Proceedings of the Twelfth International Conference on
Engineering Computational Technology
Edited by: P. Iványi, J. Kruis and B.H.V. Topping
Civil-Comp Conferences, Volume 8, Paper 6.4
Civil-Comp Press, Edinburgh, United Kingdom, 2024
ISSN: 2753-3239, doi: 10.4203/ccc.8.6.4

First Passage of Shannon Entropy Computations in Navier-Stokes Flow Problems

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Abstract

The main aim here is the numerical solution to the Navier-Stokes equations for incompressible, non-turbulent, and subsonic fluid flows with some Gaussian physical random parameters. The stochastic finite volume method implemented according to the generalized stochastic perturbation technique is engaged for this purpose. It is based upon the polynomial bases for the PVT solutions obtained with the weighted least squares method algorithm. The deterministic problem is solved using the freeware OpenFVM in conjunction with the computer algebra software MAPLE, where the LSM local fittings and the resulting probabilistic quantities are computed. The first two probabilistic moments as well as the Shannon entropy spatial distributions are determined with this apparatus and visualized in the FEPlot software. The spatial distribution of Shannon entropy has been completed thanks to the Monte-Carlo simulation scheme applied at the discrete volume level for each polynomial basis. Such an implementation of the stochastic finite volume method is applied to model 2D lid-driven cavity flow problem for statistically homogeneous fluid with limited uncertainty in its viscosity and heat conductivity. Further numerical extension of this technique is seen in an application of the Taylor-Newton-Gauss approximation technique, where polynomial approximation may be replaced with some exponential or hyperbolic bases.

Keywords: stochastic finite volume method, Shannon entropy, Navier-Stokes equation, lid-driven cavity flow, weighted least squares method, Monte-Carlo simulation, stochastic perturbation technique.

1 Introduction

Uncertainty in fluid flows is less frequently studied in computational mechanics [1] than for solids and structures deformations [2,3] but is usually characterized by decisively larger statistical scattering of physical parameters; additionally, they are all usually state-dependent, so that uncertainty propagation may have unpredictable character. Uncertainty quantification in both fluids and solids is delivered with the aid of different implementations of the Stochastic Finite Element Method (SFEM) [4], whereas analogous extensions of other discrete numerical methods are definitely less popular, and even scarce. It specifically concerns the Finite Volume Method (FVM), which seems to be more efficient than the FEM in many fluid flow problems described by the Navier-Stokes equations [5-8].

Another important topic is the fact that stochastic analysis benefits from a few probabilistic moments and coefficients of the state functions throughout the given computational domain. This makes a discussion and justification of possible statistical correlations in-between different physical fields very difficult. An alternative way is the estimation (or integration) of probabilistic entropy [9], which is determined using discrete or continuous probability measures for the physical quantity of the interest. Some mathematical models applied successfully in probability, information theory or economics may have some importance in such an analysis [10].

The main idea of this work is a utilization of the Stochastic Finite Volume Method (SFVM) [11] towards the determination of the spatial distribution of the Shannon theory for fully coupled Navier-Stokes equations relevant to the fluid flow problems, where heat flow may have an important contribution to the final fluid velocities and pressure gradients. It is based upon the Weighted Least Squares Method (WLSM) recovery of polynomial bases linking the PVT solutions with the physical parameters of the analyzed fluid. Then, some of these parameters are randomized, and their random polynomials serve in the stochastic perturbation method for Taylor expansions to calculate probabilistic moments in the given flow problem [4]. The same polynomials are engaged in Monte-Carlo simulations enabling Shannon entropy computations at the discrete finite volume level.

The well-known lid-driven cavity flow benchmark CFD study is adopted here and enriched with the Gaussian heat conductivity and fluid viscosity. This case study enables a contrast of the first two probabilistic moments maps with these representing Shannon entropy. This comparison confirms several observations made in solid analyses, especially the fact that extreme values of the resulting coefficients of variation of the PVT solution coincide very well with Shannon entropy. This work documents additionally a coincidence of the maps for these two parameters, which may affect further studies in computational mechanics.

2 Uncertainty in Navier-Stokes equations

The system of basic equilibrium Navier-Stokes equations to be extended towards stochastic analysis and to be solved numerically can be written with boundary conditions as follows [12]:

$$\rho\left(\frac{\partial v_i}{\partial t}+v_{i,j}v_j\right)=\sigma_{ij,j}+\tilde{f}_i, \tag{1}$$

$$v_{i,i}=0, \tag{2}$$

$$\sigma_{ij}=-p\delta_{ij}+2\mu\varepsilon_{ij}, \tag{3}$$

$$\rho c\left(\frac{\partial \theta}{\partial t}+\theta_{,i}v_i\right)=\left(k\theta_{,i}\right)_{,i}+\tilde{q}_i, \tag{4}$$

where the following notation is adopted:

$$\varepsilon_{ij}=\frac{1}{2}\left(v_{i,j}+v_{j,i}\right)=\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right),\quad i=1,2,3. \tag{5}$$

State variables in Eqns. (1-5) represent the velocities v_i, pressure p in the given fluid, the stress σ_{ij} and strain ε_{ij} tensors as well as the temperature θ. Conventional notation is used where fluid viscosity μ, heat conductivity k, heat capacity c as well as mass density ρ are provided. The following boundary conditions are adopted here:

- for the velocity

$$v_i=\hat{v}_i;\mathbf{x}\in\partial\Omega_v, \tag{6}$$

- for the stress tensor

$$\sigma_{ij}n_j=\hat{f}_i;\mathbf{x}\in\partial\Omega_\sigma, \tag{7}$$

- for the temperature

$$\theta=\hat{\theta};\mathbf{x}\in\partial\Omega_\Theta \tag{8}$$

- and for the heat flux

$$k\frac{\partial\theta}{\partial x}=\hat{q};\mathbf{x}\in\partial\Omega_q. \tag{9}$$

Variational formulation of this problem is proposed as follows:

$$\int_\Omega \delta v_i\rho\left(\dot{v}_i+v_{i,j}v_j\right)\mathrm{d}\Omega+\int_\Omega \delta v_{i,j}\left(2\mu\varepsilon_{ij}-p\delta_{ij}\right)\mathrm{d}\Omega=\int_\Omega \delta v_i\tilde{f}_i\mathrm{d}\Omega+\int_{\partial\Omega}\delta v_i\hat{f}_i\mathrm{d}(\partial\Omega_\sigma). \tag{10}$$

$$\int_\Omega \delta p v_{i,i}\mathrm{d}\Omega=0, \tag{11}$$

$$\int_\Omega \delta\theta\rho c\left(\dot{\theta}+\theta_{,i}v_i\right)\mathrm{d}\Omega+\int_\Omega k\delta\theta_{,i}\theta_{,i}\mathrm{d}\Omega=\int_\Omega \delta\theta\tilde{q}\mathrm{d}\Omega+\int_{\partial\Omega_q}\delta\hat{\theta}\hat{q}\mathrm{d}(\partial\Omega). \tag{12}$$

It is further assumed that some physical parameters of the analyzed fluid exhibit Gaussian uncertainty within the given first two moments [13]. An extension of the

aforementioned equations to uncertainty analysis undergoes using the generalized stochastic perturbation technique. Let us consider for this purpose a random variable b and its probability density function (PDF) by $p_b(x)$ so that its expectation can be defined as

$$E(b)=\int_{-\infty}^{+\infty} x\ p_b(x)\,dx \tag{13}$$

assuming no additional truncation in this case. Further, one can define the central probabilistic moment of the m^{th} order as

$$\mu_m(b)=\int_{-\infty}^{+\infty}(b-E[b])^m\ p_b(x)dx. \tag{14}$$

Let us consider the following representation of the random function $\mathbf{v}(b)$ with respect to its parameter b around its mean value [4,11]:

$$\mathbf{v}(b)=\mathbf{v}^0\left(b^0\right)+\varepsilon\frac{\partial\mathbf{v}(b)}{\partial b}\bigg|_{b=b^0}\Delta b+\ldots+\frac{\varepsilon^n}{n!}\frac{\partial^n\mathbf{v}(b)}{\partial b^n}\bigg|_{b=b^0}\Delta b^n, \tag{15}$$

where ε is a given perturbation parameter, while the nth-order variation of a random variable is given as follows:

$$\varepsilon^n\Delta b^n=(\delta b)^n=\varepsilon^n\left(b-b^0\right)^n. \tag{16}$$

Then, the expected values are sufficiently accurate with the use of the 10^{th} order expansion (and for ε=1) and they are calculated as

$$\begin{aligned}E[\mathbf{v}(b)]=\mathbf{v}^0\left(b^0\right)&+\frac{1}{2}\frac{\partial^2\mathbf{v}(b)}{\partial b^2}\bigg|_{b=b^0}\mu_2\left(b^0\right)+\frac{1}{4!}\frac{\partial^4\mathbf{v}(b)}{\partial b^4}\bigg|_{b=b^0}\mu_4\left(b^0\right)\\&+\frac{1}{6!}\frac{\partial^6\mathbf{v}(b)}{\partial b^6}\bigg|_{b=b^0}\mu_6\left(b^0\right)+\frac{1}{8!}\frac{\partial^8\mathbf{v}(b)}{\partial b^8}\bigg|_{b=b^0}\mu_8\left(b^0\right)+\frac{1}{10!}\frac{\partial^{10}\mathbf{v}(b)}{\partial b^{10}}\bigg|_{b=b^0}\mu_{10}\left(b^0\right)\end{aligned} \tag{17}$$

The central moments of the variable b may be simply recovered here as

$$\mu_p(b)=\begin{cases}0; & p=2k+1\\ \{\sigma(b)\}^p(p-1)!!=\{\sigma(b)\}^p(p-1)\cdot(p-3)\cdot\ldots\cdot5\cdot3; & p=2k\end{cases}, \tag{18}$$

for any natural $k\geq1$, which is the consequence of Gaussian distribution's symmetry. The expansions relevant to higher-order statistics in this methodology can be found in [4]. Uncertainty analysis based upon probabilistic moments and coefficients has some well-known limitations and may be biased with some unpredictable numerical errors, therefore a concept of probabilistic entropy has been proposed by Shannon [9] and then extended by many researchers. It states that uncertainty in the given technical system may be quantified by a real number h defined for this system's response f as

$$h\left(f\left(b\right)\right)=-\sum_{i=1}^{n}p_i\left(f\left(b\right)\right)\ln\left(p_i\left(f\left(b\right)\right)\right)\,, \tag{19}$$

where *n* stands here for the number of possible different states of this system. Because a coefficient of variation (CoV) was dominantly used in stochastic computational mechanics to discuss uncertainty importance and propagation in the given boundary value problem, a comparison of Shannon entropy distribution with analogous distribution of the CoV for the given benchmark problem is delivered in the next sections.

3 Stochastic Finite Volume Method

The following polynomial basis is proposed for the resulting temperature field in the presence of some uncertainty source *b* [4]:

$$T_{\beta}=D_{\beta m}^{T}b^{m}\,, \qquad m=0,\ldots,n\text{-}1;\ \beta=1,\ldots,N. \tag{20}$$

where $D_{\beta m}^{T}$ is a rectangular matrix of the unknown polynomial coefficients, so that the following continuous approximation is adopted:

$$\theta\left(x_i\right)=\varphi_{\beta}\left(x_i\right)T_{\beta}=\varphi_{\beta}\left(x_i\right)D_{\beta m}^{T}b^{m};\qquad i=1,2;\ \beta=1,2,...,N,\ m=0,\ldots,n\text{-}1; \tag{21}$$

where φ_{β} are traditional deterministic shape functions and T_{β}. The temperatures' gradients are similarly determined as

$$\theta_{,j}=\varphi_{\beta,j}T_{\beta}=\varphi_{\beta,j}D_{\beta m}^{T}b^{m}\,, \qquad i=1,2,\ m=0,\ldots,n\text{-}1. \tag{22}$$

Analogous representation is proposed for the pressures

$$P_{\beta}=D_{\beta m}^{p}b^{m}\,, \qquad m=0,\ldots,n\text{-}1;\ \beta=1,\ldots,N, \tag{23}$$

and also velocities. As it is well known, the basic idea behind the FVM is an application of the Ostrogradski-Gauss divergence theorem to replace the volumetric integrals inherent in the governing equations (10-12) with the surface integrals rewritten for all the finite volumes completely composing the entire computational domain. The contribution of each finite volume to the global equilibrium equation is represented by the contribution of its center as well as its outer faces. It remarkably differs from the FEM discretization [12,14], where a contribution of each element is traditionally composed of their nodal points contributions. Therefore, Eqn (10) is discretized in each local finite volume *l* as [15,16,17]

$$\left(\frac{\rho^{(\alpha)}\Delta U^{(\alpha)}}{\Delta t}\right)_l + \frac{1}{V_l}\sum_{j=1}^{n_s}\rho_j^{(\alpha)}U_j^{(\alpha)}U_j^{(\alpha)}A_j - \frac{1}{V_l}\sum_{j=1}^{n_s}\mu_j^{(\alpha)}\nabla U_j^{(\alpha)}A_j \tag{24}$$
$$= \left(\nabla U^{(\alpha)}\right)_l \nabla\mu_l^{(\alpha)} - \left(\nabla P^{(\alpha)}\right)_l + \rho_l^{(\alpha)}g^{(\alpha)}$$

where V_l denotes the lth finite volume (in Figure 1).

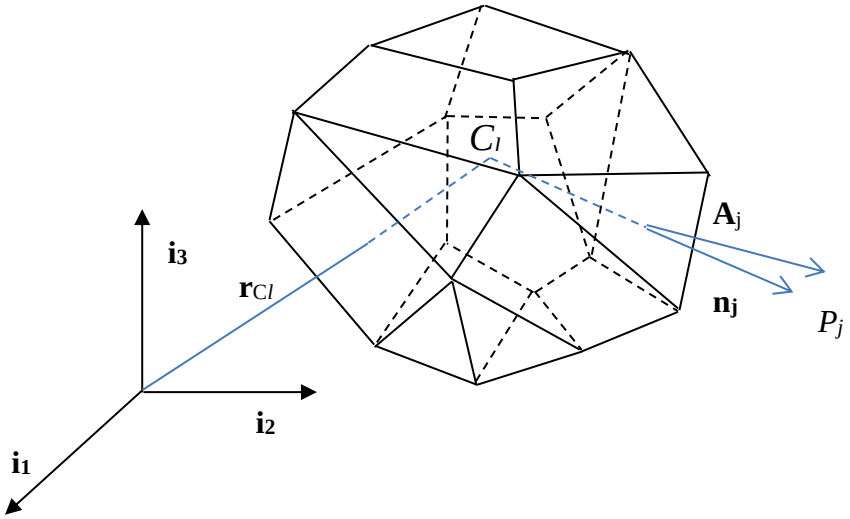

Figure 1: 3D view of a single finite volume.

The pressure gradient in the x_i direction is calculated with the use of the Gauss integration scheme as [11,15]

$$\nabla P_l^{(\alpha)}(x_i) = \frac{1}{V_l}\sum_{j=1}^{n_s}P_j^{(\alpha)}A_j n_j \tag{25}$$

where A_j is the area of the face j, n_j denotes the versor of this surface directed outwards, and $\alpha=1,\ldots, M$. Analogous procedure is proposed for the velocities, e.g.

$$\nabla U_l^{(\alpha)} = \frac{1}{V_l}\sum_{j=1}^{n_s}U_j^{(\alpha)}A_j n_j \tag{26}$$

where the central differencing scheme is applied to determine the given value at the cell face center. The following definitions are adopted and then yield

$$\begin{cases} K_l^{U(\alpha)} = \dfrac{\rho_l^{(\alpha)}}{\Delta t} + \dfrac{1}{V_l}\displaystyle\sum_{j=1}^{n_s}\left\{(1-\chi)\,\rho_j^{(\alpha)}U_j^{(\alpha)}A_j + \mu_j^{(\alpha)}\,\dfrac{A_j}{|d_j|}\right\} \\ \overline{K}_{lj}^{U(\alpha)} = \dfrac{1}{V_l}\left(\chi\rho_j^{(\alpha)}U_j^{(\alpha)}A_j - \mu_j^{(\alpha)}\,\dfrac{A_j}{|d_j|}\right) \\ Q_l^{U(\alpha)} = \dfrac{\rho_l^{(\alpha)}U_l^{(\alpha)}(t-\Delta t)}{\Delta t} - \dfrac{1}{V_l}\displaystyle\sum_{j=1}^{n_s}P_j^{(\alpha)}A_j n_j - \rho_l^{(\alpha)}g^{(\alpha)} \\ \qquad + \left(\nabla U_l^{(\alpha)}(t-\Delta t)\right)\left(\nabla\mu_l^{(\alpha)}(t-\Delta t)\right) \end{cases} \tag{27}$$

Finally, the following algebraic equations system is obtained for the *l*th finite volume

$$K_l^{U(\alpha)}U_l^{(\alpha)}(t) + \sum_{j=1}^{n_s}\overline{K}_{lj}^{U(\alpha)}\overline{U}_{lj}^{(\alpha)}(t) = Q_l^{U(\alpha)}. \tag{28}$$

The variable $\overline{U}_{lj}^{(\alpha)}(t)$ is the so-called velocity face flux adjacent to the finite volume *l* and its *j* outer plane computed at time *t* for the response function test indexed with α. The global momentum equation in the RFM-based FVM is rewritten as

$$\sum_{l=1}^{N}K_l^{U(\alpha)}U_l^{(\alpha)}(t) + \sum_{l=1}^{N}\sum_{j=1}^{n_s}\overline{K}_{lj}^{U(\alpha)}\overline{U}_{lj}^{(\alpha)}(t) = \sum_{l=1}^{N}Q_l^{U(\alpha)} \tag{29}$$

The central differencing scheme with the coefficient χ as the (linear) interpolation factor connecting the given finite volume and its particular face *j* is introduced to evaluate the given scalar field at the cell face center. The continuity equation (11) is discretized similarly on the finite volume level as

$$\sum_{j=1}^{n_s}U_j^{(\alpha)}A_j = 0 \tag{30}$$

Then, the following matrix equation for pressures (for the finite volumes center contribution and the finite volumes face, separately):

$$K_l^{P(\alpha)}P_l^{(\alpha)}(t) + \sum_{j=1}^{n_s}\overline{K}_{lj}^{P(\alpha)}\overline{P}_{lj}^{(\alpha)}(t) = Q_l^{P(\alpha)} \tag{31}$$

where its global version is provided as

$$\sum_{l=1}^{N} K_l^{P(\alpha)} P_l^{(\alpha)}(t) + \sum_{l=1}^{N}\sum_{j=1}^{n_s} \overline{K}_{lj}^{P(\alpha)} \overline{P}_{lj}^{(\alpha)}(t) = \sum_{l=1}^{N} Q_l^{P(\alpha)} \tag{32}$$

Finally, the SFVM discretization of the heat transfer equation is proposed as

$$K_l^{T(\alpha)} T_l^{(\alpha)}(t) + \sum_{j=1}^{n_s} \overline{K}_{lj}^{T(\alpha)} \overline{T}_{lj}^{(\alpha)}(t) = Q_l^{T(\alpha)} \tag{33}$$

where

$$\begin{cases} K_l^{T(\alpha)} = \dfrac{\rho_l^{(\alpha)} c_l^{(\alpha)}}{\Delta t} + U_{li}^{(\alpha)} \dfrac{1}{V_l} \rho_l^{(\alpha)} c_l^{(\alpha)} \displaystyle\sum_{j=1}^{n_s} \left\{ (1-\chi) A_{lj} n_{lji} + k_l^{(\alpha)} \dfrac{A_j}{|d_j|} \right\} \\ \overline{K}_{lj}^{T(\alpha)} = U_{li}^{(\alpha)} \dfrac{1}{V_l} \rho_l^{(\alpha)} c_l^{(\alpha)} \chi A_{lj} n_{jli}\,, \quad i = 1,2,3 \\ Q_l^{T(\alpha)} = \dfrac{\rho_l^{(\alpha)} c_l^{(\alpha)}}{\Delta t} T_l^{(\alpha)}(t - \Delta t) + \phi_l^{(\alpha)} \end{cases} \tag{34}$$

and $\phi_l^{(\alpha)}$ is the viscous dissipation in the *l*th finite volume and the αth RFM numerical test. Therefore, the global heat transfer equation for the SFVM yields [11]

$$\sum_{l=1}^{N} K_l^{T(\alpha)} T_l^{(\alpha)}(t) + \sum_{l=1}^{N}\sum_{j=1}^{n_s} \overline{K}_{lj}^{T(\alpha)} \overline{T}_{lj}^{(\alpha)}(t) = \sum_{l=1}^{N} Q_l^{T(\alpha)} \tag{35}$$

Further processing of the solution towards statistical moments is performed with the use of the Weighted Least Squares Method.

4 Computer simulation and discussion

Let us consider a cube of unit dimensions divided into 400 equal cubic finite volumes containing a fluid with the following physical parameters – density $\rho = 1 \frac{kg}{m^3}$, specific heat $c = 100 \frac{J}{kg\,K}$, thermal conductivity $E[k] = 10 \frac{W}{m\,K}$ and viscosity $E[\mu] = 10^{-1} Pa \cdot s$ (both CoVs equal 0.10). These two parameters are randomized separately according to the Gaussian distribution to distinguish the influence of their uncertainty on the PVT solution of the given fluid flow problem. Imposed boundary conditions for this cube are shown schematically in Figure 2 – the problem is restricted to 2D analysis to make a more apparent final visualization of the resulting state functions and their probabilistic characteristics. The time increment has been set as Δt=0.10 sec and the computations have been stopped after 10 seconds. It is clear that a composition of the physical parameters of the fluid is artificial, and is taken to complete this benchmark test, while realistic fluids analysis would be more demanding.

Computational analysis has been performed with hybrid usage of three different computer systems, namely (a) OpenFVM (series of the deterministic Navier-Stokes problems with varying physical parameters) [18], (b) symbolic environment of the mathematical package MAPLE [19] (WLSM and all probabilistic procedures), (c) the freeware FEPlot 3.1 [20] (probabilistic visualization).

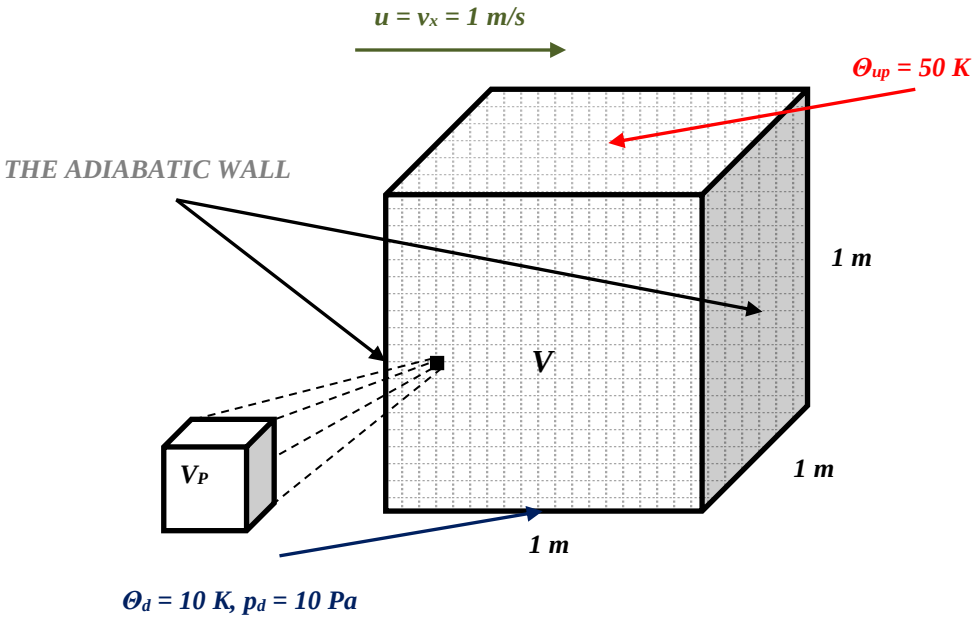

Figure 2: Boundary conditions for the lid-driven cavity flow benchmark

The expected values, coefficients of variation as well as Shannon entropies of the resulting temperatures in two tests including random viscosity (left column) and heat conductivity (right column) have been collected in Figures 3-5 below. It is rather natural and intuitively clear that expected values in both problems are equal to each other (Figure 3) increasing moderately from the upper to the lower surface of this quadratic cavity. It is due to the temperature boundary conditions presented in Figure 2. Small boundary temperature fluctuations throughout the upper and lower edges are caused by the rotational flow.

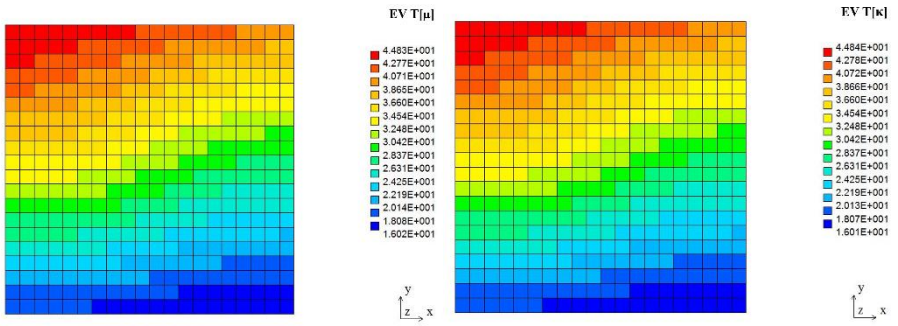

Figure 3: Expected values of the temperature in the lid-driven cavity flow test for Gaussian viscosity (left) and heat conductivity (right)

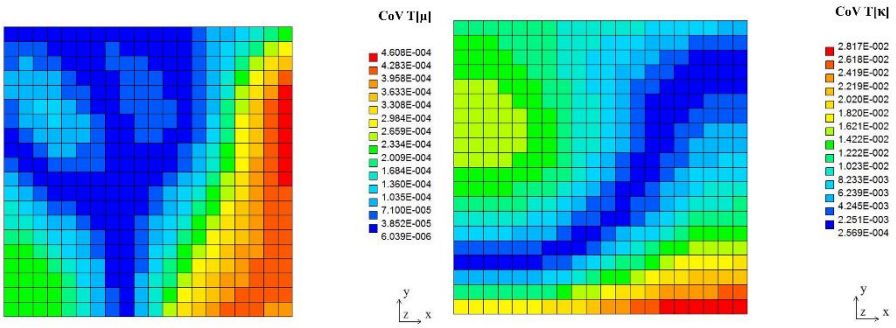

Figure 4: Coefficients of variation of the temperature in the lid-driven cavity flow test for Gaussian viscosity (left) and heat conductivity (right)

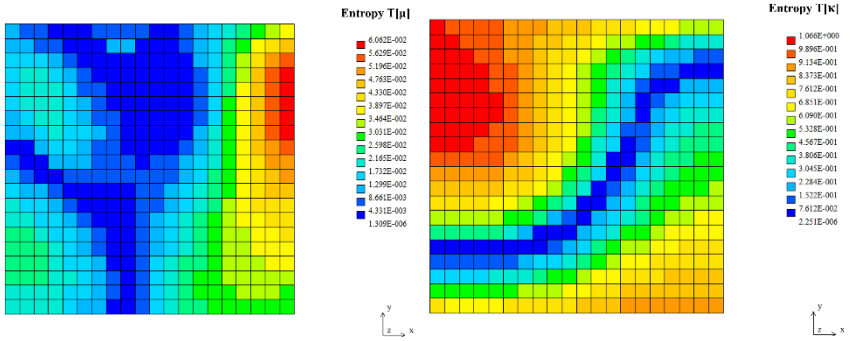

Figure 5: Shannon entropies of the temperature in the lid-driven cavity flow test for Gaussian viscosity (left) and heat conductivity (right)

Both coefficients of variation (Figure 4), as well as probabilistic entropies (Figure 5), have their spatial distributions similar to each other but completely different than a distribution of the expectations; this similarity holds for the same random input parameter, of course. Uncertainty in fluid viscosity returns extreme uncertainty of a temperature (largest values of the CoV and entropy) on some part of the right vertical edge. Analogous uncertainty in the heat conductivity has its extreme value close to the upper left corner, where extreme expectations have been noticed (cavity inlet). Quite interestingly, minimum values of the resulting temperature's uncertainty (close to 0, which is adjacent to the deterministic situation) form the same tree in the given 2D domain for the fluid viscosity and almost the same path – for random heat conductivity. Finally, it is remarkable that larger CoVs and Shannon entropies at the same time are noticed while randomizing heat conductivity than fluid viscosity – it agrees well with engineering intuition and may serve as some verification of the probabilistic solution.

5 Concluding remarks

1. Shannon entropy determination for the PVT solution of the fluid flow problem with uncertainty solved using the Stochastic Finite Volume Method has been presented in this work. This approach follows fully coupled Navier-Stokes equations and dual probabilistic methodology based on the generalized stochastic perturbation method as well as the Monte-Carlo simulation

technique. It has been demonstrated here that the spatial distribution of probabilistic entropies is very close to the additional distribution of the coefficients of variation of the given fluid state function and may be useful in further uncertainty analysis for flow problems. This coincidence is observed for two different physical properties of the fluid, namely heat conductivity and viscosity, so it does not seem to be accidental. Therefore, following computational studies delivered in the area of linear and nonlinear solid mechanics, Shannon entropy would be advisable to illustrate uncertainty propagation in the flow problem instead of a series of the probabilistic moments and coefficients, which need to be studied altogether to achieve the same goal. It needs to be underlined that contrary to the existing research in computational mechanics, this study enables spatial distributions of Shannon entropy throughout the entire computational domain and this entropy has local character connected with the discrete finite volume.

2. The numerical solution is based upon hybrid usage of the open source FVM program, computer algebra system for probabilistic analyses, and the LSM fittings as well as FEPlot software to complete a visualization of the resulting probabilistic moments and entropies. Further implementations should be focused on closer interfacing of these three systems as well as on the parameter sensitivity of the resulting entropy concerning the histogram partitioning, Monte-Carlo random trials number, input uncertainty level as well as FVM time and spatial discretization of the given flow problem. It may happen that due to the numerical error of the solution itself or erroneous definition of the aforementioned problem parameters' settings, Shannon entropy distribution computation would be inefficient. In case of any possible numerical discrepancies, some other probabilistic entropy models could be considered.

Acknowledgments

This work contains the results obtained in the framework of the research grant OPUS no. 2021/41/B/ST8/02432 entitled "*Probabilistic entropy in engineering computations*" and sponsored by the National Science Center in Cracow, Poland, 2022–2025.

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