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Reaction-diffusion Problems with Random Parameters Using the Generalized Stochastic Finite Difference Method

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Abstract. *The main idea here is to demonstrate the new stochastic discrete computational approach consisting of the generalized stochastic perturbation technique based on the Taylor expansions of the random variables and, at the same time, classical Finite Difference Method on the regular grids. As it is documented by the computational illustrations, it is possible to determine using this approach also higher probabilistic moments and to provide full hybrid analytical-discrete analysis for any random dispersion of input variables unlike in the second order second moment technique worked out before. A numerical algorithm is implemented here using the straightforward partial differentiation of the reaction-diffusion equation with respect to the random input quantity; all symbolic computations of probabilistic moments and characteristics are completed by the computer algebra system MAPLE.*
Keywords: *reaction-diffusion problem, computer algebra system, stochastic finite difference method, the generalized stochastic perturbation technique.*

1. Introduction

The Finite Difference Method (FDM) [1, 2] plays an important role in computational engineering in all those cases, where the additional differential equations

(ordinary or partial) may be solved straightforwardly – i.e. in the heat transfer [3], electromagnetics [4] and geodynamics. So that, it seems to be natural that this method is extended towards its new stochastic versions for some real systems with random parameters solved before using the traditional FDM in deterministic cases. One of such extension methods is the generalized perturbation-based stochastic technique, where the Taylor series expansions of all random quantities lead to the system of equilibrium equations of the ascending order. This method was employed before for different stochastic versions of the Finite Element Method, Boundary Element Method as well as even Finite Difference Method (according to the second order second moment approach [5]) but this implementation for the first time enables for [6] (1) any order stochastic expansion, (2) any probability density function of the random input variable, (3) parametric study with respect to the perturbation parameter and coefficient of variation for the random input as well as (4) analytical derivations of most of discrete hierarchical equations implemented in the symbolic package MAPLE (the other systems like freeware Scilab are also available for this purpose).

The major difference in the comparison to the stochastic versions of the FEM and BEM is the necessity of double differentiation – with respect to the space variable discretized by Δx (4th order derivatives transformed to the finite differences) as well as with respect to the input random variables. Fortunately, since an application of the symbolic calculus, this second differentiation is performed analytically for any available derivatives orders but in the case of a general computer program those derivatives must be implemented into it in a form of the ready-to-use-formulas (or we need to assure the interoperability with the MAPLE environment). The remaining implementation issues are almost the same like in the case of the SFEM and the SBEM, but in a further perspective a comparison with the other stochastic methods like polynomial chaos expansions or Monte-Carlo simulations would be interesting.

Probabilistic implementation of the Finite Difference Method is displayed and discussed here on the example of the reaction-diffusion differential equation and seems to be quite natural because of the numerous sources of uncertainty in chemical reactions and processes; such a computational methodology may essentially influence reliability modeling in the area of chemical engineering. The other reason to deal with this equation comes from various traditional and modern biotechnological applications related to the reaction-diffusion problems [7], which makes them still attractive for the mathematical extensive studies also [8]. Although the general computer program is written in the internal language of the symbolic com-

puting environment MAPLE, the algorithm has a general character and the grid applied to any beam may be essentially densified without any larger programming issues, where a formation and the solution of the ascending order hierarchical equations typical for the perturbation-based methodology will remain the same. This methodology will be further extended towards 2 and 3-dimensional applications, also for transient and nonlinear problems with the random coefficients. Of course, the stochastic perturbation method is not the only one to solve the reaction-diffusion problem with random parameters – we can use the Monte-Carlo simulation [9] or the polynomial chaos expansions [10] as well, however our method fits perfectly into the modern computer algebra systems.

2. Deterministic model

Let us consider the linear boundary value problem relevant to the steady state concentration profiles C(x) in the reaction-diffusion problem in the domain $0 \leq x \leq 1$ [11]. Schematic representation of such a random concentration, but related to the molecules distributed in the planar domain, is given in Fig. 1 below.

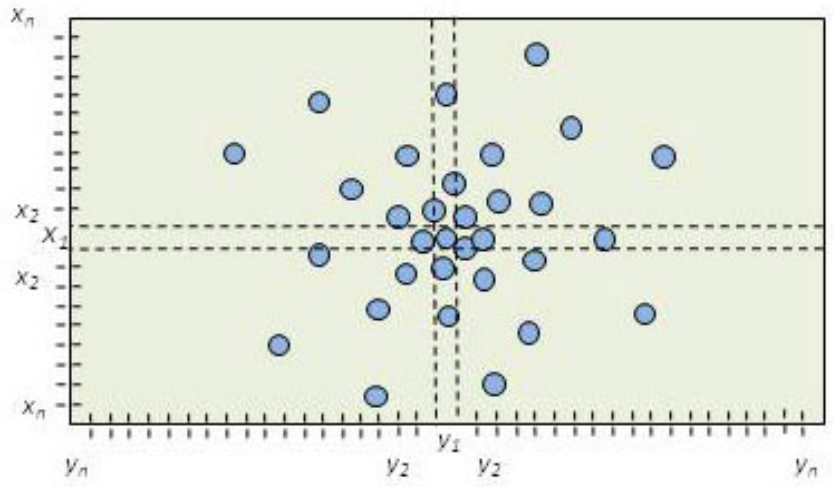

Figure 1. A simple illustration of the example of diffusion problem

Our initial problem is constituted by the following system of equations:

$$\begin{cases} \frac{d^2C}{dx^2} - C = 0 \\ C|_{x=0} = 1 \\ \frac{dC}{dx}|_{x=1} = 0 \end{cases} \tag{1}$$

This equation may be solved using the Finite Difference Method, where the domain $[0, 1]$ is partitioned into the certain number n of the subintervals with the length h, so that $x_i = (i-1)h$ for $i = 1, .., n+1$ and where the resulting concentration is noted as C_i. Now, we express the partial derivatives of this concentration using the central differential approximations as

$$\left(\frac{dC}{dx}\right)_i = \frac{C_{i+1} - C_{i-1}}{2h} \tag{2}$$

$$\left(\frac{d^2C}{dx^2}\right)_i = \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2} \tag{3}$$

Further numerical solution needs an explicit definition of the boundary conditions like

$$C_1 = 1 \tag{4}$$

$$\frac{C_{n+2} - C_n}{2h} = 0 \tag{5}$$

for x_{n+2} being a fictitious node. Therefore, we solve for C_i, $i = 1, \ldots, n$ from the following linear equations system:

$$\begin{cases} C_1 = 1 \\ C_3 - (2 + h^2)C_2 + C_1 = 0 \\ ... \\ C_{n+2} - (2 + h^2)C_{n+1} + C_n = 0 \\ C_{n+2} - C_n = 0 \end{cases} \tag{6}$$

which can be represented as the matrix equation

$$\mathbf{KC} = \mathbf{F} \tag{7}$$

where the coefficients matrix is symmetric and tri-diagonal

$$\mathbf{K} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -(2+h^2) & 1 & 0 & \dots & 0 \\ 0 & 1 & -(2+h^2) & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 1 & -(2+h^2) & 1 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}, ...\mathbf{F} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dots \\ 0 \\ 0 \end{pmatrix} \tag{8}$$

As it is known, the solution to this problem by the FDM has the quadratic convergence since the discretization errors for both first and second order derivatives equal to $O(h^2)$. The solution to the non-linear boundary value problem equivalent to the reaction-diffusion problem like

$$\frac{d^2C}{dx^2} = \alpha C + x^2 + \beta C^3 \tag{9}$$

with the boundary conditions

$$C(0) = 0 = C(1) \tag{10}$$

may proceed with the discretization *nxh* in quite a similar way until one can get

$$\begin{cases} C_1 = 0 \\ C_{i+1} - 2C_i + C_{i-1} - h^2(\alpha C_i + (i-1)^2h^2 + \beta C_i^3) = 0 \\ C_{n+1} = 0 \end{cases} \tag{11}$$

As we will see in the next section, we can also provide for the needs of the stochastic solution the multipoint versions of the Finite Difference Method or apply the error analysis techniques to determine the accuracy of determination of the particular probabilistic moments [8].

3. Reaction-diffusion with random parameter

Now, the following problem is to be solved [11]:

$$\begin{cases} \frac{d^2C(x,\omega)}{dx^2} - C(x,\omega) = 0 \\ C(x,\omega)|_{x=0} = 1 \\ \frac{dC(x,\omega)}{dx}|_{x=b(\omega)} = 0 \end{cases} \tag{12}$$

where $b(\omega)$ is the Gaussian random variable with the probability density function denoted by $p(b)$. The mth order central probabilistic moment of any random function of this parameter, namely $F(b)$, is defined as

$$\mu_m(F(b)) = \int_{-\infty}^{+\infty} (F(b) - E[F(b)])^m p(b) db \tag{13}$$

The basic idea of the stochastic perturbation approach follows the classical expansion idea and is based on an approximation of all input variables and the state functions of the problem via truncated Taylor series about their spatial expectations in terms of a parameter $\varepsilon > 0$. For example, in the case of a random concentration C, the nth order truncated Taylor expansion with random coefficients may be written as

$$C(b) = C(b^0) + \sum_{k=1}^{n} \frac{\varepsilon^k}{k!} (\Delta b)^k \frac{\partial^k C}{\partial b^k} \Big|_{b=b^0} \tag{14}$$

The first component in this expansion, $C(b^0)$, denotes the mean value of the concentration parameter C determined for the expectation $b^0 \equiv E[b]$, where $\Delta b = b - b^0$. Traditionally, the stochastic perturbation approach to all the physical problems is entered by the respective perturbed equations of the zeroth, first and successively higher orders being a modification of the variational integral formulation. Hence, there holds

- one zeroth order partial differential equation

$$\frac{d^2 C^0}{dx^2} - C^0 = 0 \tag{15}$$

- nth order partial differential equation

$$\frac{d^2}{dx^2} \left(\frac{\partial^n C}{\partial b^n} \Big|_{b=b^0} \right) - \frac{\partial^n C}{\partial b^n}|_{b=b^0} = 0 \tag{16}$$

Having solved those equations for C^0 and their higher orders, respectively, (specifically its partial derivatives w.r.t. random input within all discrete points of the grid), we derive the expressions for the expected values and the other moments of the concentration function. Since we propose the Finite Difference scheme to

solve those equations numerically, additionally we need to expand eqn (7) to obtain the Stochastic Finite Difference Method scheme. There holds

- one zeroth equation

$$\mathbf{K}^0\mathbf{C}^0 = \mathbf{F}^0 \tag{17}$$

- one linear equation for the each next perturbation order k

$$\sum_{i=1}^{k}\binom{k}{i}\frac{\partial^i K}{\partial b^i}\frac{\partial^{k-i}C}{\partial b^{k-i}}\bigg|_{b=b^0} = \frac{\partial^k F}{\partial b^k} \tag{18}$$

which need to be solved all consecutively to determine the probabilistic characteristics of the random output. In order to calculate the expected values and higher order probabilistic moments of the random field $C(x;b)$ with x denoting the only spatial coordinate in this system, the same Taylor expansion is employed for the definitions of its probabilistic moments; there holds

$$E[C(b)] = \int_{-\infty}^{+\infty} C(b)p(b)db = \int_{-\infty}^{+\infty}\Big(C(b^0)+\sum_{k=1}^{n}\frac{\varepsilon^k}{k!}(\Delta b)^k\frac{\partial^k C}{\partial b^k}\bigg|_{b=b^0}\Big)p(b)db \tag{19}$$

If there is a high random dispersion in the input random variable and the symmetric probability density function is chosen, then the generalized expansion simplifies for $n = 2m$ to

$$E[C(b)] = C(b^0) + \sum_{k=1}^{m}\frac{\varepsilon^{2k}}{2k!}\frac{\partial^{2k}C}{\partial b^{2k}}\bigg|_{b=b^0}\mu_{2k}(b) \tag{20}$$

where $\mu_{2k}(b)$ denote $2k$th order probabilistic moment of the variable b. When the probability density function is defined as the Gaussian one with the standard deviation $\sigma(b)$, we obtain additionally

$$\mu_{2k+1}(b) = 0, \quad \mu_{2k}(b) = (2k-1)!!\sigma^{2k}(b) \tag{21}$$

Using such an extension of the random input, a desired efficiency of the expected values can be achieved by the appropriate choice of the perturbation parameter and maximum order corresponding to the particular input probability density

function type, probabilistic moments interrelations, acceptable error of the computations, etc. This choice can be made reasonably by the comparative studies with the Monte-Carlo simulations or theoretical results obtained from the direct (i.e. symbolic) integration. Using a definition (13) in a conjunction with the expansion (14) one may provide the second order formula for the third order central probabilistic moment $\mu_3(C(b))$, where, using (19), one obtains

$$\mu_3(C(b)) = \int_{-\infty}^{+\infty} \left(\varepsilon(\Delta b - E[\Delta b]) \frac{\partial C}{\partial b}\Big|_{b=b^0} + \frac{\varepsilon^2}{2}(\Delta b - E[\Delta b])^2 \frac{\partial^2 C}{\partial b^2}\Big|_{b=b^0} \right)^3 p(b)db = \int_{-\infty}^{+\infty} \left(\varepsilon \Delta b \frac{\partial C}{\partial b}\Big|_{b=b^0} + \frac{\varepsilon^2}{2}(\Delta b - E[\Delta b])^2 \frac{\partial^2 C}{\partial b^2}\Big|_{b=b^0} \right)^3 p(b)db \tag{22}$$

Quite similarly one derives the fourth central probabilistic moment of the random concentration in terms of the input random variable b as

$$\mu_4(C(b)) = \int_{-\infty}^{+\infty} \left(\varepsilon(\Delta b - E[\Delta b]) \frac{\partial C}{\partial b}\Big|_{b=b^0} + \frac{\varepsilon^2}{2}(\Delta b - E[\Delta b])^2 \frac{\partial^2 C}{\partial b^2}\Big|_{b=b^0} \right)^4 p(b)db = \int_{-\infty}^{+\infty} \left(\varepsilon \Delta b \frac{\partial C}{\partial b}\Big|_{b=b^0} + \frac{\varepsilon^2}{2}(\Delta b - E[\Delta b])^2 \frac{\partial^2 C}{\partial b^2}\Big|_{b=b^0} \right)^4 p(b)db \tag{23}$$

4. Numerical illustration

The computational domain is partitioned into 20 equal subintervals with the random length, so that the expected values are equal to $E[b] = 1$ and $E[h] = 0.05$. Following the properties of random variables one can easily notice that the coefficients of variations of both random variables are equal – they are both assumed to be truncated Gaussian random variables. First we consider the case, where the perturbation parameter value is adopted as equal to 1; as one may notice from Figs. 2 and 3, the 6th order perturbation expansion appeared to be quite sufficient in this particular case.

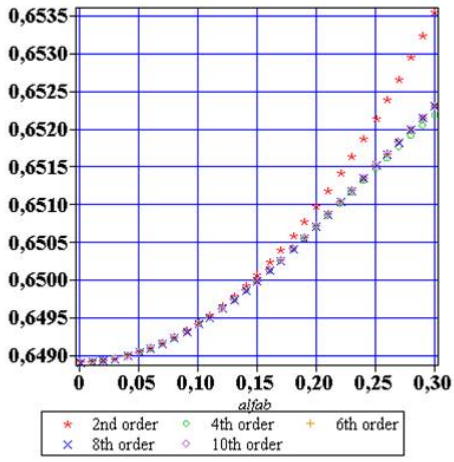

Figure 2. The expected values for the concentration C

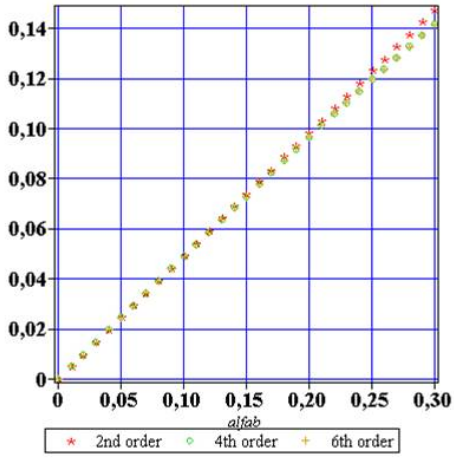

Figure 3. The standard deviations for the concentration C

The results of the analysis are presented in Figs. 2 – 5 – the first graph contains the expected values, next – the standard deviations of the concentration computed for the upper boundary of the domain ($x = l$). The third and the fourth figures show in turn the variability of the third and the fourth central probabilistic moments with

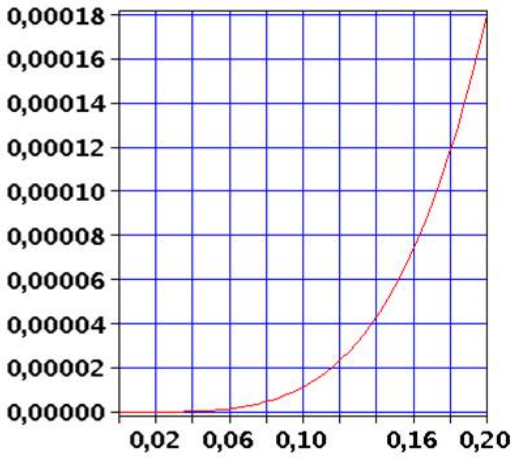

Figure 4. The third central probabilistic moments for the concentration C

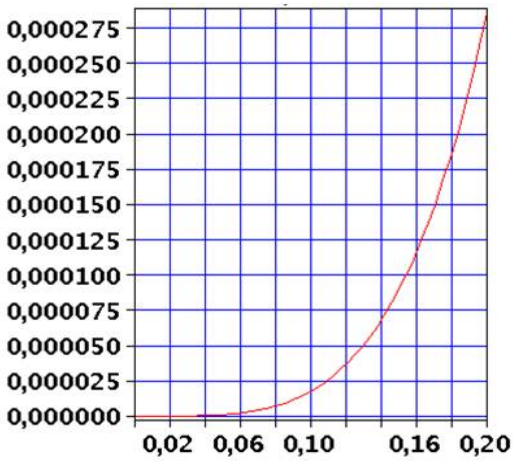

Figure 5. The fourth central probabilistic moments for the concentration C

respect to the input coefficient of variation $\alpha(b) \in [0.0, 0.3]$. The lower limit of this interval is adequate to the deterministic solution, so that the expectations become the deterministic solution and the remaining moments equal 0 for this particular value. Higher orders than the sixth are omitted here for a brevity of the presentation since they do not introduce any extra components to this analysis. As it

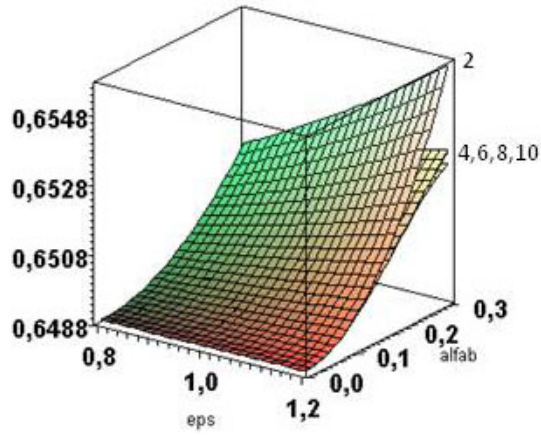

Figure 6. The expected values for the concentration $C = C(\varepsilon, \alpha)$

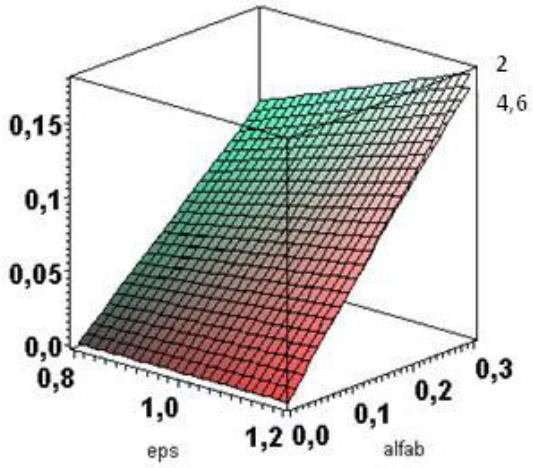

Figure 7. The standard deviations for the concentration $C = C(\varepsilon, \alpha)$

is clear (and can be initially presumed), all central probabilistic moments increase together with an increase of the input coefficient of variation. All those functions

have also positive second derivative with respect to $\alpha(b)$; the exception is noticed in the case of standard deviation, which (equals square root of the second central probabilistic moment) shows almost linear dependence on $\alpha(b)$. Intuitive interpretation of those figures is that the higher uncertainty in the upper edge location, the larger probabilistic moments computed. As we noticed before, the probabilistic convergence of this method is rather fast, at least for the first two probabilistic moments (see Figs. 2 and 3). All of those moments as well as the probabilistic coefficients recovered algebraically from the values collected in Figs. 2 – 5 may be further used in reliability analysis of the first or second order.

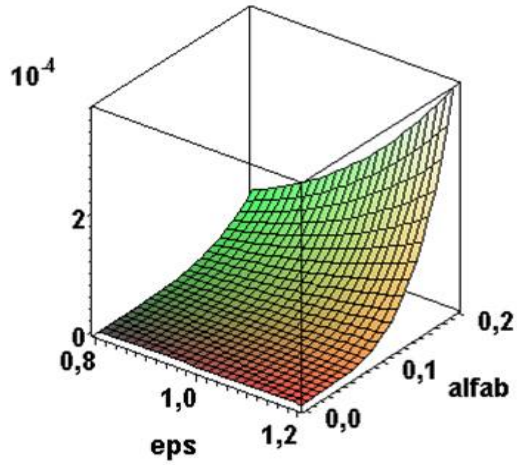

Figure 8. The third central probabilistic moments for the concentration $C = C(\varepsilon, \alpha)$

Next, the first four probabilistic moments are computed and presented with respect to two parameters – the coefficient of variation of the input random variable (as above) and, additionally, the perturbation parameter. There are in turn – the expected values (Fig. 6), the standard deviation (Fig. 7), the third (Fig. 8) and the fourth central probabilistic moments (Fig. 9). All the surfaces presented in those figures lead to the conclusion that the coefficient of variation seems to be more decisive for all the probabilistic moments variations than the perturbation parameter (for the ranges given on both figures). Further, it is apparent that the variations of the expected values and the standard deviations with respect to the perturbation parameter are almost linear, while for the third and fourth probabilistic moments this

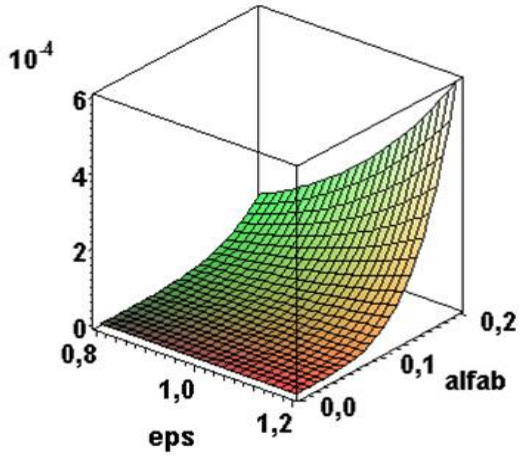

Figure 9. The fourth central probabilistic moments for the concentration $C = C(\varepsilon, \alpha)$

interrelation become highly nonlinear. Let us note that, in the same time, the interrelation between the expected values of the solution and the input coefficient of variation remains nonlinear, while between the solution's standard deviation and this input coefficient – linear; therefore, the influences of those two parameters on the final probabilistic moments remain fully independent. As one may expect, the perturbation parameter, the coefficient of random input and the solution probabilistic moments increase together and there is no exception from this rule in our computational experiment evidence; this type of monotonous behavior follows directly the analytical relations derived above. Let us underline that the polynomial expansions for the probabilistic moments of the FDM solution are available for the computer algebra software applications only, unlike for the FORTRAN implementations of the SOSM methodology [12].

5. Conclusions

The generalized Stochastic Finite Difference Method seems to be the efficient probabilistic computational tool to model the reaction-diffusion problems and should be further developed for the nonlinear and unsteady problems, also for the inhomogeneous domains [13] in 2D [14] or 3D. As it was demonstrated

before, it can be applied to the problems with physical (mechanical or chemical) parameters but stochastic boundary waviness, although essentially more complicated, may be also modeled. It is seen that the stochastic methodology described above may be applied directly to the implementations of the FDM on the irregular grids also [15].

As it was documented above, the application of the symbolic algebra environment enabled for the solution to the generalized stochastic-perturbation based discrete equations system as well as to introduce the perturbation parameter ε into the final solution expansions and the resulting probabilistic moments. Thanks to the very extended linear algebra tools in MAPLE (as well as the remaining CAS programs) we can provide a solution to the linear equations systems with both symmetric and non-symmetric coefficients matrix using the same algorithm for the stochastic perturbation scheme. Such a dual implementation is completely unavailable for the academic software (Finite Difference Method or Finite Element Method) coded traditionally in FORTRAN or C++, for instance.

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