Variational multiscale stabilized FEM formulations for stochastic advection-diffusion equations

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Abstract

An extension of the deterministic variational multiscale approach with algebraic subgrid scale modeling is considered for developing stabilized finite element formulations for the stochastic advection-diffusion equations. The stabilized formulations are numerically implemented using the spectral stochastic formulation of the finite element method. Generalized Askey polynomial chaos and Karhunen-Loève expansion techniques are used for the representation of uncertain quantities. The proposed stabilized formulations are finally evaluated against a standard natural convection example with uncertainty in boundary conditions.

Introduction

Uncertainty quantification in natural convection has received considerable research interest in recent times. This can be attributed to the strong dependence of flow and temperature patterns on system inputs via flow geometry, temperature and flow inlet boundary conditions, initial perturbations and material data like diffusivity, viscosity and porosity. Also, the numerical simulation of natural convection using techniques like finite element analysis presents difficulties when the exact solution is characterized by the presence of narrow boundary or internal layers and vanishing diffusion.

This has fuelled extensive research towards the development of stabilized FE techniques for addressing fluid-flow and other advection dominant problems. In particular, the Variational Multiscale VMS method (Hughes 1995, Brezzi 1997, Guermond 1999) has been established as a paradigm for derivation of stabilized finite element schemes.

Following the pioneering work of (Ghanem and Spanos 1991) in the development of a spectral stochastic finite element method, significant advances have been made in addressing uncertainty propagation in fluid-flow and transport via finite-difference methods (Le Maitre et al. 2001, 2002), and spectral techniques (Xiu et al. 2001, 2003). However, none of these techniques utilize the inherent advantages of finite element methods owing to the lack of a consistent stabilization framework. This paper attempts at extending the VMS approach to address the above issue in the context of convection dominant systems.

The paper is organized as follows: We start with a brief description of input and output uncertainty quantification schemes. We proceed by stating the governing equations for stochastic natural convection under the Boussinesq assumption and a presentation of the stabilized weak formulation. The proposed stabilized formulation is then numerically evaluated against the stochastic version of Rayleigh-Bènard flow in a square cavity with an adiabatic body at the center.

Mathematical Framework for Probabilistic Representation of Uncertainty

Consider a probability space $(\Omega, \mathcal{F}, \mathcal{P})$ referred to in this work using the short notation Ω, where, Ω is the sample space, $\mathcal{F}$ is the minimal σ-algebra of the subsets of Ω and $\mathcal{P}$ is the probability measure defined on $\mathcal{F}$. Any random variable is expressed as a function of $\omega \in \Omega$.

Karhunen-Loéve expansion and lower dimensional representation of stochastic processes - Let $W(\mathbf{x}, t, \omega)$ be a second order stochastic processes i.e. at each given spatial and temporal location $\mathbf{x}_1$ and t_1, the random variable corresponding to $W(\mathbf{x}_1, t_1, \omega)$ belongs to the function space $L_2(\Omega)$. The covariance function $R_{\mathrm{hh}}(\mathbf{y}_1, \mathbf{y}_2)$ is defined as

$$R_{\mathrm{hh}}(\mathbf{y}_1, \mathbf{y}_2) := \mathbb{E}[(W(\mathbf{y}_1, \omega) - \mathbb{E}[W](\mathbf{y}_1))(W(\mathbf{y}_2, \omega) - \mathbb{E}[W](\mathbf{y}_2))] \tag{1}$$

where, $\mathbf{y}_1$ and $\mathbf{y}_2$ refer to sets of spatial and temporal locations $(\mathbf{x}_1, t_1)$ and $(\mathbf{x}_2, t_2)$, respectively. By definition, the covariance function is symmetric positive definite, bounded and hence has real positive eigenvalues and an orthogonal set of eigen-functions that form a complete basis. The KLE takes takes the following form

$$W(\mathbf{x}, t, \omega) = \mathbb{E}[W](\mathbf{x}, t) + \sum_{\mathrm{i}=1}^{\infty} \sqrt{\lambda_{\mathrm{i}}} W_{\mathrm{i}}(\mathbf{x}, t) Z_{\mathrm{i}}(\omega) \tag{2}$$

where, λ_{i} and $W_{\mathrm{i}}(\mathbf{x}, t)$ are defined through the eigenvalue problem

$$\int_{\mathcal{D}\times\mathcal{T}} R_{\mathrm{hh}}(\mathbf{y}_1, \mathbf{y}_2) W_{\mathrm{i}}(\mathbf{y}_2) d\mathbf{y}_2 = \lambda_{\mathrm{i}} W_{\mathrm{i}}(\mathbf{y}_1) \tag{3}$$

Typically, by employing KLE the inputs to a stochastic continuum system can be represented in terms of a finite set of independent random variables $(Z_1, \ldots, Z_{\mathrm{n}})$, where the quantity n is called the dimensionality of the stochastic input or simply the KL dimension.

Generalized polynomial chaos expansion GPCE - Consider a continuum system with random inputs represented as a collection of random variables $\{Z_1(\omega), \ldots, Z_{\mathrm{n}}(\omega)\}$. The output response $W(\mathbf{x}, t, \omega)$ of the system can be represented in a Generalized polynomial chaos expansion as follows

$$\begin{aligned} W(\mathbf{x}, t, \omega) &= a_0(\mathbf{x}, t) I_0 + \sum_{\mathrm{i}_1=1}^{\mathrm{N}} a_{\mathrm{i}_1}(\mathbf{x}, t) I_1(Z_{\mathrm{i}_1}(\omega)) + \sum_{\mathrm{i}_1=1}^{\mathrm{N}} \sum_{\mathrm{i}_2=1}^{\mathrm{i}_1} a_{\mathrm{i}_1\mathrm{i}_2}(\mathbf{x}, t) I_2(Z_{\mathrm{i}_1}(\omega), Z_{\mathrm{i}_2}(\omega)) \cdots \\ &:= \sum_{\mathrm{i}=0}^{\infty} W_{\mathrm{i}}(\mathbf{x}, t) \psi_{\mathrm{i}}(\omega) \end{aligned} \tag{4}$$

where, $I_{\mathrm{k}}(Z_{\mathrm{i}_1}(\omega), \ldots, Z_{\mathrm{i}_2}(\omega))$ denotes a hypergeometric polynomial from the Wiener-Askey series of orthogonal polynomials. The functions $\psi_{\mathrm{i}}(\omega)$ are one-to-one functions of $I_{\mathrm{k}}(Z_{\mathrm{i}_1}(\omega), \ldots, Z_{\mathrm{i}_2}(\omega)) : k \geq 0$ and are introduced for notational convenience.

Problem Definition

A brief detail of the VMS stabilized weak formulation for a natural convection system is presented in this section. The complete derivation follows along the lines of (Badri Narayanan and Zabaras, 2004). Consider $\mathcal{D}$ to be a closed region with piecewise smooth boundary Γ in d-dimensional Euclidean space $\mathbb{R}^{\mathrm{d}}$. Let $\mathcal{D}$ be occupied by a constant property fluid. It is further assumed that the temperature variations in the domain are negligible and hence the Boussinesq approximation holds.

The set of equations (in non-dimensional form) governing the natural convection of the fluid occupying $\mathcal{D}$ can be specified in the form of the following conservation equations for the velocity $\boldsymbol{v}$, pressure p and temperature θ:

$$\nabla \cdot \boldsymbol{v} = 0, \quad (\mathbf{x}, t, \omega) \in \mathcal{D} \times \mathcal{T} \times \Omega \tag{5}$$

$$\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} = \nabla \cdot \boldsymbol{\sigma} - \mathrm{Pr}(\omega)\mathrm{Ra}(\omega)\theta \boldsymbol{e}_{\mathrm{g}} \tag{6}$$

$$\frac{\partial \theta}{\partial t} + \boldsymbol{v} \cdot \nabla \theta = \nabla^2 \theta \tag{7}$$

where the constitutive relation describing the stress tensor is given as

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\mathrm{Pr}(\omega)\boldsymbol{\epsilon}(\boldsymbol{v}), \quad \boldsymbol{\epsilon}(\boldsymbol{v}) = [\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T]/2 \tag{8}$$

In the above equations, $\mathcal{T}$ is a closed time interval, $\boldsymbol{I}$ is the second-order unit tensor, p is the modified pressure and $\boldsymbol{e}_{\mathrm{g}}$ is the unit vector in the direction of gravity. The following scales were used to non-dimensionalize the governing equations:

$$\mathbf{x} = \frac{\mathbf{x}^*}{L}, \quad t = \frac{t^* \alpha}{L^2}, \quad p = \frac{p^* L^2}{\rho \alpha^2}, \quad \boldsymbol{v} = \frac{\boldsymbol{v}^* L}{\alpha}, \quad \text{and} \quad \theta = \frac{\Delta T^*}{\Delta T^*_{\mathrm{ref}}} \tag{9}$$

where the superscript * refers to the dimensional quantities, L is an appropriate length scale for the problem and α is the thermal diffusivity. It should be noted that we can allow α to be a random variable. This assumption just implies that the exact scaling information for the quantities is not known. The quantities ΔT^* and $\Delta T^*_{\mathrm{ref}}$ are problem dependant scaling parameters for temperature and are used to represent the induced and reference temperature gradients, respectively.

The above non-dimensionalization scheme results in two critical dimensionless parameters: Prandtl number $\mathrm{Pr}(\omega) = \nu(\omega)/\alpha(\omega)$ and Rayleigh number $\mathrm{Ra}(\omega) = g\beta L^3 \Delta T_{\mathrm{ref}}/\nu(\omega)\alpha(\omega)$ where, β is the volume expansion coefficient.

We further assume that the boundary is sub-divided as $\Gamma^{\mathrm{m}}_{\mathrm{g}}$ and $\Gamma^{\mathrm{m}}_{\mathrm{h}}$, where velocity and traction are specified, respectively and $\Gamma^{\mathrm{t}}_{\mathrm{g}}$ and $\Gamma^{\mathrm{t}}_{\mathrm{h}}$, where temperature θ_{g} and heat flux $\mathbf{h}$ are specified. The following relations hold $\Gamma = \Gamma^{\mathrm{m}}_{\mathrm{g}} \cup \Gamma^{\mathrm{m}}_{\mathrm{h}} = \Gamma^{\mathrm{t}}_{\mathrm{g}} \cup \Gamma^{\mathrm{t}}_{\mathrm{h}}$ and $\emptyset = \Gamma^{\mathrm{m}}_{\mathrm{g}} \cap \Gamma^{\mathrm{m}}_{\mathrm{h}} = \Gamma^{\mathrm{t}}_{\mathrm{g}} \cap \Gamma^{\mathrm{t}}_{\mathrm{h}}$.

Multiscale Decomposition - Consider an overlapping sum decomposition for the velocity, pressure and temperature fields of the form $\boldsymbol{v} = \bar{\boldsymbol{v}} \oplus \boldsymbol{v}'$, $p = \bar{p} \oplus p'$ and $\theta = \bar{\theta} \oplus \theta'$, where the quantities with a bar denote the large-scale resolved solution components and the quantities with a dash indicate the unresolved small-scale solution components. This a priori scale decomposition of the solution results in a similar decomposition for the function spaces as follows: $(H^1(\mathcal{D}) \times L_2(\Omega) \times L_2(\mathcal{T}))^{\mathrm{d}} = \bar{\boldsymbol{U}} \oplus \boldsymbol{U}'$ and $L_2(\mathcal{D}) \times L_2(\Omega) = \bar{X} \oplus X'$. The large scale function spaces often refer to piecewise polynomial finite element representations.

A priori assumptions -Though the velocity and temperature fields are coupled, we will assume that when we solve for the velocity field, the temperature field values are known and vice-versa. We will also assume that the unresolved small-scale solutions are quasi-static whereby $\partial_{\mathrm{t}} \boldsymbol{v}' = \partial_{\mathrm{t}} \theta' \approx 0$ and that a one step Picard linearization holds for the nonlinear convection term $\boldsymbol{v} \bullet \nabla \boldsymbol{v} \approx \bar{\boldsymbol{v}} \bullet \nabla \bar{\boldsymbol{v}} + \bar{\boldsymbol{v}} \bullet \nabla \boldsymbol{v}'$. These assumptions are valid for laminar flows where the small scale solutions typically manifest as small fluctuations about the large scale solutions.

Weak formulation for large scale conservation equations -

$$(\nabla\bullet(\bar{\boldsymbol{v}}+\boldsymbol{v}'),\bar{q})=0 \tag{10}$$

$$(\partial_{\mathrm{t}}\bar{\boldsymbol{v}},\bar{\boldsymbol{w}})+(\mathrm{Pr}(\omega)\nabla(\bar{\boldsymbol{v}}+\boldsymbol{v}'),\nabla\bar{\boldsymbol{w}})+(\bar{\boldsymbol{v}}\bullet\nabla\bar{\boldsymbol{v}}+\bar{\boldsymbol{v}}\bullet\nabla\boldsymbol{v}',\bar{\boldsymbol{w}})-(\bar{p}+p',\nabla\bullet\bar{\boldsymbol{w}})= (\mathrm{Pr}(\omega)\mathrm{Ra}(\omega)\theta,\bar{\boldsymbol{w}})+(\boldsymbol{h},\bar{\boldsymbol{w}})_{\Gamma_{\mathrm{h}}^{\mathrm{m}}} \tag{11}$$

$$(\partial_{\mathrm{t}}\bar{\theta},\bar{w})+(\boldsymbol{v}\bullet\nabla(\bar{\theta}+\theta'),\bar{w})+(\nabla(\bar{\theta}+\theta'),\nabla\bar{w})=(q_0,\bar{w})_{\Gamma_{\mathrm{h}}^{\mathrm{t}}} \tag{12}$$

Strong formulation for small scale conservation equations

$$\bar{\boldsymbol{v}}\bullet\nabla\boldsymbol{v}'-\mathrm{Pr}(\omega)\nabla^2\boldsymbol{v}'+\nabla p'=\mathcal{R}_{\mathrm{m}}(\bar{\boldsymbol{v}},\bar{p}) \tag{13}$$

$$\nabla\bullet\boldsymbol{v}'=\mathcal{R}_{\mathrm{c}}(\bar{\boldsymbol{v}},\bar{p}) \tag{14}$$

$$\boldsymbol{v}\bullet\nabla\theta'-\nabla^2\theta'=\mathcal{R}_{\mathrm{t}}(\bar{\theta}) \tag{15}$$

In the above equations, the mass, momentum and energy residuals $\mathcal{R}_{\mathrm{m}}(\bar{\boldsymbol{v}},\bar{p})$, $\mathcal{R}_{\mathrm{c}}(\bar{\boldsymbol{v}},\bar{p})$ and $\mathcal{R}_{\mathrm{t}}(\bar{\theta})$, respectively are defined as follows:

$$\mathcal{R}_{\mathrm{m}}(\bar{\boldsymbol{v}},\bar{p}) = \mathrm{Pr}(\omega)\mathrm{Ra}(\omega)\theta-\partial_{\mathrm{t}}\bar{\boldsymbol{v}}-\bar{\boldsymbol{v}}\bullet\nabla\bar{\boldsymbol{v}}+\mathrm{Pr}(\omega)\nabla^2\bar{\boldsymbol{v}}-\nabla\bar{p} \tag{16}$$

$$\mathcal{R}_{\mathrm{c}}(\bar{\boldsymbol{v}},\bar{p}) = -\nabla\bullet\bar{\boldsymbol{v}} \tag{17}$$

$$\mathcal{R}_{\mathrm{t}}(\bar{\theta}) = -\partial_{\mathrm{t}}\bar{\theta}-\boldsymbol{v}\bullet\nabla\bar{\theta}+\nabla^2\bar{\theta} \tag{18}$$

Following along the lines of (Badri Narayanan and Zabaras, 2004 and Codina, 2002a,b), we model the subgrid solutions in each element as $\boldsymbol{v}'\approx\tau_{(\mathrm{m})}\mathcal{R}_{\mathrm{m}}(\bar{\boldsymbol{v}},\bar{p})$, $p'\approx\tau_{(\mathrm{c})}\mathcal{R}_{\mathrm{c}}(\bar{\boldsymbol{v}},\bar{p})$ and $\theta'\approx\tau_{(\mathrm{t})}\mathcal{R}_{\mathrm{t}}(\bar{\theta})$, respectively. Substituting the subgrid solutions back in Eqs. (10, 11, 12), we obtain the following stabilized weak formulation for the large scale conservation equations:

$$(\nabla\bullet\bar{\boldsymbol{v}},\bar{q})-(\mathcal{R}_{\mathrm{m}}(\bar{\boldsymbol{v}},\bar{p}),\tau_{(\mathrm{m})}\nabla\bar{q})=0 \tag{19}$$

$$(\partial_{\mathrm{t}}\bar{\boldsymbol{v}},\bar{\boldsymbol{w}})+(\mathrm{Pr}(\omega)\nabla\bar{\boldsymbol{v}},\nabla\bar{\boldsymbol{w}})-(\mathcal{R}_{\mathrm{m}}(\bar{\boldsymbol{v}},\bar{p}),\tau_{(\mathrm{m})}\mathrm{Pr}(\omega)\nabla^2\bar{\boldsymbol{w}})-(\mathcal{R}_{\mathrm{m}}(\bar{\boldsymbol{v}},\bar{p}),\tau_{(\mathrm{m})}\bar{\boldsymbol{v}}\bullet\nabla\bar{\boldsymbol{w}}) +(\bar{\boldsymbol{v}}\bullet\nabla\bar{\boldsymbol{v}},\bar{\boldsymbol{w}})-(\bar{p},\nabla\bullet\bar{\boldsymbol{w}})-(\mathcal{R}_{\mathrm{c}}(\bar{\boldsymbol{v}},\bar{p}),\tau_{(\mathrm{c})}\nabla\bullet\bar{\boldsymbol{w}})=(\mathrm{Pr}(\omega)\mathrm{Ra}(\omega)\theta,\bar{\boldsymbol{w}})+(\boldsymbol{h},\bar{\boldsymbol{w}})_{\Gamma_{\mathrm{h}}^{\mathrm{m}}} \tag{20}$$

$$(\partial_{\mathrm{t}}\bar{\theta},\bar{w})+(\boldsymbol{v}\bullet\nabla\bar{\theta},\bar{w})-(\mathcal{R}_{\mathrm{t}}(\bar{\theta}),\tau_{(\mathrm{t})}\boldsymbol{v}\bullet\nabla\bar{w})+(\nabla\bar{\theta},\nabla\bar{w})-(\mathcal{R}_{\mathrm{t}}(\bar{\theta}),\tau_{(\mathrm{t})}\nabla^2\bar{w})=(q_0,\bar{w})_{\Gamma_{\mathrm{h}}^{\mathrm{t}}} \tag{21}$$

Model derivations for the intrinsic time scales $\tau_{(\mathrm{c})}$, $\tau_{(\mathrm{m})}$ and $\tau_{(\mathrm{t})}$ and issues related therein are discussed in further detail in (Badri Narayanan and Zabaras, 2004). We just state the final results of these models here for the sake of completion.

$$\tau_{(\mathrm{m})} = \left[\left(c_1(\omega)\frac{\nu(\omega)}{h^2}\right)^2+\left(c_2(\omega)\frac{|\bar{\boldsymbol{v}}|}{h}\right)^2\right]^{-1/2}, \quad \tau_{(\mathrm{c})}=\left[\nu(\omega)^2+\left(\frac{c_2(\omega)|\bar{\boldsymbol{v}}|}{c_1(\omega)h}\right)^2\right]^{1/2} \tag{22}$$

where, $c_1(\omega)$ and $c_2(\omega)$ are in general random constants and h is the elemental length. Also, $\tau_{(\mathrm{t})}$ is defined by the following relations

$$\tau_{(\mathrm{t})}=\frac{h}{2|\boldsymbol{v}(\mathbf{x},\omega)|}f(\mathrm{Pe}),\quad f(\mathrm{Pe})=\frac{\mathrm{Pe}}{3}\mathbb{I}_{[Pe:0<\mathrm{Pe}\leq 3]}(Pe)+\mathbb{I}_{[Pe:\mathrm{Pe}>3]}(Pe)\quad \mathrm{Pe}=\frac{|\boldsymbol{v}(\mathbf{x},\omega)|h}{2} \tag{23}$$

where, $\mathbb{I}_A(\boldsymbol{x})$ is the indicator function for set $\{\mathrm{A}\}$ and Pe is the element Pèclet number.

Natural Convection in a Square Cavity with an Adiabatic Body at the Center

We consider natural convection of air at 293 K in a square enclosure with a square adiabatic body at the center as shown in Figs. 1(a,b). The simulations are carried out away from critical points and thus, the solution does not exhibit a highly nonlinear dependance on the input parameters. The Prandtl number is ≈ 0.7 and the Rayleigh number based on the dimensions of the square cavity is assumed to be 10^4. The non-dimensional temperature boundary condition at the hot wall is assumed to be uniformly distributed random variable

$$\theta_H = 1.0 + 0.05\xi, \quad \xi \sim [-1, 1]$$

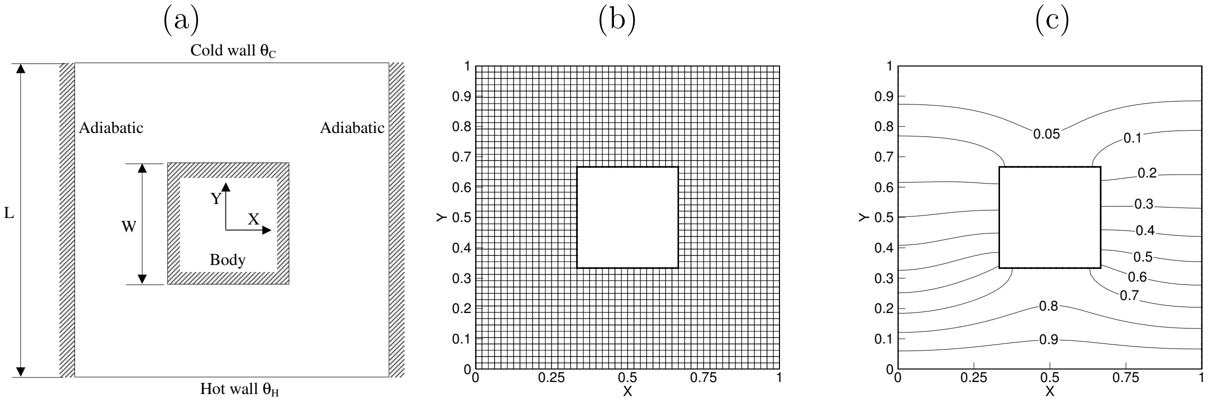

Figure 1. a. Schematic of the computational domain, b. Finite element mesh, c. Mean non-dimensional temperature isotherms at $t = 0.01$.

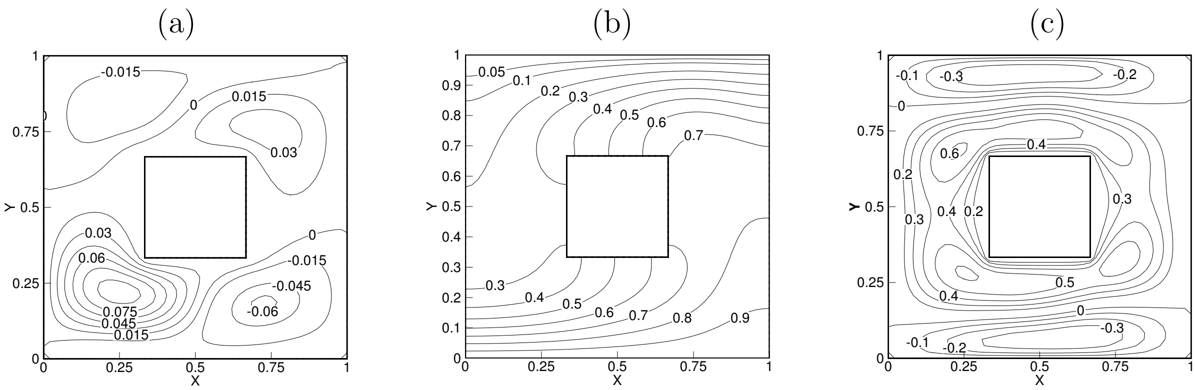

Figure 2. a. Mean streamfunction at $t = 0.01$, b. Mean non-dimensional temperature isotherms at steady state, c. Mean streamfunction at steady state.

A third-order Legendre chaos expansion was used for the representation of temperature and flow fields. The mean temperature field at a non-dimensional time of 0.01 is shown in Fig. 1(c). The system initially proceeds towards an equilibrium state characterized by isotherm contours that are symmetric about the centerlines of the square cavity. The mean streamfunction at this time is shown in Fig. 2(a). This equilibrium state is unstable and the symmetry of the isotherms is not attained. The system proceeds to a steady state as shown in Figs. 2(b,c). The first-order term in the Legendre chaos expansion of temperature at a non-dimensional time of 0.01 and at steady state are shown in Figs. 3(a,b). The higher

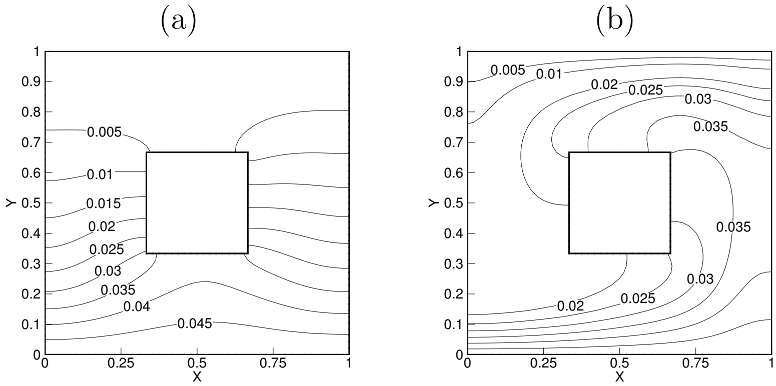

Figure 3. a. First-order term in the Legendre chaos expansion of non-dimensional temperature isotherms at $t = 0.01$, b. First-order term in the Legendre chaos expansion of non-dimensional temperature isotherms at steady state.

order terms in the Legendre chaos expansion of temperature and velocity were negligible in comparison to the mean and first order terms, hence they are not plotted.

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