Optimizing generation of multiple turbulent flow states

B Krasnopolyky, N Nikitin and A Lukyanov
Institute of Mechanics of Lomonosov Moscow State University, 1 Michurinsky prosp., Moscow 119192, Russia
E-mail: krasnopolyky@imec.msu.ru

Abstract. The problem of generation multiple uncorrelated turbulent flow states subject to low computational costs is among the key questions affecting the overall performance of algorithms for modeling incompressible turbulent flows. The current paper proposes the computational procedure that can be used to generate multiple initial turbulent flow fields. This procedure is based on the fact of exponential divergence of the phase trajectories for turbulent flows and allows to perform the corresponding simulations without priori information about the characteristic decorrelation time scale. The preliminary validation results of the proposed procedure demonstrate a possibility of additional 10% speedup when modeling turbulent flows by using proposed in this paper numerical algorithm with the algorithms combining averaging in time with ensemble averaging.

1. Introduction
Despite constant growth of computational capabilities of modern high performance computing systems, the problem of modeling turbulent flows using high-fidelity eddy resolving methods is still a challenging task. Extremely high computational costs for these simulations strongly limit their range of applicability in engineering and scientific applications. This motivates researchers to develop novel computational methods with the focus on improvement of the overall simulations performance. Recently, the method for modeling incompressible turbulent flows with the averaging over multiple ensembles has been proposed in [1]. The method combines averaging in time to obtain turbulent statistics together with the averaging over multiple uncorrelated flow realizations. This allows to replace a long integration in time for a single flow state with the integration of multiple flow states, but over much shorter time interval, thus allowing to parallelize the simulation in time.

The time integration schemes typically used for high-fidelity turbulent flow simulations allow to rearrange the simulations of multiple flow states in a single run, thus transforming the solution of pressure Poisson equation at each time step, used to project the velocity field to a space of divergence-free functions, to a system of equations with multiple right-hand sides. The architecture of modern compute systems allows to obtain observable speedup when solving systems of linear algebraic equations with multiple right-hand sides compared to multiple solutions of the systems with single right-hand side vector [1]. Using this fact, it is possible to speedup the turbulent flow simulations with ensemble averaging compared to conventional simulations with averaging in time only.

The paper [1] provides simple theoretical estimate showing the range of applicability for the proposed simulation methodology. The achieved speedup for this approach is strongly affected by the
computational overhead due to the need to obtain multiple uncorrelated initial turbulent flow states. These states were obtained in a trivial way by simulating transition intervals to reach statistically steady turbulent flow states from different initial conditions (e.g., with random perturbations added, figure 1a). While this approach guarantees obtained solutions to be uncorrelated with a large enough transition interval [2], it is definitely not the optimal one in terms of computational costs, and the corresponding overhead can be reduced. One of the possible scenarios to generate multiple turbulent flow states has been investigated in [3]. Here, an option to introduce the perturbations inside the transition interval has been examined (figure 1b). The presented results have demonstrated that the reduction of computational overhead to generate multiple turbulent flow states by a factor of 1.5 can be achieved for the test problem of modeling turbulent flows in a channel with a matrix of wall-mounted cubes [4] considered in the paper. The observed improvement in the overhead reduction allows to obtain an additional speedup by approximately 20% and increases the range of applicability of the proposed approach which is based on combining averaging in time together with ensemble averaging as a whole.

While the proposed approach to generate multiple initial turbulent flow states allows to significantly improve the overall performance, the main drawback was related to the choice of the time instant to introduce the corresponding perturbations. On the one hand, this bifurcation point is reasonable to be chosen close to the end of the transition interval. On the other hand, the time interval before the end of the transition interval must be large enough to ensure the corresponding turbulent flow states to become uncorrelated. The paper [3] demonstrates that the problem of optimization the procedure to generate multiple turbulent flow states is of paramount importance for further algorithm performance improvements, but does not provide the formal criteria on how to choose the corresponding time instant to introduce the perturbations. The current paper attempts to extend ideas presented in [3] and suggests the corresponding algorithm for the generation of multiple uncorrelated turbulent flow states.
The paper is organized as follows. The second section contains the description of the proposed computational algorithm together with the formal criterion to choose the corresponding simulation intervals. The third section contains numerical simulation results, validating the proposed numerical procedure. Finally, the fourth section concludes the paper.

2. Algorithm description
The development of the optimized procedure to generate multiple turbulent flow states is among the key factors for further improvements of the computational algorithm to model turbulent flows, combining averaging in time together with ensemble averaging. The procedure is based on the injection of small perturbations at the intermediate point \( T_B \) inside the transition interval \( T_T \) allowed to obtain significant performance gain, but does not provide formal criteria, applicable for a wide range of applications. The current paper suggests the modification of the approach discussed above.

It is known, that the stochastic processes demonstrate exponential divergence of the phase trajectories, and the corresponding growth rate is determined by the highest Lyapunov exponent [2]. Thus, having the single statistically steady turbulent flow state, one can obtain multiple states by modeling the evolution in time the flows with introduced small random perturbations. The growth rate of the norm of difference of two velocity fields can be used as a formal criterion in practical simulations: the deviation of the residual norm behavior over time from the exponential growth indicates the flow states to become uncorrelated. This guides to split the overall simulation in three stages (figure 1c): (1) obtaining the single statistically steady turbulent flow state (performing the simulation over the time interval \( T_T \)); (2) introducing random perturbations and modeling the evolution of \( m \) flow states until they become uncorrelated; (3) averaging in time of multiple flow states over the time interval \( T_A/m \). The proposed procedure differs from the one suggested in [3]: here, it is suggested to introduce the perturbations after reaching the statistically steady state, while previously the perturbations were introduced at the transition stage.

The current procedure assumes minor increase in the overall computational costs compared the one discussed in [3]. However, it can be shown with simple theoretical estimates that the overall simulation slowdown is only within several percent if the decorrelation intervals for both approaches coincide. Otherwise, the modified procedure can even be beneficial, as it does not need any priori information about the decorrelation time scale.

3. Simulation results
The proposed computational procedure has been validated using the test case of modelling turbulent flows in a channel with a matrix of wall-mounted cubes [4] using an “in-house” computational code for direct numerical simulations of turbulent flows on orthogonal curvilinear coordinates [5]. Some details of the computational code and the test case formulation can be found in [1, 3]. The grid of 2.32 mln. cells was used for the benchmark purpose. The overall simulation time was set to \( T = 2100 \) time units, which comprises of the transition interval \( T_T = 100 \) and averaging interval \( T_A = 2000 \) time units. The simulations were performed on “Lomonosov-2” supercomputer using 32 compute nodes per each run.

In the current test session, four runs are compared, including the conventional simulation with the averaging over the single flow state and simulation of 4 flow states with various strategies to obtain initial turbulent flow states. The corresponding simulation times are summarized in table 1. The conventional approach to model this test problem took 44 min. to obtain the turbulent flow from the prescribed initial state, and 892 min. to perform 2000 time units and collect turbulent statistics. The overall computational time was equal to 936 min. The second run includes the simulation of 4 flow states with basic approach to generate multiple initial flow states, i.e. the computation of full transition intervals for each of flow realizations. In this case, the simulation of the transition interval took 114 min., and the averaging over 500 time units was performed in 531 min. The overall simulation for this run took 645 min. The third run reiterates the simulation strategy, suggested in [3]: the first stage of the transition interval (77 time units) with the single flow state took 34 min.; the second stage,
decorrelation of flow states, took 22 minutes (23 time units), and finally the averaging was performed in 537 min. Thus, the simulation result was obtained in 593 minutes. The last run, focused on validating the approach to generate multiple turbulent flow states proposed in this paper, started with modeling of the transition for the single flow state, i.e. $T_T = 100$ time units in 44 min. After that, the simulation was restarted for 4 flow states with the random perturbations injected to each of the states (the amplitude of the perturbations did not exceed $10^{-4}$). The norms of the difference of streamwise velocity components for the modeled flow states were monitored at the second stage. The strong deviation from the exponential growth was observed starting from the $T_D = 120$, which indicated the decorrelation was achieved in 20 time units (figure 2). The indicated time scale for the considered test problem correlates with the one identified in [3], where the interval of 23 time units was denoted. The simulation of the corresponding stage took 21 min. Finally, the averaging over 500 time units with 4 flow states was performed in 538 min., that allowed to obtain the overall solution in 603 min.

| Flow states, m | Transition time, min ($T_T$) | Averaging time, min ($T_A$) | Overall simulation time, min |
|---------------|------------------------------|-----------------------------|-----------------------------|
|               | Evolution time, min ($T_E$) | Decorrelation time, min ($T_D$) |                             |
| 1             | 44 (100)                     | 892 (2000)                  | 936                         |
| 4             | 114 (100)                    | 531 (500)                   | 645                         |
| 4             | 34 (77)                      | 537 (500)                   | 593                         |
| 4             | 44 (100)                     | 538 (500)                   | 603                         |

Figure 2. Evolution of the norms of difference of velocity fields after the introduction of random perturbations.

The presented preliminary validation results demonstrate that the proposed procedure allows to obtain the turbulent flow states without any priori information about the characteristic decorrelation time scale. This procedure has higher computational costs compared to the one discussed in [3], but decreases the overall speedup by only 1-2%. After the detailed validation using a wider range of test cases, the proposed procedure, as expected, can be suggested as an efficient algorithm for generation of multiple initial turbulent flow states thus supplementing the general algorithm for modeling turbulent flow states with ensemble averaging.
4. Conclusions
The paper discusses the problem of the generation of multiple initial turbulent flow states used in the simulations of turbulent flows with the algorithm which combines averaging in time together with ensemble averaging. The proposed computational algorithm is based on the exponential divergence of the phase trajectories for the turbulent flow states. The strong deviation from the exponential divergence is suggested as a criterion of the decorrelation of obtained turbulent flow states. The corresponding algorithm is validated with the test problem of modeling turbulent flows in a channel with a matrix of wall-mounted cubes. The preliminary validation results demonstrate the speedup comparable to the algorithm suggested in [3], which uses additional a priori information about the characteristic decorrelation time scale.

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