Some Notes on Numerical Convergence of the Stochastic Perturbation Method

Marcin Kamiński

Division of Mechanics of Materials, Technical University of Łódź
Al. Politechniki 6, tel/fax 48-42-6313551, 93-590 Łódź, POLAND
marcin@kmm-lx.p.lodz.pl
http://kmm.p.lodz.pl/pracownicy/Marcin_Kaminski

Abstract. This paper concerns numerical convergence studies of the general n-th order stochastic perturbation technique applied frequently to randomize some boundary value of boundary initial problems in computational mathematics as well as to additionally modify numerical methods in engineering. The general scheme of the technique is introduced and invented in terms of the coupled viscous fluid dynamics problem. Symbolic mathematics package MAPLE and its visualization tools are engaged to perform computational studies on convergence of the first two probabilistic moments for the simple unidirectional Couette Newtonian fluid flow. The methodology and its implementations need many further improvements, however their efficient applications in various engineering problems are possible now.

1 Introduction

Various stochastic computational techniques have been implemented until now using both theoretical and computational methods, i.e. stochastic spectral approaches, some Monte-Carlo simulation (MCS) techniques [3,5] and various numerical realizations of the perturbation technique [6,7]. As it is known, the usage, precision and computational implementation algorithms strongly depend on the input random fields types, their correlation functions as well as the interrelations between the first few probabilistic moments. Some of those issues are raised in the paper in terms of the Gaussian input inserted in the boundary value problem with random parameters being solved by the stochastic perturbation method. This method applied frequently in its second order moment version has the well-known limitations on the input coefficients of variation and that is why the traditional approach is extended to the sixth order technique.

Convergence of the perturbation method is discussed next using a simple symbolic computations comparison of second, fourth and sixth order approximation of the expected values with deterministic solution for a simple test problem for the random output being inversion of the Gaussian variable. It shows that widely discussed in the literature convergence of perturbation technique applications strongly depends on the transformation type between the output and input random variables. Further numerical studies especially of comparative nature with another stochastic methods are necessary – improved Monte-Carlo analyses of analogous flow problems to establish

P.M.A. Sloot et al. (Eds.): ICCS 2003, LNCS 2657, pp. 521–530, 2003.

the most efficient perturbation orders for various input and perturbation parameters (to be performed using the FEM [1,2] package ANSYS, for instance) and theoretical analysis for the non-Gaussian variables as well.

2 General Stochastic Perturbation Technique

Let us introduce the random vector by $b_r(\mathbf{x})$ and its probability density functions by $p(b_r)$ and $p(b_r,b_s)$, respectively, for r,s=1,...,R, where R represents the total number of different input random fields. Then, the first two probabilistic moments of $b_r(\mathbf{x})$ are defined by [9]

$$E[b_r] \equiv b_r^0 = \int_{-\infty}^{+\infty} b_r p(b_r) db_r , \tag{1}$$

and

$$\mathrm{Cov}(b_r; b_s) \equiv S_{rs} = \int_{-\infty}^{+\infty} \left[b_r - b_r^0\right]\left[b_s - b_s^0\right] p(b_r; b_s) db_r db_s . \tag{2}$$

The basic idea of the stochastic perturbation approach is to expand all input variables and all the state functions of the given problem via Taylor series about their spatial expectations using some small parameter $\psi>0$. For example, in case of random parameter ρ the following expression is employed:

$$\rho = \rho^0 + \psi \rho^{,r} \Delta b_r + \tfrac{1}{2}\psi^2 \rho^{,rs} \Delta b_r \Delta b_s + \ldots + \tfrac{1}{n!}\psi^n \rho^{(n)} \prod_{i=1}^{R} \Delta b_{r_i} , \tag{3}$$

where

$$\psi \Delta b_r = \psi\left(b_r - b_r^0\right) \tag{4}$$

is the first variation of b_r about its expected value

$$\psi^2 \Delta b_r \Delta b_s = \psi^2 \left(b_r - b_r^0\right)\left(b_s - b_s^0\right) \tag{5}$$

is the second variation of b_r, b_s about b_r^0 and b_s^0, respectively. Analogously, n^{th} order variation can be expressed as

$$\psi^n \prod_{i=1}^{R} \Delta b_{r_i} = \psi^n \left(b_{r_1} - b_{r_1}^0\right)\ldots\left(b_{r_R} - b_{r_R}^0\right). \tag{6}$$

Symbol $(.)^0$ represents value of any function (.) taken at the expectations b_r^0, while $(.)^{,r}$ and $(.)^{,rs}$ denote the first and the second partial derivatives with respect to b_r

evaluated at b_r^0, respectively. Let us analyze further the expected values of any state function defined as

$$E[f(t,b_R);b_R] = \int_{-\infty}^{+\infty} f(t)p(b_R)db_R$$
$$= \int_{-\infty}^{+\infty}\left(f^0 + \psi f^{,r}\Delta b_r + \frac{1}{2}\psi^2 f^{,rs}\Delta b_r \Delta b_s + \ldots + \frac{1}{n!}\psi^n f^{(n)}\prod_{i=1}^{R}\Delta b_{r_i}\right)p(b_r)db_r \tag{7}$$

Adopting perturbation parameter ψ as equal to 1 and eliminating higher than the second order terms, it yields

$$E[f(t,b_R);b_R] = \int_{-\infty}^{+\infty} f(t)p(b_R)db_R =$$
$$\int_{-\infty}^{+\infty}\left(f^0 + f^{,r}\Delta b_r + \frac{1}{2}f^{,rs}\Delta b_r \Delta b_s\right)p(b_r)db_r \tag{8}$$
$$= 1\times f^0(t) + 0\times f^{,r}(t) + \frac{1}{2}\times f^{,rs}(t)S^{,rs} = f^0(t) + \frac{1}{2}f^{(2)}(t)$$

If higher order terms are necessary (because of a great random deviation of the input random variable about its expected value), then the following extension can be proposed:

$$E[f(t,b_R);b_R] =$$
$$= 1\times f^0(t,b_R) + \frac{1}{2}\times f^{,rs}(t,b_R)\times Cov(b_r,b_s)$$
$$+ \frac{1}{4!}\times f^{,rstu}(t,b_R)\times Cov(b_r,b_s,b_t,b_u) + \tag{9}$$
$$+ \frac{1}{6!}\times f^{,rstuvw}(t,b_R)\times Cov(b_r,b_s,b_t,b_u,b_v,b_w) + \ldots =$$
$$= f^0(t,b_R) + \frac{1}{2}f^{(2)}(t,b_R) + \frac{1}{4!}f^{(4)}(t,b_R) + \frac{1}{6!}f^{(6)}(t,b_R) + \ldots$$

when all terms with the odd orders are equal to 0 for the Gaussian random deviates. Thanks to such an extension of the random output, any desired efficiency of the expected values as well as higher probabilistic moments can be achieved by the appropriate choice of the parameters m and ψ corresponding to the input probability density function (PDF) type, probabilistic moments interrelations, acceptable error of the computations etc. This choice can be made by comparative studies with the long (almost infinite) series Monte-Carlo simulations or theoretical results obtained from the direct symbolic integration.

Similar considerations for the second order expansion only lead to the following result on the cross-correlations of any state function:

$$Cov\left(f\left(x_i^{(1)};t\right), f\left(x_j^{(2)};t\right)\right) = f^{,r}\left(x_i^{(1)};t_1\right)f^{,s}\left(x_j^{(2)};t_2\right)S^{rs} \tag{10}$$

It can be relatively easy extended to the 6th order approach, for instance. There holds

$$
\begin{aligned}
&\mathrm{Cov}(f,g)= \\
&\int_{-\infty}^{+\infty}\Big(f^{0}+\Delta b_r f^{,r}+\tfrac{1}{2}\Delta b_r\Delta b_s f^{,rs}+\tfrac{1}{3!}\Delta b_r\Delta b_s\Delta b_t f^{,rst}+ \\
&+\tfrac{1}{4!}\Delta b_r\Delta b_s\Delta b_t\Delta b_u f^{,rstu}+\tfrac{1}{5!}\Delta b_r\Delta b_s\Delta b_t\Delta b_u\Delta b_v f^{,rstuv}-E[f]\Big)\times \\
&\Big(g^{0}+\Delta b_c g^{,c}+\tfrac{1}{2}\Delta b_c\Delta b_d g^{,cd}+\tfrac{1}{3!}\Delta b_c\Delta b_d\Delta b_e g^{,cde} \\
&\tfrac{1}{4!}\Delta b_c\Delta b_d\Delta b_e\Delta b_h g^{,cdeh}+\tfrac{1}{5!}\Delta b_c\Delta b_d\Delta b_e\Delta b_h\Delta b_l g^{,cdehl}-E[g]\Big)\times \\
&p(f(b),g(b))db
\end{aligned}
\tag{11}
$$

Hence

$$
\begin{aligned}
&\mathrm{Cov}(f,g)= \\
&\int_{-\infty}^{+\infty}\Delta b_r f^{,r}\Delta b_c g^{,c}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\tfrac{1}{4}\Delta b_r\Delta b_s f^{,rs}\Delta b_c\Delta b_d g^{,cd}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\Delta b_r f^{,r}\,\tfrac{1}{3!}\Delta b_c\Delta b_d\Delta b_e g^{,cde}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\Delta b_c g^{,c}\,\tfrac{1}{3!}\Delta b_r\Delta b_s\Delta b_t f^{,rst}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\tfrac{1}{3!}\Delta b_r\Delta b_s\Delta b_t f^{,rst}\,\tfrac{1}{3!}\Delta b_c\Delta b_d\Delta b_e g^{,cde}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\tfrac{1}{4!}\Delta b_c\Delta b_d\Delta b_e\Delta b_h g^{,cdeh}\,\tfrac{1}{2}\Delta b_r\Delta b_s f^{,rs}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\tfrac{1}{4!}\Delta b_r\Delta b_s\Delta b_t\Delta b_u f^{,rstu}\,\tfrac{1}{2}\Delta b_c\Delta b_d g^{,cd}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\tfrac{1}{5!}\Delta b_r\Delta b_s\Delta b_t\Delta b_u\Delta b_v f^{,rstuv}\Delta b_c g^{,c}p(f(b),g(b))db+ \\
&\int_{-\infty}^{+\infty}\tfrac{1}{5!}\Delta b_c\Delta b_d\Delta b_e\Delta b_h\Delta b_l g^{,cdehl}\Delta b_r f^{,r}p\big(f(b),g(b)\big)db
\end{aligned}
\tag{12}
$$

As it can be recognized from eqn (12), first integral corresponds to the second order perturbation, next three completes 4[th] order approximation and the rest needs to be included to achieve full 6[th] order expansion. After multiple integration and indices transformations one can show

$$\begin{aligned}
&\mathrm{Cov}(f,g) = \mathrm{Cov}(b_r, b_s) \times f^{,r} g^{,s} + \\
&\mathrm{Cov}(b_r, b_s, b_t, b_u) \times \left(\tfrac{1}{4} f^{,rs} g^{,tu} + \tfrac{1}{3!} f^{,r} g^{,stu} + \tfrac{1}{3!} f^{,rst} g^{,u}\right) + \\
&\mathrm{Cov}(b_r, b_s, b_t, b_u, b_v, b_w) \times \\
&\left(\left(\tfrac{1}{3!}\right)^2 f^{,rst} g^{,uvw} + \tfrac{1}{4!}\left(g^{,cdeh} \tfrac{1}{2} f^{,rs} + f^{,rstu} \tfrac{1}{2} g^{,cd}\right) + \tfrac{1}{5!}\left(f^{,rstuv} g^{,w} + g^{,rstuv} f^{,w}\right)\right)
\end{aligned} \tag{13}$$

3 An Application to the Computational Fluid Dynamics Problems

Let us consider for illustration a viscous incompressible flow of a Newtonian fluid in the domain Ω, which can be written as the standard Navier-Stokes formulas

$$\rho\left(\frac{\partial v_i}{\partial t} + v_{i,j} v_j\right) = \sigma_{ij,j} + f_i^B \tag{14}$$

$$v_{i,i} = 0 \tag{15}$$

$$\sigma_{ij} = -p\delta_{ij} + 2\mu\varepsilon_{ij} \text{ where } \varepsilon_{ij} = \tfrac{1}{2}\left(v_{i,j} + v_{j,i}\right) \tag{16}$$

The state variables v_i, ε_{ij}, σ_{ij} denote velocity of the fluid, components of velocity strain and stress tensors, while f_i^B denote the body force vector components. The variables ρ, p, μ denote mass density, pressure, and viscosity, correspondingly; typical boundary conditions for these equations hold for fluid velocities:

$$v_i = \hat{v}_i \,;\; \mathbf{x} \in \partial\Omega_v \quad \text{and} \quad \sigma_{ij} n_j = \hat{f}_i \,;\; \mathbf{x} \in \partial\Omega_\sigma . \tag{17}$$

A weak variational formulation of the problem follows on integration by parts in the weighted residual integral statement with the stress and velocity boundary conditions. Inserting the stochastic expansion of all input parameters and the state functions and equating the same order terms, the following coupled equations are obtained:

$$\begin{aligned}
&\int_\Omega \delta v_i \left(\sum_{k=0}^{n} \binom{n}{k} \rho^{(k)} \dot{v}_i^{(n-k)} + \sum_{k=0}^{n} \binom{n}{k} \rho^{(k)} \left(\sum_{m=0}^{n-k} \binom{n-k}{m} v_{i,j}^{(m)} v_j^{(n-k-m)} \right) \right) d\Omega \\
&+ 2 \int_\Omega \delta\varepsilon_{ij} \left(\sum_{k=0}^{n} \binom{n}{k} \mu^{(k)} \varepsilon_{ij}^{(n-k)} - p^{(n)} \delta_{ij} \right) d\Omega \\
&= \int_\Omega \delta v_i \left(f_i^B\right)^{(n)} d\Omega + \int_\sigma \delta v_i \left(\hat{f}_i\right)^{(n)} d(\partial\Omega)
\end{aligned} \tag{18}$$

$$\int_\Omega \delta p v_{i,i}^{(n)} d\Omega = 0 , \tag{19}$$

$$\int_{\Omega}\delta\theta\left(\sum_{k=0}^{n}\binom{n}{k}\left(\sum_{m=0}^{k}\binom{k}{m}\rho^{(k)}c_p^{(k-m)}\right)\dot{\theta}^{(n-k)}\right)d\Omega+$$
$$+\int_{\Omega}\delta\theta\left(\sum_{k=0}^{n}\binom{n}{k}\left(\sum_{m=0}^{k}\binom{k}{m}\rho^{(k)}c_p^{(k-m)}\right)\left(\sum_{l=0}^{n-k}\binom{n-k}{l}\theta_{,i}^{(l)}v_i^{(n-k-l)}\right)\right)d\Omega+ \tag{20}$$
$$+\int_{\Omega}\delta\theta_{,i}\sum_{k=0}^{n}\binom{n}{k}k_i^{(k)}\theta_{,i}^{(n-k)}d\Omega=\int_{\Omega}\delta\theta\left(q^B\right)^{(n)}d\Omega+\int_{\partial\Omega_q}\delta\hat{\theta}(\hat{q})^{(n)}d(\partial\Omega)$$

It is necessary to multiply each of these equations by the n^{th} order probabilistic moments of the input random variables or fields to get the algebraic form convenient for any symbolic computations. Because of a great complexity of such a solution, the second order perturbation approach is usually preferred. Recursive derivation of the particular perturbation order equilibrium equations can be powerful in conjunction with symbolic packages with automatic differentiation tools only; it can extend the area of stochastic perturbation technique applications in computational physics and engineering outside the random processes with small dispersion about their expected values. Hence, there is no need to implement directly exact formulas for a particular k^{th} order equations extracted from the perturbation – they can be symbolically generated in the system MAPLE, and next converted to the FORTRAN or C++ source codes of the relevant computer software; there has been no software available until now to demonstrate any numerical illustrations in that area. Finally, it should be emphasized that the random input variables must express here the uncertainty in space or in time, separately.

4 Computational Illustration

Stochastic convergence of the perturbation method in flow problems is demonstrated below on the example of unidirectional Couette flow described by deterministic function as [7,8]

$$\rho\nu u=\frac{y^2}{2}\left(\frac{\partial p}{\partial x}\right)+\frac{y}{h}\left\{\rho\nu U-\frac{h^2}{2}\left(\frac{\partial p}{\partial x}\right)\right\}, \tag{21}$$

where ν is the fluid kinematic viscosity. In case of zero pressure gradient from the classical definitions it yields in case of the second order perturbation approach [9]

$$E\left[u\big|_{y=h/2}\right]=\frac{U}{2}+\frac{1}{4}\frac{U}{E^2[h]}\mathrm{Var}(h),\quad \mathrm{Var}\left(u\big|_{y=h/2}\right)=\frac{1}{2}\frac{U^2}{E^2[h]}\mathrm{Var}(h). \tag{22}$$

In case of a single input random variable a general expansion can be proposed as

$$E[f(t,h);h,\psi,m]= \\ = f^0(t,h)+\frac{1}{2}\psi^2\frac{\partial^2 f}{\partial h^2}\mu_2(h)+\frac{1}{4!}\psi^4\frac{\partial^4 f}{\partial h^4}\mu_4(h) \\ +\frac{1}{6!}\psi^6\frac{\partial^6 f}{\partial h^6}\mu_6(h)+...+\frac{1}{(2m)!}\psi^{2m}\frac{\partial^{2m} f}{\partial h^{2m}}\mu_{2m}(h) \tag{23}$$

for any natural m with μ_{2m} being the ordinary probabilistic moment of $2m^{th}$ order. As far as Gaussian variables are analyzed, all central probabilistic moments can be expressed in terms of variances (standard deviations) as

$$\mu_{2m+1}(h)=0, \quad \mu_{2m}(h)=1\cdot 3\cdot ...\cdot(2k-1)\sigma^{2m}(h) \tag{24}$$

and can be included into computational analysis without any further modifications what gives for the 6^{th} order expansion

$$\mu_2(h)=\sigma^2(h)=\mathrm{Var}(h), \mu_4(h)=3\sigma^4(h)=3\mathrm{Var}^2(h), \\ \mu_6(h)=15\sigma^6(h)=15\mathrm{Var}^3(h) \tag{25}$$

Deterministic values are compared against the second, third, fourth, fifth and sixth order perturbation based approximation of the expected values for U=10.0, E[h]=2.0 and its coefficient of variation equal to 0.1 and collected in Fig. 1 for the entire fluid flow domain, whereas for $y \to h$ in Fig. 2.

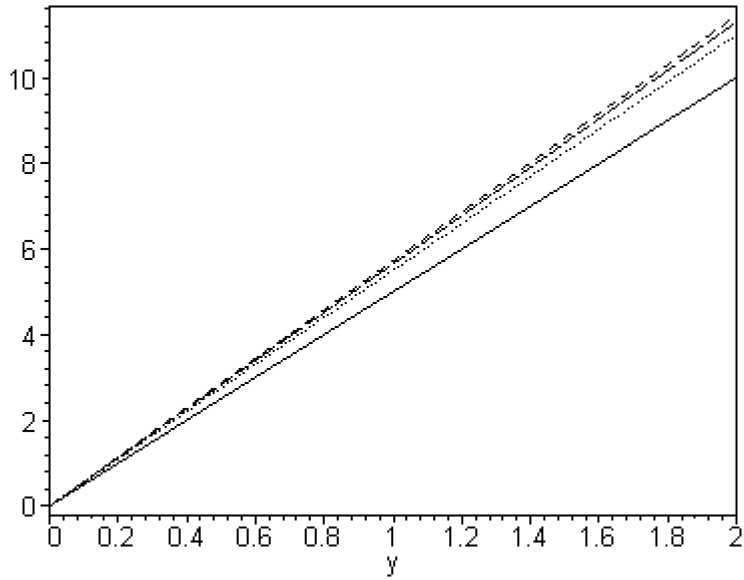

Fig. 1. Stochastic convergence of the expected values for the entire domain

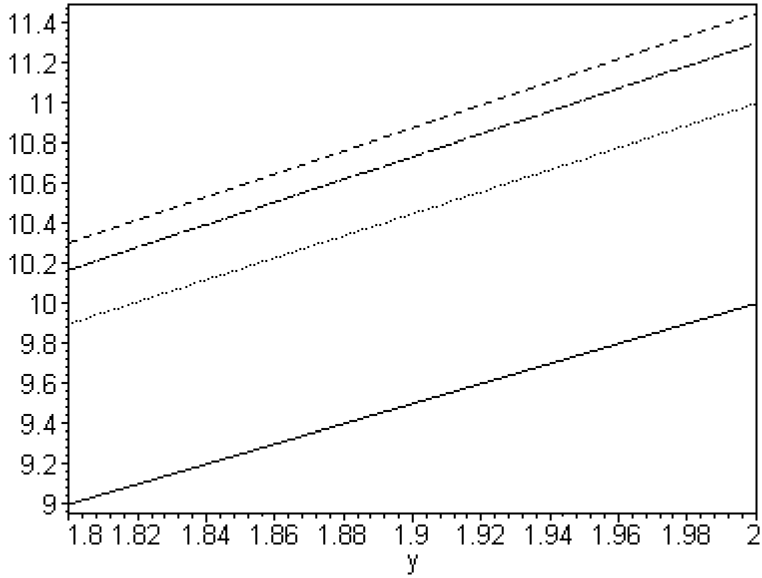

Fig. 2. Stochastic convergence of the expected values near the end

The test function is good illustration because it has infinite number of nonzero partial derivatives with respect to the random input parameter, so that each new perturbation order introduces new components into the probabilistic output. In case of linear or even polynomial transformation between output and input the differences between various perturbation-based approximations monotonously and systematically decrease. Another visible aspect is that we can speed up the effectiveness of the stochastic Taylor expansion through decreasing of the perturbation parameter ψ value what needs separate further detailed computational studies. Generally, it can be concluded that the application of polynomial transformation can be successful even in case of the second order approximation with unitary perturbation parameter, whereas in case of random input in denominator the convergence is very slow and that is why it is recommended to reduce the expansion coefficient ψ after some analogous probabilistic computational convergence studies.

Analogously to the previous considerations, the formula for 6[th] order perturbation variance of a single random variable v in terms of the Gaussian random input given by h is introduce. There holds

$$\begin{aligned}\mathrm{Var}(v)=&\left(v^{,h}\right)^2\times\mu_2(h)+\left(\frac{1}{4}\left(v^{,hh}\right)^2+\frac{2}{3!}v^{,h}v^{,hhh}\right)\times\mu_4(h)+\\&+\left(\left(\frac{1}{3!}\right)^2\left(v^{,hhh}\right)^2+\frac{1}{4!}v^{,hhhh}v^{,hh}+\frac{2}{5!}v^{,hhhhh}v^{,h}\right)\times\mu_6(h)\end{aligned} \tag{26}$$

Including here eqns (27), the second order probabilistic moment of the variable v can be determined as a function of the relevant partial derivatives of v with respect to U as well as its expected value and variance. The relevant results are collected in Figs. 3 and 4 in case of standard deviations and the coefficients of variations computed for the second, fourth and sixth order stochastic expansions of the basic solutions.

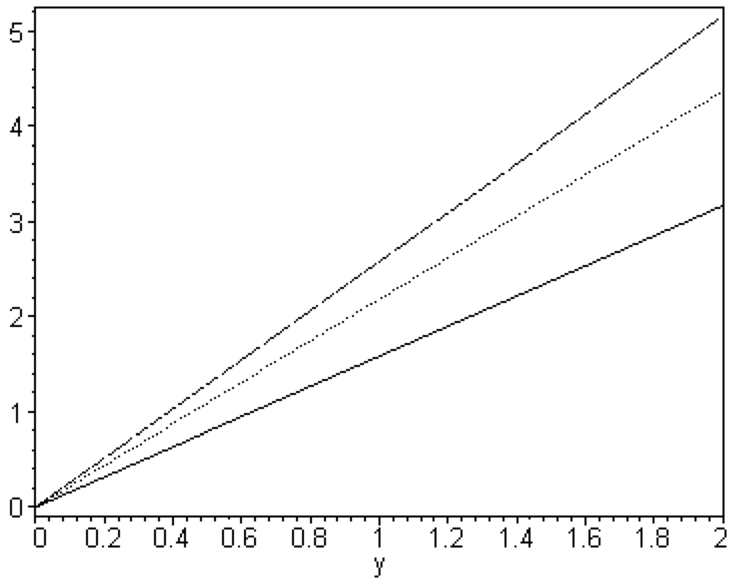

Fig. 3. Stochastic convergence of the standard deviations

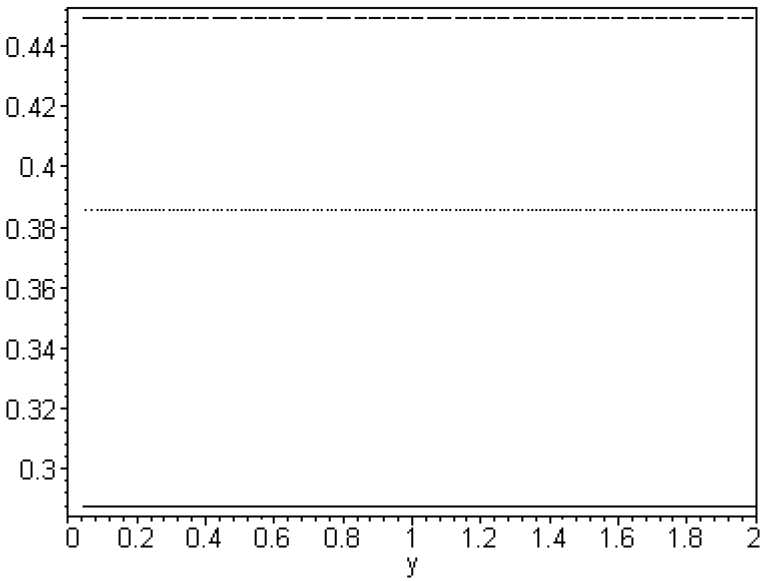

Fig. 4. Stochastic convergence of the coefficients of variations

Computational results presented in Figs. 1-4 show that the differences between the stochastic perturbation-based solutions sequential orders decrease together with the increasing order of the applied perturbation. This convergence is obtained for symmetric and very specific random input and generally depends on numerous stochastic perturbation parameters what should be verified next in details.

It should be emphasized that, in contrast to the stochastic simulation method, the stochastic n^{th} order perturbation nth moment analysis makes it possible to derive probabilistic moments of the state functions up to n^{th} order only; higher order expansion is necessary to calculate higher order probabilistic moments from the perturbation-based solution.

5 Concluding Remarks

The comparison between the second and higher as well as the generalized n^{th} order perturbation stochastic second moment approach is demonstrated theoretically and verified numerically in case of some viscous incompressible fluid flow with some input random parameter. As it is shown in the symbolic computations, the stochastic convergence of this methodology strongly depends on the character of the transformation between input and output random functions. In case when infinite number of partial derivatives of the output with respect to the input random variable exists, this convergence can be speeded up by some additional reduction of the perturbation parameter. It may be precisely established using some further numerical tests where the analytical solution of a similar nature is available.

The appropriate FEM (or similar techniques [6]) implementations [1,2] can be proposed according to the general n^{th} order perturbation approach proposed. Higher order probabilistic approaches for the general random deviates (as the Weibull Second Order Third Moment) can be applied in all those cases where the asymmetry about the expectations cannot be neglected; further mathematical and numerical studies on other type than Taylor expansions are also necessary. On the other hand, the symbolic-numeric PDE-solvers developments would substantially increase the stochastic perturbation method applications in the applied sciences and engineering.

References

1. Bathe, K.J.: Finite Element Procedures. Prentice Hall, 1996.
2. Carey, G.F., Oden, J.T.: Finite Elements: Fluid Mechanics. Prentice-Hall, Englewood Cliffs, 1986.
3. Ghanem, R.G, Spanos, P.D.: Stochastic Finite Elements: A Spectral Approach. Springer-Verlag, 1991.
4. Grigoriu, M.: Stochastic mechanics. Int. J. Sol. & Struct. **37** (2000) 197–214.
5. Hurtado, J.E., Barbat, A.H.: Monte Carlo techniques in computational stochastic mechanics. Arch. Comput. Meth. Engrg. **5**(1) (1998) 3–30.
6. Kamiński, M.: Stochastic perturbation approach in vibration analysis using Finite Difference Method. Int. J. Sound Vibr. **251**(4) (2001) 651–670.
7. Kamiński, M.: On probabilistic viscous incompressible flow of some composite fluids. Comput. Mech. **28**(6) (2002) 505–517.
8. Spurk, J.H.: Fluid Mechanics. Problems and Solutions. Springer, Berlin Heidelberg, 1997.
9. Vanmarcke, E.: Random Fields. Analysis and Synthesis. MIT Press, 1983.