusted at each step according to the canonical diffusion and CFL conditions

$$\Delta t = C\min\left(\frac{h}{\lambda_{\max}}, \frac{2h^2}{D}\right), \quad h = \min(\Delta x, \Delta y), \tag{12}$$

where $\lambda_{\max}$ is the spectral radius and C is a safety factor set to 0.75 for all test cases to ensure the stability of the numerical scheme. Notice that the number of time steps (integer) is given as

$$NTS := \left[\frac{T}{\Delta t}\right] \quad \text{for } T \in \mathbb{R}^+. \tag{13}$$

Reaction-diffusion equation. This example considers the stochastic Reaction-diffusion problem of a uniform constant function one. The equation is of the form

$$\partial_t u(x,y,t) - \nabla \cdot (D\nabla u(x,y,t)) = F(x,y,t); \quad x,y \in \mathbb{R}, t \in [0,T],$$

$$u^0(x,y,0) = 1, \quad F(x,y,t) = 1 + \sum_{i=1}^{5} \delta_{[a_i,b_i]\times[c_i,d_i]}(x,y)\Delta W, \tag{14}$$

where $D = 5 \cdot 10^{-4}$ is a diffusion coefficient, ξW represents a space dependents random noise and the initial solution is $u^0(x,0)$ is given a constant one for all our simulations. The term $\delta_{[a_i,b_i]\times[c_i,d_i]}$ represents a local random excitation. The energy of each concentration is given as:

$$E(t)^2(w) := \int_0^1 \int_0^1 u^2(x,y,t)(w)dxdy, \quad w \in \Omega, \tag{15}$$

where by discritizing the computation domain, we compute in each time step the following term

$$E(t)^2 := \sum_{i=1}^{N}\sum_{i=1}^{N} U_{i,j}^2 \Delta x_i \Delta y_j. \tag{16}$$

The figure 1 illustrate the computational domain and the spatial positions of the randomness sources, which we have called stochastic excitation.

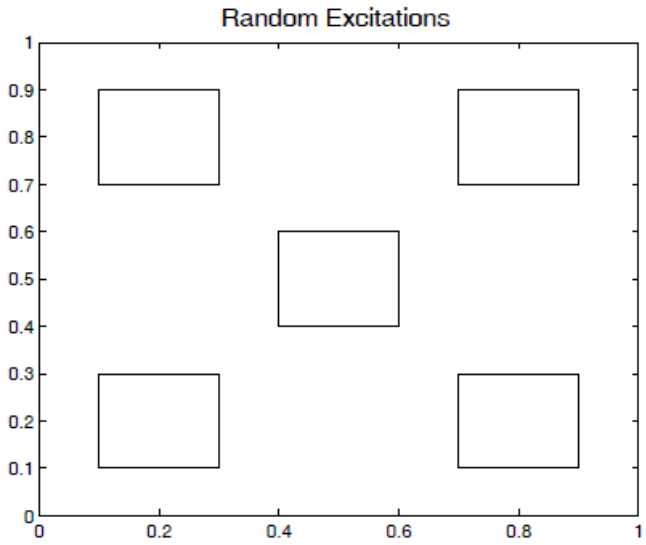

Figure 1 : Spatial positions of stochastic excitation sources.

We run our code to simulate synchronously Euler-Maruyama and Runge-Kutta schemes to compute 1000 realizations solutions of (14). For each scheme, we observe the numericalbehavior of the mean solutions of the 1000 realizations, and compute the standard deviation and the energy.

Using Euler-Maruyama and Runge-Kutta schemes, we present in Figures 2 and 3 respectively, three realizations and the corresponding means at time $T = 5$, $T = 150$ and $T = 200$ of the evolution of the diffusion of test (14). It should be pointed out that with a smaller diffusion coefficient; the effect of uncertainties becomes more visible. This is due to the fact that a stochastic forcing term adds extra diffusion to the reaction-diffusion problem, which could be neglected if the physical diffusion D is large.

In Figures 4 and 5, we show the corresponding contour plots of the same results above. In Figure 6 we present the cut plots of the obtained solutions along with those obtained for the deterministic problem at $t = 5$, 150 and 200. Compared to the deterministic solution, it can be observed that the presence of random perturbation introduces extra diffusion in the mean solution. Note that for this particular type of random perturbation, fluctuations remain in the mean solution at final time $t = T$, compare Figure 6. These fluctuations are inherited from the stochastic structure of (14) and can be removed by increasing the number of realizations used to calculate the mean solution in the method of lines. We should also mention that, one of the key aspects of the present method of lines is that the mass conservation property is satisfied.

In Figure 7 we plot the energy of the solution using both schemes. Notice that the large randomness behavior of realizations using Euler scheme in comparison of Runge-Kutta one is due to its order of convergence. Figures 8 presents the corresponding standard divinations using Euler and RK schemes. The highly indeterminacy of the euler schemes is clearly shown on the first row.

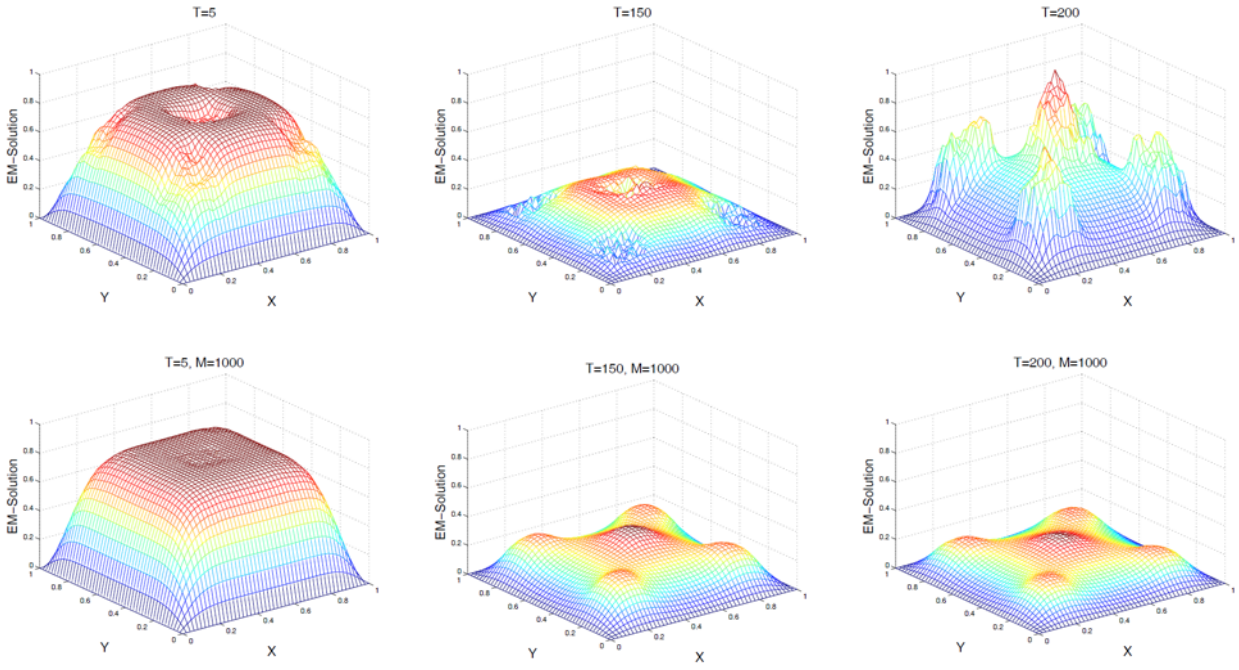

Figure 2: EM simulation (first row) and the corresponding mean solutions (second row).

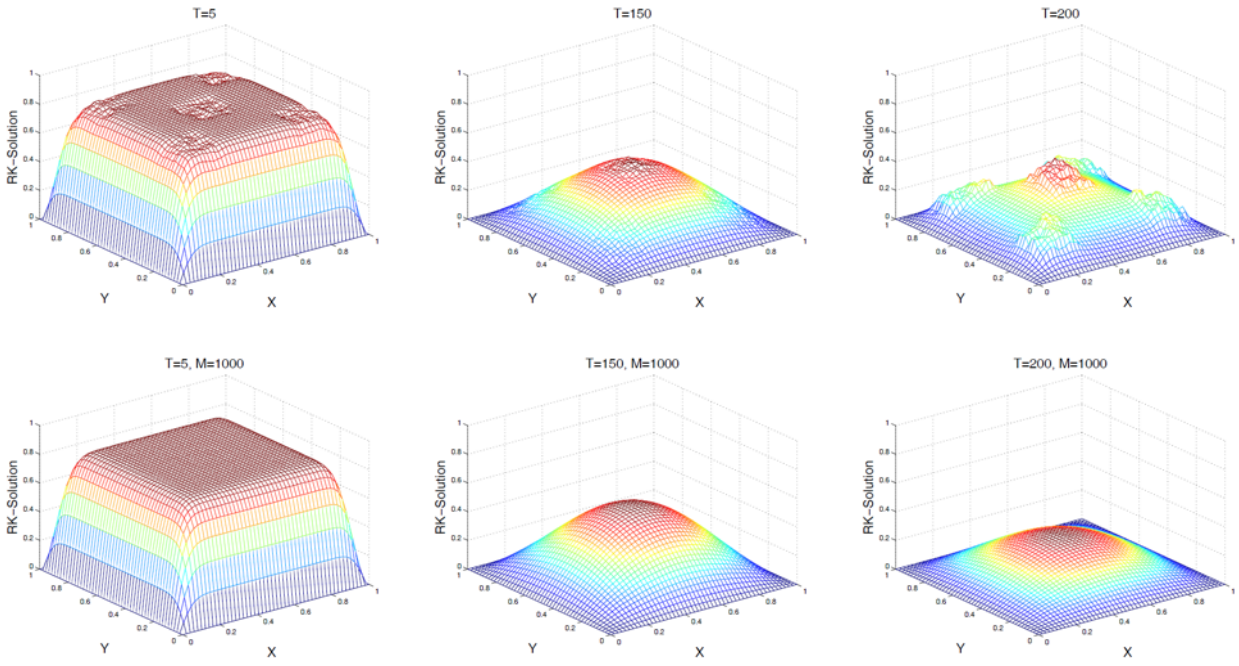

Figure 3: RK simulation (first row) and the corresponding mean solutions (second row).

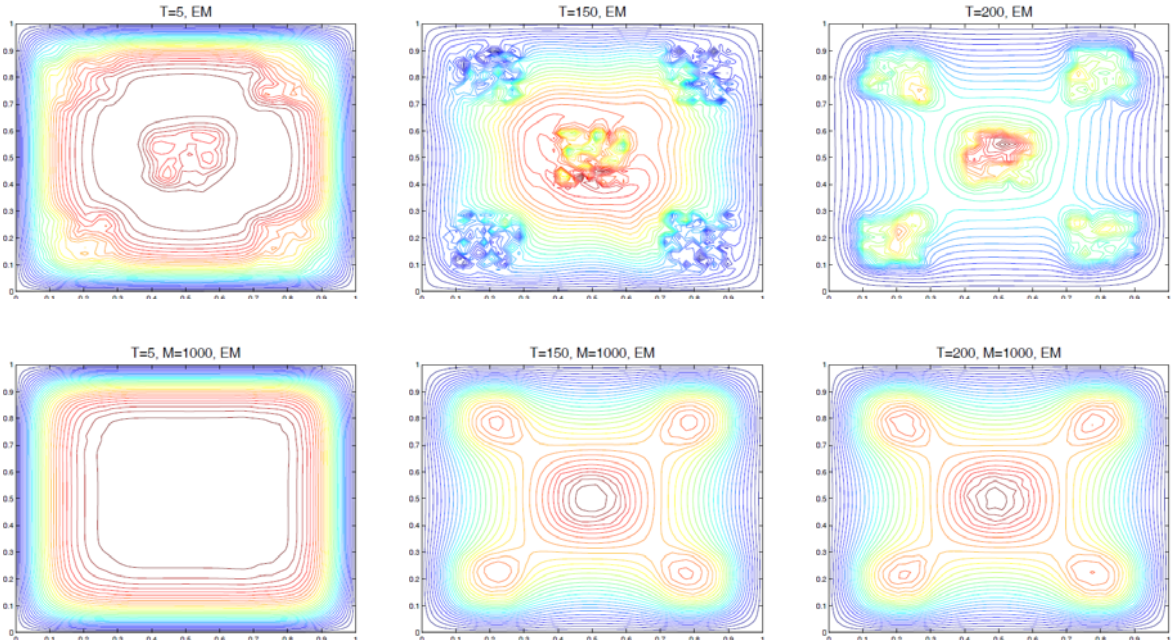

Figure 4: Contour of EM-simulation (first row) and the corresponding means (second row).

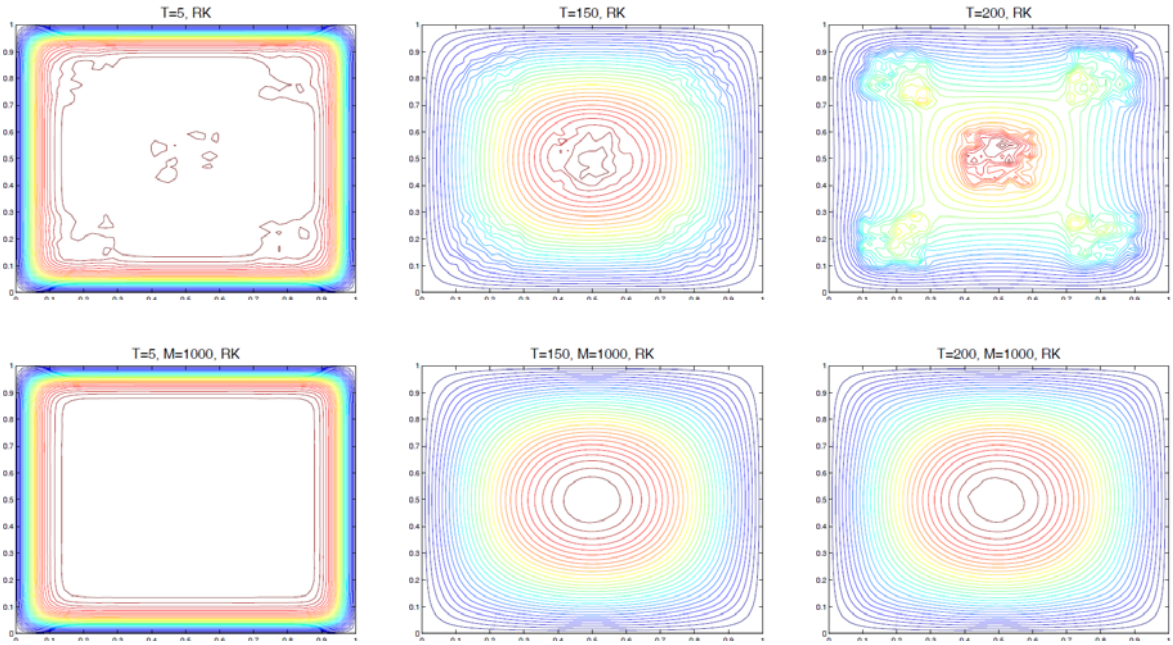

Figure 5: Contour of RK-simulation (first row) and the corresponding means (second row).

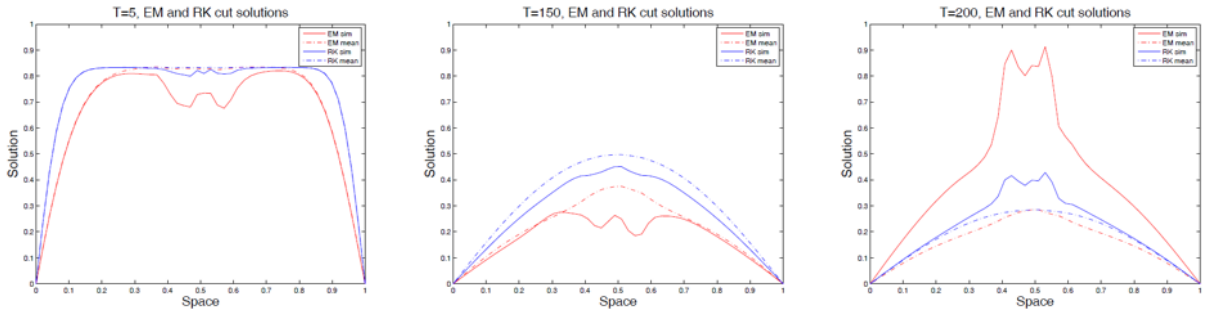

Figure 6: Cut of EM and RK solutions.

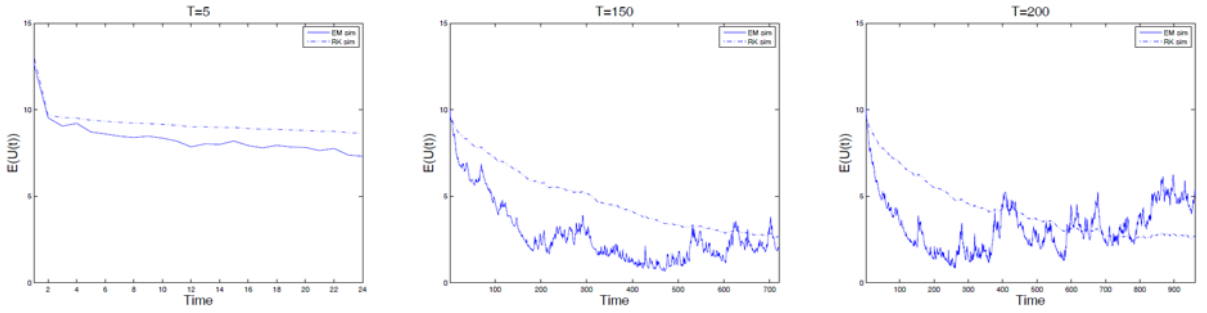

Figure 7: Energy of EM and RK solutions

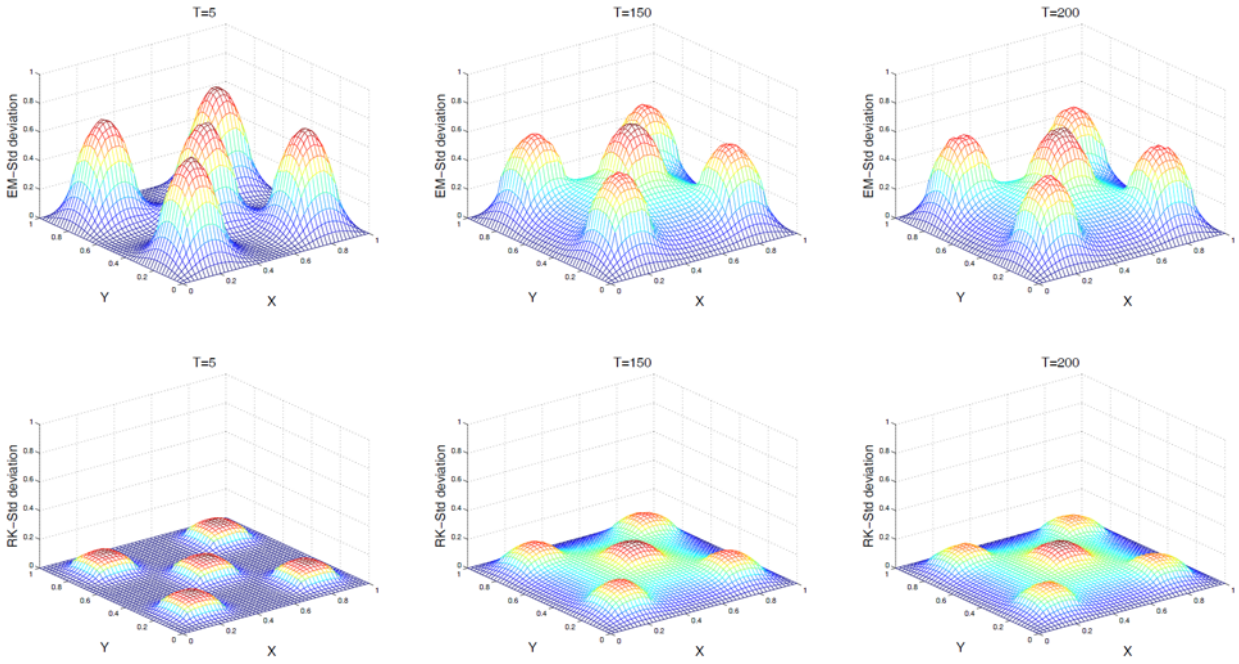

Figure 8: Standard deviation of all simulations EM (first row) RK (second row).

5. Concluding Remarks

We have studied the performance of stochastic Euler-Maruyama and Runge-Kutta methods for solving stochastic reaction-diffusion problems with additive noise. Using method of lines, we implemented and numerically solved the stochastic reaction diffusion equation. Moreover, a numerical comparison is done in order to compare not only the diffusibility behavior of the solutions carried out by using the stochastic schemes mentioned above but also to observe the irregularities of each scheme. We have observed that even if the diffusibility behavior of the two schemes is similar, the Runge-Kutta solution are smoother than the Euler-Maruyama. This is due to the fact that Runge-Kutta is second order scheme. It is important to note that uncertainties in the considered stochastic reaction-diffusion problems have a smoothering influence on the numerical solution. In addition, this procedure combines the attractive attributes of the two methods to yield a procedure for linear or nonlinear stochastic reaction-diffusion problems. The method retains all the attractive features of finite element method such as monotonicity and conservation properties. Furthermore, the scheme does require neither linear solvers for systems of algebraic equations nor special treatment of random fields.

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