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STOCHASTIC NATURAL CONVECTION IN SQUARE ENCLOSURES WITH HORIZONTAL ISOTHERMAL WALLS

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ABSTRACT
The effectiveness of two well established stochastic approaches, i.e. the generalized polynomial chaos method and the multi-element generalized polynomial chaos method, is investigated to simulate the onset of convection in bidimensional square enclosures with horizontal isothermal walls. The Boussinesq's approximation for the variation of physical properties is assumed. The stability analysis is first carried out in a deterministic sense, to determine steady state solutions and the primary bifurcation which identifies the transition from conduction to convection regime. Stochastic simulations are then conducted around discontinuities and transitional regimes. Randomness is introduced into the system through the Rayleigh number which is assumed to be a random variable following a uniform distribution. By a comparison with an accurate Monte-Carlo simulation it is shown that the statistics for the velocity and the temperature fields can be efficiently captured by the multi-element generalized polynomial chaos method.

1 Introduction

Heat transfer analysis relies heavily on obtaining accurate physical properties of the medium, precise boundary conditions, and well defined geometries. In many situations, experimental data for such quantities are available, but there exist cases where obtaining them is a difficult task and appropriate models and hypotheses have to be used. This lack of knowledge about the system has been traditionally neglected in numerical investigations of heat transfer where physical parameters, boundary conditions, geometry and initial conditions are usually set to be deterministic. Further developments toward physically relevant results raise the need to account for more realistic operating conditions, eventually represented in terms of random processes. The recent rapid advances in computational fluid dynamics open this possibility and allow the integration and the propagation of randomness in numerical simulations of convective heat transfer.

Uncertainty can be implemented by using either a *statistical* approach or a *non-statistical* approach. The statistical approach, e.g. Monte Carlo techniques, essentially amount to performing deterministic simulations for randomly selected conditions and then conducting a statistical analysis on the resulting set of realizations in order to extract the relevant statistics of the process. The Monte Carlo approach [1] is known to be robust and to be able to deal with very complex situations. However, as it is well known, it tax the computational resources heavily and therefore it is often restricted to problems involving a small number of uncertain parameters and/or degrees of freedom. For example, the Monte Carlo-based evaluation of statistical moments of 3D Navier-Stokes equations is notorious for its computational difficulties. Even supercomputer-based simulations are often too slow to provide a sufficient and timely number of samples for effective estimation. In addition, performing computer simulations by Monte Carlo methods entails generating random numbers. This is often a delicate problem that requires a careful selection of pseudo-random number generators.

On the other hand, the non-statistical approach is based upon an analytical treatment of the uncertainty. In many cases, it has advantages over the statistical approach in terms of computer time and in ease of interpretation. Thus recent research effort has been focusing on developing efficient non-statistical methods for uncertainty quantification. Several non-statistical methods have been developed with different treatment of stochastic fields. The perturbation method is based on the expansion of random quantities around their mean values, and is widely used in practice. The solution is often expressed in terms of their first and second moment, resulting in the so-called "second moment analysis" [2]. Another approach is based on the manipulation of the stochastic operator. Methods along this line include the weighted integral method [3] and Neumann expansion method [4]. Another approach is based on the Fokker-Plank equation [5].

A non-statistical approach, called *polynomial chaos* (PC), is based on the homogeneous chaos theory of Wiener [6] and it involves a spectral expansion of random fields based on *Hermite* orthogonal polynomials in terms of *Gaussian* random variables. By considering all the physical observables (velocity, temperature, etc.) as second order random processes, i.e. processes with *finite* variance, the chaos expansion decouples deterministic effects from randomness though a Fourier transform in random space. This is at the basis of the so called spectral stochastic finite element method [10], which has several advantages over Monte Carlo approaches. In particular it generally results in efficient uncertainty propagation schemes (in many situations orders of magnitude faster than Monte-Carlo methods) and yields quantitative estimates of the sensitivity of the solution with respect to uncertainties in model data. In addition, this quantitative information is expressed in a format that permits it to be readily used to probe the dependence of specific observables on particular components of the input data, to design experiments in order to better calibrate and test the validity of postulated

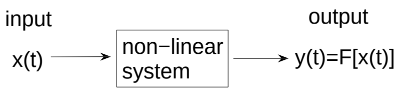

Figure 1. Functional relation between input and output of a non-linear system. The functional F[·] can be expanded in functional power series.

models. The Wiener-Hermite stochastic finite element method was first applied by Ghanem and his collaborators to various problems in mechanics; applications to thermal convection at steady state were published in [11; 12].

A broader framework, called *generalized polynomial chaos* (gPC), was proposed in [13; 14] in order to deal with more general random inputs effectively. This method represents a generalization of the Wiener-Hermite expansion since the orthogonal set of random polynomials used to represent the stochastic solution is no longer the Hermite set but it is chosen according to the probability distribution of the random input. This leads to the least possible dimensionality and thus minimum computational complexity of the stochastic problem. Results have been obtained for different flows such as 2D incompressible flow past an oscillating cylinder [15], pressure driven channel flow [12], natural convection in square enclosures [12; 11], compressible flows induced by a piston moving inside an adiabatic tube. Although generalized polynomial chaos works effectively for many problems, e.g., elliptic and parabolic partial differential equations with stochastic coefficients, it has been recognized that it cannot deal with some other differential equations, e.g., the Kraichnan-Orszag's three-mode system for modeling turbulence [16] or the Navier-Stokes equations for unsteady noisy flows such as the flow past a stationary cylinder with random inflow [17; 15].

In order to deal with such situations and increase the accuracy of the generalized polynomial chaos spectral representation (p-type) it was proposed in [18; 19] an h-type extension called *multi element generalized polynomial chaos* (ME-gPC). The key idea is to partition the domain of the random input into finite elements and consider a *local* generalized polynomial chaos basis in each element. Clearly as the number of these elements goes to infinity the multi-element method approaches Monte Carlo. Preliminary results and applications to forced stochastic thermal convection are obtained in [21] and [20].

This paper is organized as follows. In section §2 we review the representation theory of random processes in terms of polynomial chaos expansions.

In section §3 we consider natural convective flows in 2D square enclosures under the Boussinesq's approximation. We study the onset of convection (primary bifurcation) both in deterministic and stochastic sense

2 Representation of the statistical solution

If we consider the statistical solution of the convection problem as a certain non-linear functional of the random variables that model the uncertainties in input on the system the question is: how do we represent such a functional?. This problem was first considered by Volterra [24] in a deterministic sense. The basic idea can be understood with reference to figure 1. We have a non-linear system that maps the input $x(t)$ onto $y(t)$. The functional F can obviously be expanded in a functional power series in the form

$$F[x(t)] = \sum_{n=0}^{\infty} F_n[x(t)],$$

$$F_n[x(t)] = \underbrace{\int \ldots \int}_{n} k_n(t-\alpha_1,..,t-\alpha_n)\, x(\alpha_1)\ldots x(\alpha_n) d\alpha_1 \ldots d\alpha_n$$

where $k_n(t-\alpha_1,..,t-\alpha_n)$ are the Volterra's kernels. Following the ideas of Volterra, N. Wiener [6] developed a functional power series expansion for nonlinear systems forced by *random inputs* $x(t)$, i.e. stochastic processes. Specifically the type of random input considered by Wiener was Brownian motion. One of the most important property of the Wiener expansion relies in the fact that the polynomial functionals are mutual orthogonal with respect to the probability measure of the Brownian motion, i.e. Gaussian probability. Therefore these polynomials are just the Hermite polynomials and for this reason this type of expansion is also known as Wiener-Hermite expansion The theoretical justification that any functional of the Brownian motion, i.e. any output of a generic non-linear system forced by Brownian motion, can be expanded in series of Wiener-Hermite functionals was given by R.H. Cameron and W.T. Martin [7] in 1947. Subsequently other Authors extended the pioneering ideas of Wiener to other types of random inputs such as the Poisson process [8] and more general independent increment stochastic processes [9]. The basic result of all these works is that given a certain non-linear system $y(t) = F[x(t)]$ forced by some stochastic process $x(t)$ one can always expand the input-output functional relation $F[\cdot]$ as

$$y(t) = \sum_{n=0}^{\infty} F_n[x(t)] \qquad (1)$$

$$F_n[x(t)] = \underbrace{\int .. \int}_{n} \Phi_n[x(\xi_1),..,x(\xi_n)]\, g_n(t-\xi_1,..,t-\xi_n)\, d\xi_1..d\xi_n$$

where $\Phi_n[x(\xi_1),..,x(\xi_n)]$ are multivariate polynomial functionals of the random process $x(t)$. Moreover these polynomials are mutual orthogonal with respect to the probability measure of $x(t)$. In the special case where $x(t)$ is Brownian motion it can be shown that

$$\left.\begin{array}{ccc} \Phi_0 & = & 1 \\ \Phi_1[x(\xi_1)] & = & x(\xi_1) \\ \Phi_2[x(\xi_1),x(\xi_2)] & = & x(\xi_1)x(\xi_2) - \delta(\xi_1-\xi_2) \\ \cdots & & \end{array}\right\} \begin{array}{l}\text{multivariate}\\ \text{Hermite}\\ \text{polynomials}\end{array}$$

This is the classical Wiener-Hermite chaos expansion.

In the finite dimensional case all the integrals become summations and we have the easier representation

$$y(t;\zeta) = \sum_{k=0}^{M} \widehat{y}_k(t)\, \Phi_k(\zeta), \qquad (2)$$

where $\Phi_k(\zeta)$ are orthogonal polynomials of the random variables ζ. The orthogonality is with respect to the probability

probability density of the random input	polynomial chaos $\{\Phi_i\}$	support
Gaussian	Hermite	$(-\infty,\infty)$
Gamma	Laguerre	$[0,\infty)$
Beta	Jacobi	$[a,b]$
Uniform	Legendre	$[a,b]$

Table 1. Correspondence between the probability density of the random input and the optimal chaos basis to represent the random output.

measure of $x(t)$, denoted by $w(\xi)$, i.e.

$$\int \Phi_k(x)\Phi_j(x)w(x)dx = \delta_{kj}\,\|\Phi_k\|\,\|\Phi_j\|\,. \tag{3}$$

Note that the chaos expansion (2) in some sense *decouples* the deterministic part of the random signal $y_k(t)$ form its random part $\Phi_k(\zeta)$ though the orthogonalization process.

Therefore we can construct a *unique* correspondence between probability distribution of the random input $x(t)$ and the polynomial chaos basis to represent the random output. This correspondence is shown in table 1 for the most common probability distributions of the random inputs. This kind of correspondence has been called *generalized polynomial chaos* by Xiu and Karniadakis [13]. In the language of finite elements this expansion exhibits p-type convergence, i.e. converges in the mean square (L_2) sense when the polynomial order is increased.

In order to increase the accuracy of the polynomial chaos spectral representation (p-type) it was recently proposed by Wan and Karniadakis [18; 19] an h-type extension. The key idea, shown in figure 2(a), is to partition the domain of the random inputs into finite elements and to consider a *local* generalized polynomial chaos basis in each of them. These finite elements are called "random finite elements" because they belong to a discretization of the support of the probability density. The type of polynomial chaos in each random element is chosen according to the *local* probability density function of the random input, shown in figure 2(b), so that we have *local* orthogonality. Practically the random element B_k is mapped onto the standard element $[-1,1]$ and the probability density function $w(\zeta)$, restricted to B_k, is transformed according to

$$\overline{w}(\eta_k) = \frac{(b_k-a_k)}{2\int_{a_k}^{b_k} w(x)\,dx} w(\zeta_k(\eta_k))\,, \qquad B_k = [a_k,b_k]\,. \tag{4}$$

Thus the orthogonal chaos basis for the random element B_k is generated using to the local weight $\widetilde{w}(\eta)$ which is the renormalized probability density function relative to the element B_k. It is worth to note that the multi element method converges towards a monte carlo method when the number of random elements goes to infinity.

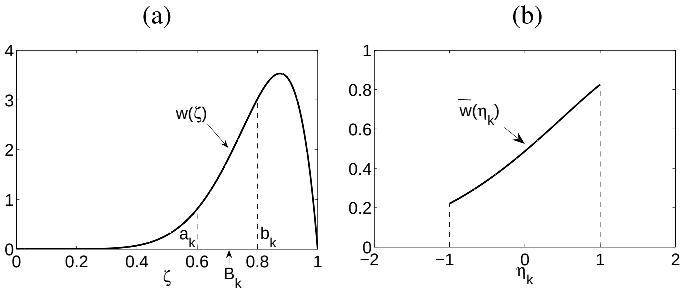

Figure 2. Basic ideas underlying the multi-element polynomial chaos method. The random element B_k is mapped onto the standard element $[-1,1]$ and the local probability density function $w(\zeta)$, restricted to B_k, is transformed accordingly (equation (4)). The orthogonal chaos basis in random element B_k is generated using to the local weight $\widetilde{w}(\eta)$ which is the renormalized probability density function relative to the element B_k.

3 Stochastic formulation of the Boussinesq's equations

We consider the dimensionless form of the Boussinesq's approximation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} = RaPrT\mathbf{j} - \nabla p + Pr\nabla^2\mathbf{u}\,, \tag{5}$$

$$\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T = \nabla^2 T\,, \tag{6}$$

$$\nabla\cdot\mathbf{u} = 0\,. \tag{7}$$

where $\mathbf{j}$ is the upward unit vector; $\mathbf{u}$ and T are the dimensionless velocity and temperature fields respectively.

As it is well known for natural convection problems it is a common practice to re-scale the Reynolds number as function of the Prandtl and/or the Rayleigh numbers. Physically this means that the reference velocity of the system is defined in terms of the buoyancy magnitude and/or the termophysical properties of the fluid. The dimensionless equations (5)-(7) are obtained using the standard scaling $Re = 1/Pr$.

We want to study the stochastic solution corresponding to a random Rayleigh number. To this end we consider

$$Ra = Ra_c\,(1+\sigma\xi) \tag{8}$$

where Ra_c plays the role of "critical Rayleigh number" and ξ is a normalized random variable.

We consider a finite dimensional representation of the velocity, the pressure and the temperature in the generalized polynomial chaos basis $\Phi_i(\xi)$ which are polynomials of the random Rayleigh number

$$\mathbf{u}(\mathbf{x},t;\xi) = \sum_{i=1}^{M} \widehat{\mathbf{u}}_i(\mathbf{x},t)\,\Phi_i(\xi)\,, \tag{9}$$

$$p(\mathbf{x},t;\xi) = \sum_{i=1}^{M} \widehat{p}_i(\mathbf{x},t)\,\Phi_i(\xi)\,, \tag{10}$$

$$T(\mathbf{x},t;\xi) = \sum_{i=1}^{M} \widehat{T}_i(\mathbf{x},t)\,\Phi_i(\xi)\,. \tag{11}$$

We substitute the expansions (9)-(11) into (5)-(7) and we perform a Galerkin projection onto $\{\Phi_i\}_{i=1,..,M}$ in order to ensure that the error is orthogonal to functional space spanned by the finite dimensional chaos basis $\{\Phi_i\}$. By employing the orthogonality conditions (3) we obtain for each $k = 0, \ldots, M$

$$\frac{\partial \widehat{\mathbf{u}}_k}{\partial t} + \frac{1}{e_{0kk}} \sum_{i,j=0}^{M} (\widehat{\mathbf{u}}_i \cdot \nabla) \widehat{\mathbf{u}}_j e_{ijk} = Ra_c Pr \left(\widehat{T}_k + \sigma \sum_{j=0}^{M} \frac{e_{1jk}}{e_{0kk}} \widehat{T}_j \right) \mathbf{j} - -\nabla \widehat{p}_k + Pr \nabla^2 \widehat{\mathbf{u}}_k \, , \quad (12)$$

$$\frac{\partial \widehat{T}_k}{\partial t} + \frac{1}{e_{0kk}} \sum_{i,j=1}^{M} \cdot \nabla \widehat{T}_j e_{ijk} = \nabla^2 \widehat{T}_k \, , \quad (13)$$

$$\nabla \cdot \widehat{\mathbf{u}}_k = 0 \, . \quad (14)$$

It should be noted that the averaging operation allows to transform effectively the stochastic problem into a system of coupled partial differential equations to be solved for the *deterministic* unknown chaos modes $\widehat{\mathbf{u}}_i(\mathbf{x},t)$. Discretization in space and time can be carried out by any conventional deterministic technique, e.g., finite element methods, finite volume methods, etc. At the heart of the polynomial chaos method is the construction of the matrix

$$e_{ijk} = \int \Phi_i(\xi) \Phi_j(\xi) \Phi_k(\xi) w(\xi) d\xi \, . \quad (15)$$

Once this is available we can easily compute other quantities such the mean and the standard deviations of the flow field

$$\langle \mathbf{u}(\mathbf{x},t;\xi) \rangle = \widehat{\mathbf{u}}_0(\mathbf{x},t) \, , \quad (16)$$

$$\sigma_{\mathbf{u}}(\mathbf{x},t) = \left(\sum_{k=1}^{M} \widehat{\mathbf{u}}_k(\mathbf{x},t)^2 e_{0kk} \right)^{\frac{1}{2}} \, . \quad (17)$$

In general it can be proved that the total number of equations $M+1$ to be solved simultaneously is related to the number of independent random inputs n and to the highest order P of the polynomials $\{\Phi_i\}$ by

$$M + 1 = \frac{(n+P)!}{n!P!} \, . \quad (18)$$

For our problem we only have one random input, the Rayleigh number so $n = 1$. Therefore if we represent the stochastic solution using a polynomial chaos of order $P = 6$ we have 6 Boussinesq-like problems to be solved *simultaneously*, which means 24 scalar coupled partial differential equations if we are in bidimensional space. Although for many problems the polynomial chaos method definitely beats the Monte-Carlo approach we can clearly see in (18) the limit of applicability of this technique. Even supercomputers based simulations cannot handle such a proliferation of the number of equations when the stochastic dimension $M+1$ is high.

4 Onset of convection in 2D square enclosures with horizontal isothermal walls

In this section we study the transition form conduction to convection (onset of convection) in 2D square enclosures under the Boussinesq's approximation. This phenomenon takes place when the buoyancy effects due to temperature gradients exceed the stabilizing viscous effects [25] or, equivalently, when the Rayleigh Ra number exceeds a "critical" Rayleigh number Ra_c which in general depends on the aspect ratio of the cavity and the boundary conditions but not on the Prandtl number. For the geometry and the boundary conditions shown in figure 3(a) it is well known [22; 23] that $Ra_c = 2585.03$; also, as shown in figure 5 the transition from conduction to convection do not depend on the Prandtl number.

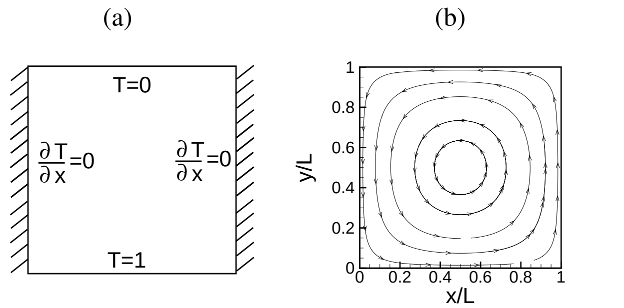

Figure 3. (a) Schematic of the geometry and boundary conditions. (b) Rayleigh-Bénard roll at Rayleigh number $Ra = 2590$.

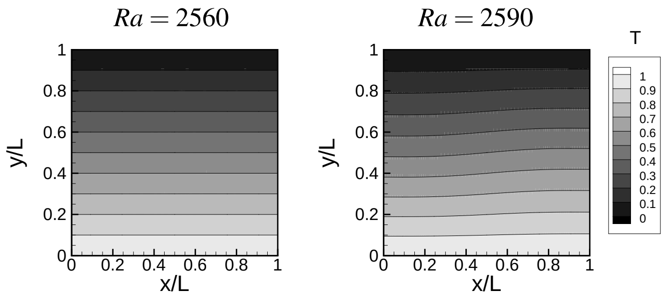

Figure 4. Dimensionless temperature fields corresponding to flows at $Ra = 2560$ (pure conduction) and $Ra = 2590$ (weak convection).

For $Ra < Ra_c$ the fluid flow is absent and the heat transfer between the horizontal isothermal walls takes place by pure conduction (figure 4(a)). For $Ra > Ra_c$ the buoyancy effect dominates, fluid flow is initiated and the temperature field is significantly transported by velocity (figure 4(b)) with development of the classical Rayleigh-Bénard rolls shown in figure 3(b). The physics of the solutions corresponding to $Ra < Ra_c$ and $Ra > Ra_c$ is completely different and at $Ra = Ra_c$ there is a branch point that divides these two ensembles.

In order to determine the properties of the flow field in proximity of the the onset of convection we use different approaches:

1. integral transform method [26] and
2. spectral element method [27].

The integral transform method allow us to perform a systematic bifurcation analysis using AUTO. The result of these computations are shown in figure 5 where a branch point located at $Ra_c = 2585.24$ is identified. We note that there is a very good agreement with other results available in the literature, see for instance [22; 23].

5 Stochastic simulations

We would like to study if polynomial chaos simulations can capture the statistics of an ensemble of solutions that include the onset of convection. This is a very important issue since this

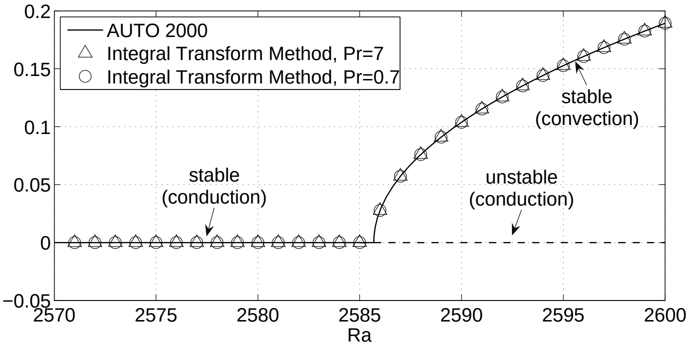

Figure 5. Stable and unstable branches of the pitchfork bifurcation. For $Ra > Ra_c$ two solutions of the Boussinesq's problem are possible: pure conduction, which is unstable, and convection, which is stable. It is shown that the transition from conduction to convection does not depend on the Prandtl number.

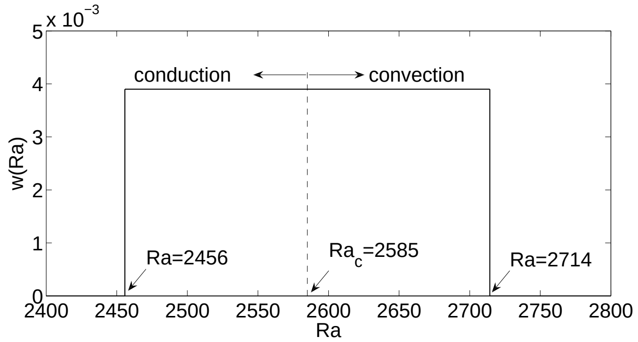

Figure 6. Probability density function of the Rayleigh number.

kind of discontinuity is one of the simplest bifurcation arising in fluid mechanics and any stochastic simulation can potentially include such bifurcations in its domain.

We consider the upper branch of the pitchfork bifurcation shown in figure 5 and figure 7 (stable branch) and we study the ensemble of solutions as function of the random Rayleigh number.

We assume that the probability density of Rayleigh number is uniform with mean $Ra_c = 2585$ and standard deviation $5\% Ra_c$, i.e.

$$Ra = Ra_c\,(1 + \sigma\xi)\,, \quad \xi \sim U\,([-1,1])\,, \quad \sigma = 5\%\,. \qquad (19)$$

With such a standard deviation the Rayleigh number ranges from 2455.75 to 2714.25, thus including the branch point (see figure 7). We study the statistics of the random flow corresponding to this distribution of Rayleigh numbers using three different stochastic approaches:

1. Monte Carlo method (based on Cotta's integral transformation method [26]) to generate a benchmark for the stochastic solution. The possibility to perform a timely and accurate Monte Carlo simulation arises from the fact that the integral transform method is computationally fast because it reduces the system of partial differential equations to a boundary value problem for an ordinary differential equation.
2. Generalized polynomial chaos (gPC) [13; 14] based on spectral element code [27].
3. Multi-element generalized polynomial chaos (ME-gPC) [18] based on spectral element code [27].

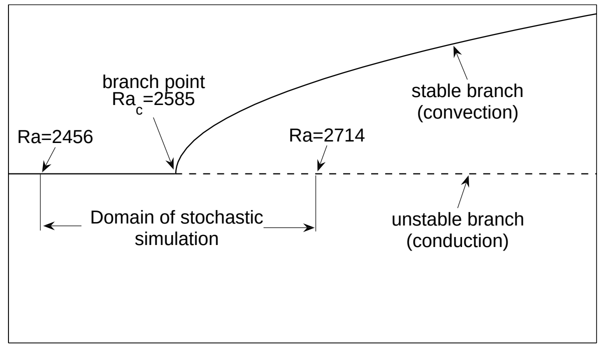

Figure 7. Sketch of the stochastic simulation domain.

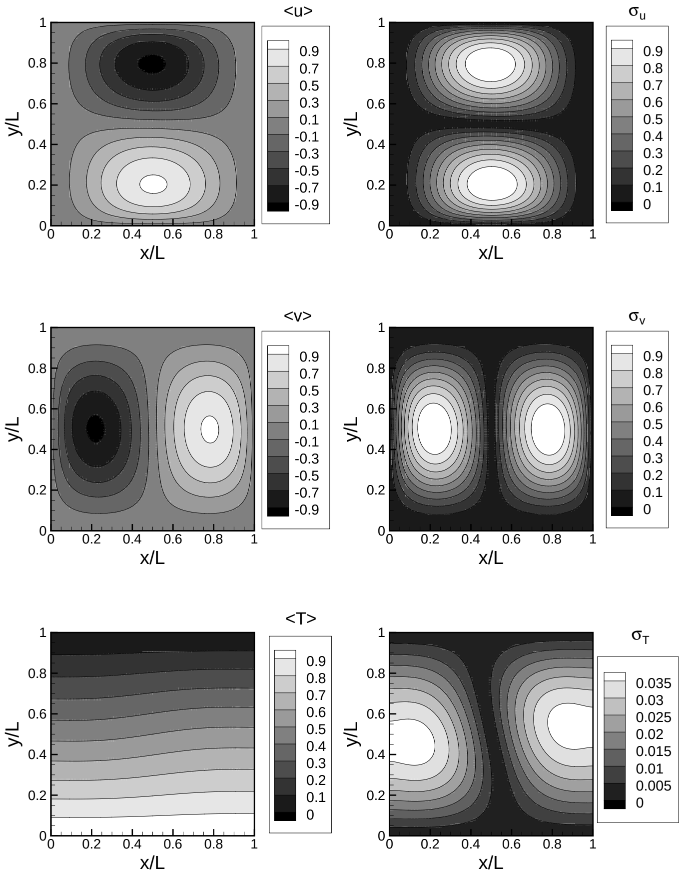

Figure 8. Monte-Carlo benchmark stochastic solution. Ensemble mean (left) and ensemble standard deviation (right) for velocity and temperature fields. The ensemble of solutions is composed of 50000 samples.

The generalized polynomial chaos basis which is orthogonal with respect the uniform measure, is the Legendre set (see table 1). In figure 8 we show the Monte Carlo ensemble mean and ensemble standard deviation for velocity and temperature fields at steady state. In figure 9 we compare the mean and the standard deviation obtained by different stochastic approaches along the crossline and $y = 0.5L$ respectively.

6 Conclusions

As shown in figure 9 the transition from conduction to convection, which is one of the simplest bifurcation arising in fluid mechanics, can be efficiently captured in a stochastic sense by the ME-gPC method. This is an important result since any stochastic simulation can potentially include these kind discon-

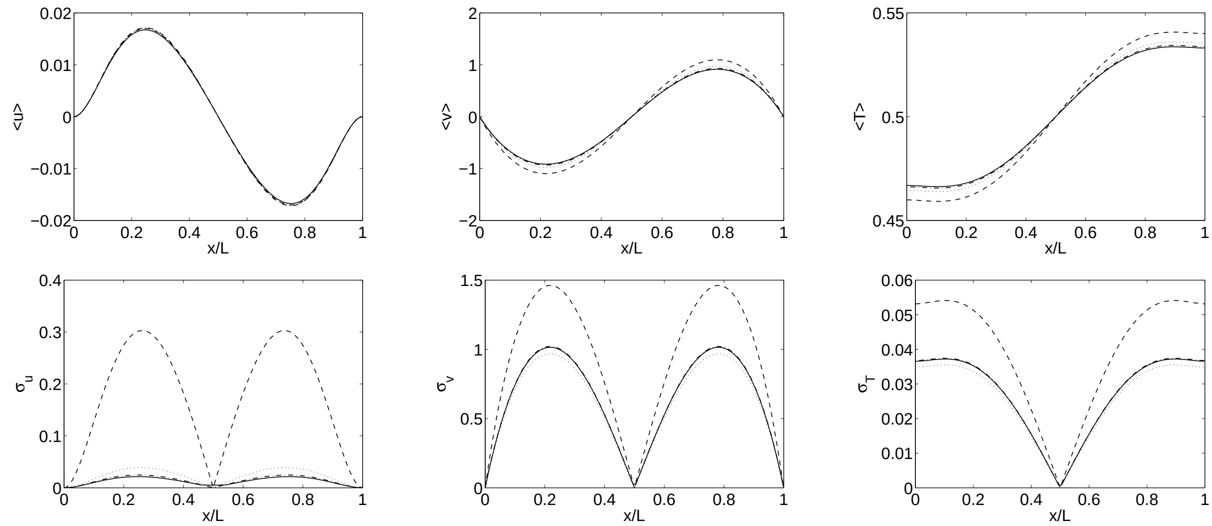

Figure 9. Velocity and temperature fields along the crossline $y/L = 0.5$. First row: means; second row: standard deviations. We plot different stochastic results: benchmark Monte Carlo simulation (−), gPC (−−) (order 3), ME-gPC (···) (2 elements of order 3), ME-gPC (−·) (8 elements of order 3).

tinuities in its domain. Differently from what it is reported by Asokan & Zabaras in [11], the classical generalized polynomial chaos method still works although it is not accurate.

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