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Chapter

Direct Numerical Simulation of Nano Channel Flows at Low Reynolds Number

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Abstract

The governing equations of viscous fluid flow are generally represented by Navier–Stokes (NS) equations. The output of Navier Stokes equations is in essence velocity vector from which rest of the flow parameters can be calculated. It is essentially a riotous task, sometimes it becomes so unmanageable that fluid flow over simplest topologies under low Reynold's numbers also needs the most powerful supercomputing facility to solve, if needed to model the fluid and its behavior under the turbulent conditions the best way out is to solve the averaged NS equations. However in the process of averaging Reynolds introduced certain new terms such as Reynolds Stresses. Therefore it is required to close the system of equations by relating the unknown variables with known ones. Hence we have turbulence models. Direct Numerical Simulation (DNS) is a method of solving NS equations directly that is by forfeiting the need of turbulence models as the equations are not averaged. However originally direct numerical simulation procedure does not need of additional closure equations, it is essential to have very fine grid elements and should be estimated for exceptionally small time steps to achieve precise solutions. In the present chapter an interesting flow through nano-channel problem has been discussed using the indispensable mathematical technique of computational fluid dynamics (CFD) which is DNS.

Keywords: direct numerical simulation (DNS), Navier stokes (NS) equation, turbulent flow, nano-channel flow Reynolds number

1. Introduction

While studying any physical phenomena be it of practical or academic importance, it is not always possible to mimic the exact system. For an example, if we want to study the flow of air past a moving train engine, we might have to build a wind tunnel along with a provision for a railway track for the engine to move in and out. We should have sensitive measuring instruments fixed at different places to measure various parameters. Again, finding the right locations for fixing these instruments can only be determined by carefully performing large number of iterations because the margin for errors in real-life problems are miniscule. For example, if the paint on the car is not done correctly even in some parts, it may contribute hugely to skin-friction drag and thereby reducing the mileage of the car.

One might argue that we can use scaled models keeping the physics of the problems same. These models induce errors during extrapolation to the actual situation besides being very costly in terms of infrastructure, resources and time. If we try to write a mathematical function and solve it, we should know all the pertinent parameters and laws that govern the flow. Then we might use various techniques like dimensional analysis and arrive at an equation. The validation of this mathematical equation again, can only be done by experiments. Once we get an equation, solving it for various cases is in itself a major challenge because we almost always end up with differential, integral or Integro-Differential equations. Till date, exact solutions to some of these equations are still open problems. So, approximate solutions are desired as against exact solutions. The advent of advanced computers brought along the solution for this in the form of Computational Fluid Dynamics (CFD). We can now analyze various types of fluid flows with numerical simulations and also develop suitable simulation algorithms. In most practical problems, the state variables of the fluids can be treated as continuous functions of space for which we already have conservation laws for mass, momentum, and energy. For many fluids that are used in engineering applications, there are well-accepted constitutive relations.

The fundamental fluid mechanics is put in the form of Navier Stokes equations way back in 1800s and thereupon many attempts were made to find the general solutions for the equations but even today it is an open millennium problem [1–3]. Based on the physics of interest, we make certain approximations to Navier–Stokes equations and therefore obtain the governing partial differential equations to be solved [4]. When tried to solve such governing equations using a numerical methods a suitable discretization procedure will be adopted and the problem will be attacked to solve using a better solver. Here we convert the mathematical model into a discrete system of algebraic equations. We even call it to be a difference equation in some gut words while the chosen method to solve the equations is Finite difference method (FDM). Many of this kind of solving methods have been evolved and to mention a few the finite element method (FEM), the finite volume method (FVM), boundary element method (BEM) are a few popular methods among so many numerical techniques. Out of many factors that influence selection, some are very crucial like problem defined on the geometry, the analyst's preference, and the predominant trend of solution may be in a selected and particular area of the problem space. Nonetheless it will be decided later about which numerical algorithm to be adopted and solve these equations and develop a computer programs [5–7]. After the advent of enormous speed in graphics processing units the computer graphics and animations formed from large output of numerical values make the visualization of the simulation results easier to human comprehension and draw the conclusions henceforth.

The nature of fluid flow is such a complicated phenomenon no matter what governing equations we formulate and try even more numerical solutions for the same, it can well be understood with a single classic statement of legendary Nobel Laureate R. P. Feynman in his popular scientific texts, in a quote "The efforts of a child trying to dam a small stream flowing in the street and his surprise at the strange way the water works its way out has its analog in our attempts over the years to understand the flow of fluids. We have tried to dam the water up—in our understanding—by getting the laws and the equations that describe the flow" depicts how novice the formulations are. The statement given by Feynman has already been proved more than quite often times in the applications of Fluid Dynamics in modern engineering and science, and more profoundly to the computational fluid dynamists.

> *Nonetheless an additional unique feature relates to the mathematical nature of Navier-Stokes equations. Steady-state Navier-stokes equations are elliptic in nature, whereas unsteady Navier-Stokes equations are parabolic in nature. As numerous problems associated with the methods of solution of the completely defined elliptic Partial differential equations the Navier-Stokes equations generally solved as an unsteady problem even in the case if the flow is steady, using a time marching schemes [8–10]. The transient solution of Navier-Stokes problem yields the solution but not be any easy compared to the steady state flow problem in more general geometric case.*

Turbulent flows involve randomly fluctuating flow variables such as velocity, pressure, and temperature.

Within the defined flow decomposition in accordance with Reynolds, a flow variable at a given spatial point at a given instant can be represented as the sum of a mean value and a random fluctuation about this mean value, and the process of obtaining the average or a mean value is represented as the technique of *Reynolds averaging*. Therefore, for any flow variable ϕ , its spatio-temporal variation can be expressed as stated below.

$$\phi(\,x_i,t\,) = \overline{\phi(\,xi\,)} + \phi'(\,x,t\,)$$

Where $\overline{\phi}$ the mean or an averaged value and ϕ' is the variations in the property which is with fluctuating values or statistically steady turbulent flows.

$\phi(x)$ is the time average defined as

$$\overline{\phi(\,xi\,)} = \lim_{T\to\infty}\frac{1}{T}\int_0^T \phi(xi)dt$$

Where T represents the averaging time interval, which must be large compared to the typical time scales of fluctuations throughout the flow length.

For unsteady flows, ϕ represents ensemble averaging defined as

$$\phi(\,x_{i,},\mathrm{t}\,) = \lim_{N\to\infty}\frac{1}{N}\sum_{i=0}^{N}\phi(x_i,t)$$

where *N* is the number of identical experiments.

The Reynolds averaging applied to the continuity and momentum equations of an incompressible fluid flow would be obtained in the following set of equations.

$$\frac{\partial(\rho\overline{vi})}{\partial xi} = 0$$

$$\frac{\partial(\rho\overline{vi})}{\partial xi} = \frac{\partial(\rho\overline{vi}\,\overline{vj})}{\partial xj} = -\frac{\partial\overline{p}}{\partial xi} + \frac{\partial\rho\left(\overline{\tau ij} - \tau ij\,R\,\right)}{\partial xj}$$

Where $\hat{o}_{ij}\mathrm{R} = -\tilde{n}\overline{\left(\acute{v}i\,v\acute{}j\;\;\right)}$ is Reynolds stress tensor.

The Reynolds averaged transport equation for a scalar ϕ

$$\frac{\partial(\rho\overline{\phi})}{\partial t}+\frac{\partial(\rho\,\overline{vj}\;\overline{\phi})}{\partial xj}=\frac{\partial\left(\mathrm{r}\,\frac{\partial(\rho\overline{\phi})}{\partial t}+qjR\right)}{\partial xj}$$

Where $q_iR=\rho\overline{v'\,j\,\phi'}$ is turbulent flux.

The higher order correlations appear in Reynold's stress equation is due to non-linearity of Navier–Stokes equation, despite the fact that we try an attempt to derive the governing equation for higher-order terms, they would always result in equations with even higher order correlations.

The Eddy viscosity models are evolved basing on the Boussinesq proposition, which defines the Reynolds stresses which would be proportional to mean velocity gradients, as that of Deviatoric Reynolds stress. This stress is proportional to the mean rate of strain. Numerical computation of eddy viscosity possibly would be required for the solution of the set of transport equations.

Thus, the Reynolds averaged NS model turbulence models are going to be categorized on some of the several additional partial differential equations that are to be solved to enforce closure and find the final flow behavior in any of the defined topology. The zero-equation model is actually the one that computes the eddy viscosity solely from the Reynolds-averaged velocity field. The transport equation that is solved simultaneously with the Reynolds-averaged Navier–Stokes equations to determine the eddy viscosity is in other words known as one-equation model that refers to the family of turbulence models [11–13].

The highly established standard k -ε model which has been developed and contributed by Launder and Spalding makes use of two model equations, one for the turbulent kinetic energy k and the dissipation rate of turbulent kinetic energy per unit mass ε. The transport equations are solved using the Reynolds averaged Navier–Stokes equations. The k-€ turbulence model is well established and the most widely validated and uses the eddy Viscosity turbulence model [14]. Diverse modifications of the standard model have been recommended to account for the near-wall flow region and low Reynolds number turbulent flows. Nevertheless the Eddy viscosity models have significant deficiencies, which are due to some eddy viscosity assumptions. The experimental measurements and numerical simulations have indicated that in the cases of three dimensional turbulent flow the eddy viscosity turns out to be a tensor quantity [15]. Therefore, the use of a scalar eddy viscosity for computation of Reynolds stresses is might not be appropriate. It would as an alternative be recommendable to compute Reynolds stresses directly using its dynamic transport equations. This idea has been the basis of the Reynolds stress model though it the most expensive methods of the turbulence models in use in the present day CFD solutions and particularly for RANS simulations. It is relatively expensive computationally in comparison to eddy diffusivity models since it requires solving seven additional PDEs for every grid solution in this case. Hence these models are not used as widely as expected from the analysis's the eddy diffusivity models in practical analyses.

In the later days one of the most adoptable and practically sensible methods that have surfaced is Large Eddy simulation (LES). The method in which the Large scales of motion or large eddies of fluids which possess more energy than a smaller one have been taken to be most critical in the solving for turbulent flow cases and has been proved to be more effective in most of the cases both in the experimental and industrial applications [16]. The most effective transporters of conserved quantities viz. mass, momentum, and energy remain to be only large eddies compared to the smaller eddies. The momentum, and energy exchange is so minimal in such cases that they can be neglected. Moreover the behavior of these smaller scales of motion is universal in turbulent flows irrespective of the flow's context and geometry.

It is moderately undemanding to capture the effect of smaller eddies through a model. The underlying principle of LES is to treat the large eddies of the flow precisely and model the more universal small scale eddies, however this method is inherently time-dependent and are highly suitable for three-dimensional simulations. Such approach is less costly than DNS but a lot more expensive than RANS model for the same flow. Large Eddy Simulation (LES) is mostly preferred method for obtaining accurate time history for high Reynolds number and complex geometry flows. It separates the larger and smaller eddies through spatial filtering operation [17].

The conceptual steps are somewhat like this, it begins with the spatial filter to decompose velocity field $v_i(x,t)$ into a sum of resolved components $v_i(x,t)$ and residual sub grid scale component $v_i(x,t)$ $v_i(x,t)$ represents the motion of large eddies. Such equations are very similar to the original Navier–Stokes equation except for an additional residual stress term arising from filtering. Thus it will be obtained that the filtered velocity, pressure, and temperature field using an appropriate Navier–Stokes solver. In large eddy simulation, the spatial filtering operation for any transported field is defined by a using filter function. In LES, a filter kernels has been used, this also includes a Gaussian filter, a top-hat or box filter, and also spectral cut-off filter. Filtering operation roughly implies that eddies of a size larger than cut off width are large eddies while eddies of size smaller must be modeled. The convective term in the preceding equation cannot be computed in terms of the resolved velocity field. To get an approximation for this term, let us introduce the so called sub-grid stress tensor. The sub grid scale (SGS) Reynolds stress represents large scale momentum flux caused by small or unresolved scales, and it must be modeled to ensure closure. The dissipation takes place is much smaller than the characteristic length scale considering the length scale η of the flow with its ratio $\frac{L}{\eta}$ and this being proportional to $\mathrm{Re}^{3/4}$. As we allow the Reynolds number of the flow is increased length scales range it is observed the space and time in the flow and hence it becomes wider.

On the other hand due to the rapid growth in the computational resource Direct Numerical Simulation (DNS) of turbulent flows has become one of the crucial tools in turbulence research. Though DNS has gained its importance and has been universally recognized about its technique and methodology the kind of resources it consumes to figure out turbulence in some of the fundamental geometries is in itself a complicated affair.

It is also able to provide statistical information difficult to obtain by experimental measurements. Among effects to be observed in the DNS prior to laboratory experiments about flow velocity and vorticity vectors such effects are not present in if the modeling is done gaussian fields. However the attainment of high Reynolds number flow analysis necessitates the use of subgrid scale model to represent the effects of the unresolved small-scale turbulence on the explicitly designed and simulated large-scale flow. The leading length scales are considered to be of the order of higher dimension of flow region in the fluid flows or of the size of largest Eddie leading to turbulence in the fluid flow. The nominal scale of size of eddies in the inertia forces and viscous forces are of comparable magnitude so that the energy is cascaded to the Eddie, it is directly dissipated. Consecutively to simulate whole scales in turbulent flows, the computational domain must be sufficiently larger than the largest characteristic length scale of the flow L and the grid size must be smaller than the finest turbulence scale η.

The turbulent flows are essentially three-dimensional in nature and to satisfactorily model it needs at least require $(L/\eta)^3$ grid points, seems to be proportional to $\mathrm{Re}^{9/4}$. The calculations must proceed for time scale of largest Eddie i.e., L/U, while the time steps must be of the order η/U which implies Re^n time steps must be taken per each run of the simulation. If we calculate the computing time necessary for the range would be of years for a single run in the limits of the magnitudes of Reynolds numbers encountered in practice. Most DNS performed does not take into account the vortices with size smaller than the grid size. To be able to obtain meaningful results from DNS sufficiently fine spatial resolution must be acquired to ensure that flow phenomena taking place at scales smaller than the grid resolution are negligible. For these reasons, DNS in many cases should be regarded as "highly accurate turbulent calculations without any use of turbulent models." The mathematical framework and numerical results therefore obtained must serve as the useful exact solutions of the physical problems only possible for limited cases and topologies for example in the region of laminar flow of fluid through a pipe and moreover that is possible if the nonlinear terms are dropped from the N-S equation which allows analytical solution in such confined and flow regions and geometries.

In the present work, turbulent flows have been selected to investigate using large eddy simulation (LES) principles and also to understand the direct numerical simulation methodology to model and study the turbulence in fluid flow in nano channels of an electronic device. The nano channel is designed to transit the fluid and therefore removes the heat from the plate. The fluid considered to be multiphase as there would be a base fluid in which the nanoparticles will be suspended and hence an Eulerian multiphase as well as VoF techniques is being implemented. The same conditions are been attempted to solve directly using the techniques of DNS code of Geris flow solver for a simple 2D model and an unified flow field has been created as an initial flow conditions to capture the turbulent flow along the length scale and adaptive mesh refinement has been adopted while selecting the flow solvers in the three dimensional flow generation in such nano channel. The problem uses a finite volume method (FVM), in which the conservation equations in their weak formulation are solved in a discrete number of cells, determining one value for the flow parameters in each cell. The visualization has been taken in paraview and the exported combined file is processed as a data file in commercial code to make a comparative study about the two well developed turbulence modeling techniques. The nano channel considered as a rectangular pipe flow shown in **Figure 1**. The turbulent channel flow is often referred to as a canonical flow of Poiseuille flow case, since it is one of the simplest flows one can think of to attack using the direct numerical simulation. Therefore, this test case is suitable to verify if a numerical solver is able to accurately predict the turbulent vortices near the wall of the tube particularly at the bottom of the channel as the fluid is incompressible.

Simulations between all the Reynolds numbers in the range of $100 \geq \mathrm{Re} \geq 320$ the grids have been selected in the stream wise, the wall-normal, and the pipe length of the computational domain are $L_x \times L_y \times L_z = 2 \times 2 \times 40$ as shown in the **Figure 1**. The grid points have been $N_x \times N_y \times N_z = 178 \times 98 \times 356$. It has been proposed as the standard condition that the computational grid is uniform in the direction of stream flow. In due course of transient time approximately 18 convective time scales it has been observed that the steady state has been reached. From this condition the time averaging has started and the flow has been simulated for more than 120 convective time steps statistically independent time levels have been considered for averaging flow velocities and vorticity in the length scale.

In the **Figures 2, 3** and **4** it has been shown about the convergence of the statistical data in the cases of turbulent intensity along the pipe length as the flow becomes steadily turbulent.

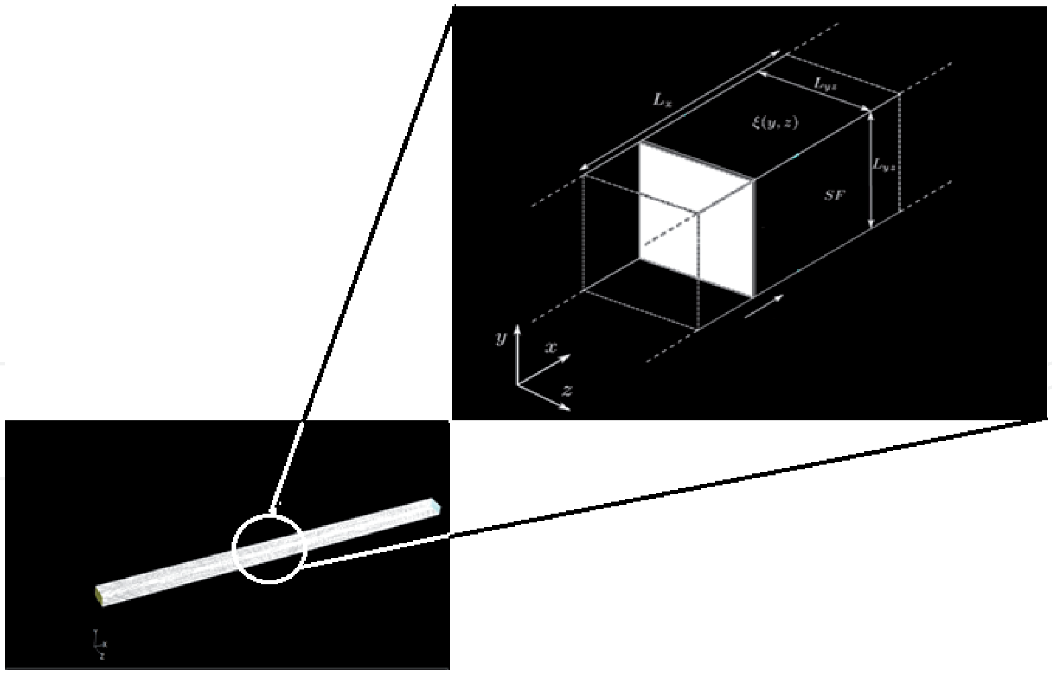

Figure 1.
Geometry of pipe.

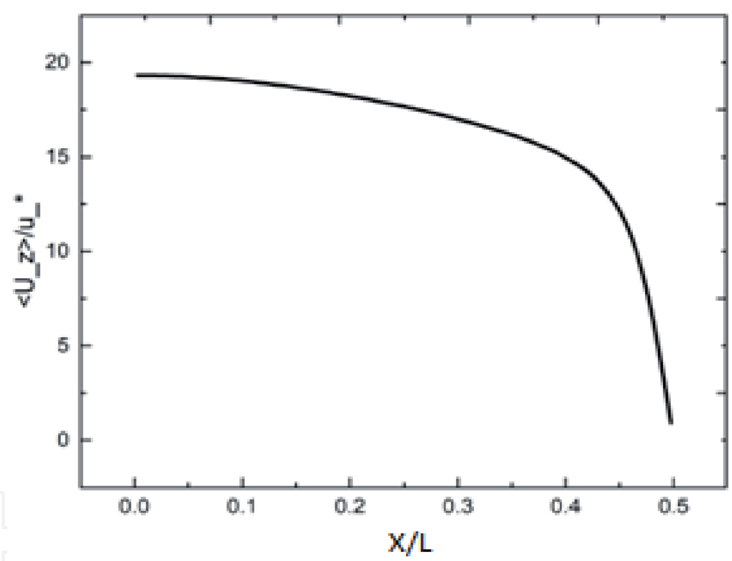

Figure 2.
Mean axial velocity.

The gradual development from uniform turbulence to a pattern at Reynolds number180 has been accounted and presented in the **Figure 4**. The energy distribution plays a key role in the flow transition and henceforth is to be tracked quantitatively and with the probability distribution. The velocity gradients near the pipe walls after the flow is fully developed would exhibit the axial flow velocity as shown in **Figure 2** and consecutively the root mean square velocity computed is presented in **Figure 3**. These plots are developed on the basis of non dimensional number along the length of the pipe. At the maximum fluid velocity along the channel it has been recorded that there is no significant raise or dip in the Reynolds number in all the runs.

The propagation velocity of the pattern is approximately that of the mean flux and is a decreasing function of Reynolds number. Examination of the time-averaged flow shows that a turbulent band is associated with two counter-rotating cells stacked in the cross-channel direction and that the turbulence is highly

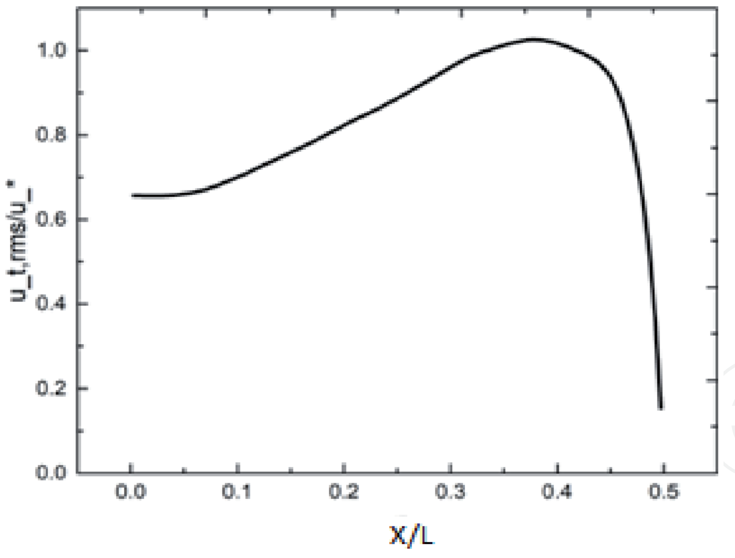

Figure 3.
RMS value along the pipe length.

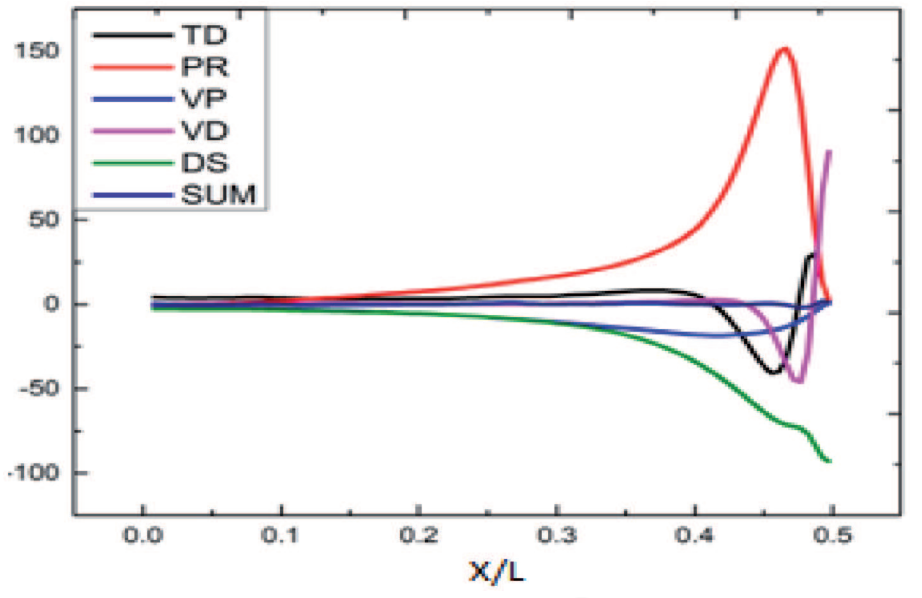

Figure 4.
Turbulent KE distribution record.

concentrated near the walls. Near the wall, the Reynolds stress force accelerates the fluid through a turbulent band while viscosity decelerates it; advection by the laminar profile acts in both directions. In the center, the Reynolds stress force decelerates the fluid through a turbulent band while advection by the laminar profile accelerates it. These characteristics are compared with those of turbulent-laminar banded patterns in plane Couette flow.

The average Reynolds number varies in the different cases, from 120 in the bare flow case to 512 in the fully developed convective flow conditions as a working nanofluid cooling device. Though the primary aspect of heat transfer is not considered until the turbulent flow did not notice during the flow through the channel, the swirling velocity component is completely ignored. The pressure drop is exactly getting equated to the experimentally verified case in the case of LES calculated value in almost all the cases as shown in **Figure 5**. Once the LES model could capture the significant turbulence properties, the problem is attempted on geris flow solver code for DNS solution for one such case to be verified with the already obtained results. Some of the results obtained are presented in **Figure 6**.

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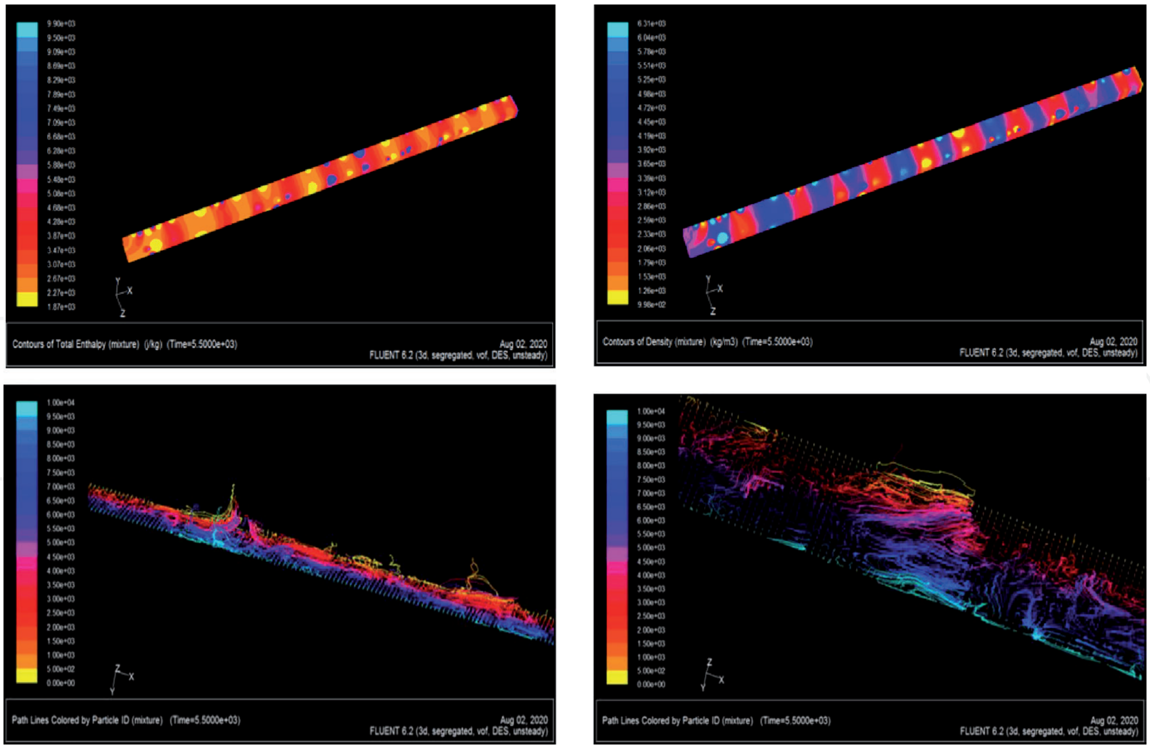

Figure 5.
LES based simulation.

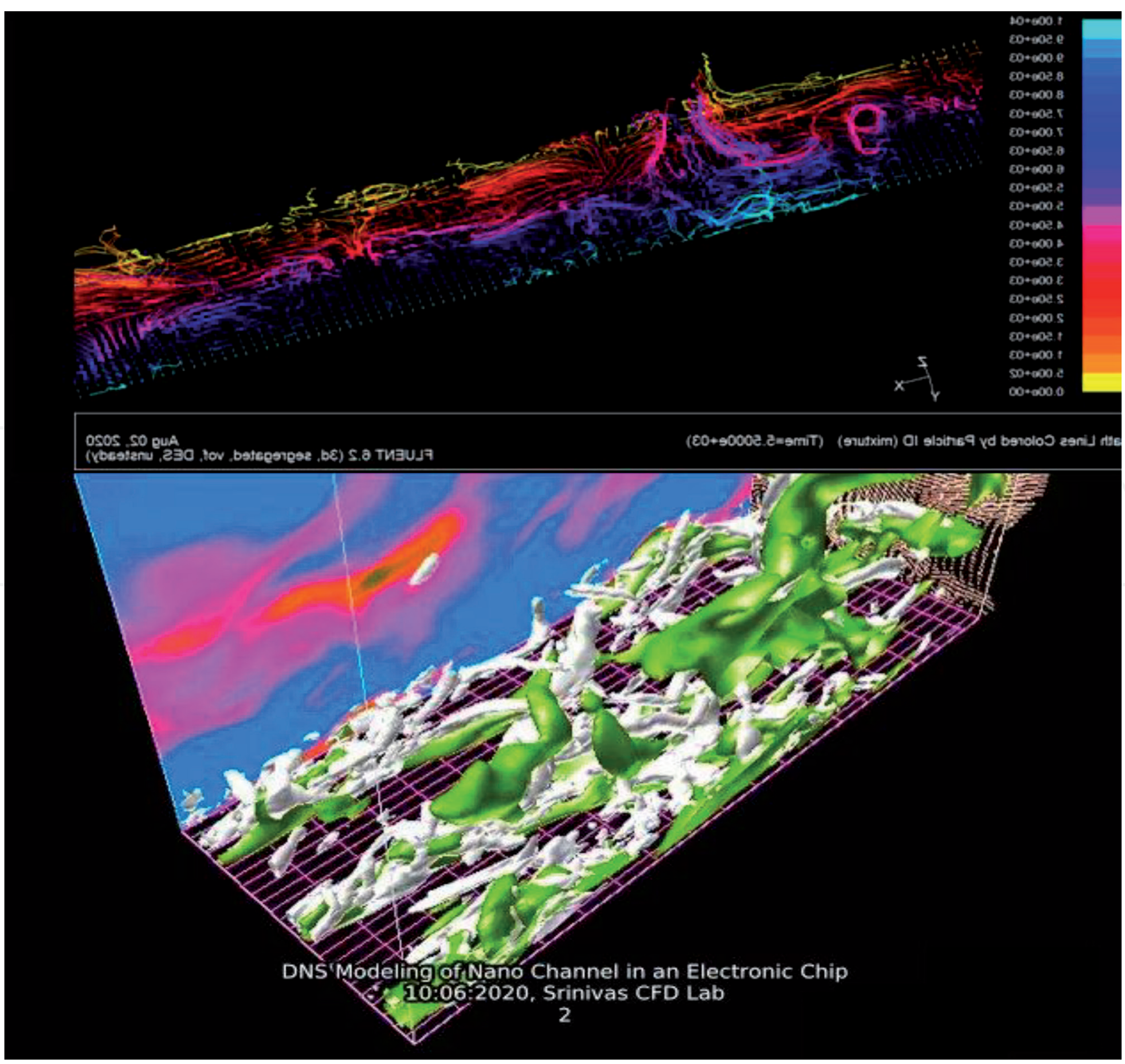

Figure 6.
DNS on LES based simulation.

2. Conclusion

A direct numerical simulations (DNS) has been performed over a nano channel considering as that of a nono pipe used for electronics cooling purpose with various set of Reynolds numbers and the effects of Reynolds number on the turbulence properties have been investigated. Since DNS of experimental-scale setups are beyond the author's computational resources, DNSs on a reduced computational domain were performed. The unified flow solver will be taking the job of adaptive mesh refinement (AMR) with automatic selection of fluid solver that has been implemented in whole range of computational domain. In contrast to the micro-channel flow the nano channel flow case has been much qualitatively trivial once the LES solution is available and further solving for a DNS solution of the problem at any particular Reynolds number. It has been shown that Kolmogrov length and velocity scales are more appropriate compared to the other such approximations while modeling DNS at significantly low Reynolds numbers including any other energy diffusion during the course of fluid flow through rectangular channels.

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