

## USE OF LAGRANGIAN STATISTICS FOR THE DIRECT ANALYSIS OF THE TURBULENT CONSTITUTIVE EQUATION

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### ABSTRACT

Turbulence models often involve Reynolds averaging, with a closure providing the Reynolds stress  $\overline{u'v'}$  as function of mean velocity gradients  $d\bar{u}/dy$ , through a turbulence constitutive equation (equation 1). The main limitation of this linear closure is that it rests on an analogy with kinetic theory. For this analogy to be valid there has to be scale separation. The aim of this work is to better understand this hypothesis from a microscopic point of view. Therefore, fluid elements are tracked in a turbulent channel flow. The flow is resolved by direct numerical simulation (DNS). Statistics on particle trajectories ending on a certain distance  $y_0$  from the wall are computed leading to estimations of the turbulent mixing length scale and the Knudsen number. Comparing the computed values to the Knudsen number in the case of scale separation we may know in which region of the flow and to what extent the turbulence constitutive equation (equation 1) is not verified.

### INTRODUCTION

Diverse industrial applications and environmental issues often involve complex turbulent flows. A better understanding of the nature of transport process in these flows is challenging since available turbulence models do not provide accurate predictions for complicated configurations possessing recirculations, anisotropy or stagnation points (Wilcox, 1998; Pope, 2000).

Turbulence models often involve Reynolds averaging, with a closure providing the Reynolds stress  $\overline{u'v'}$  as function of mean velocity gradients  $d\bar{u}/dy$ , through a turbulence constitutive equation:

$$-\overline{u'v'} = \nu_T \frac{d\bar{u}}{dy} \quad (1)$$

The main limitation of this linear closure (equation 1) is that it rests on an analogy with kinetic theory. For this analogy to be valid there has to be scale separation between the mean velocity variations and the turbulent Lagrangian free path whose mean value is the turbulent mixing length. The aim of this work is to better understand this hypothesis from a microscopic point of view using DNS data.

Since turbulent transport process depend to a large extent upon the dynamics of fluid particle motion, considerable benefit may be taken from analysing the Reynolds stress

from a Lagrangian point of view. This perspective has been explored by Deardorff and Peskin (1970) for channel flow computed on relatively coarse meshes. Later, Bernard et al. (1989) and Bernard and Handler (1990) investigated the mechanisms for momentum transport in the wall region of channel flow by using ensembles of computed particle paths with direct numerical simulation (DNS). The authors showed that the gradient mechanism overpredicts the Reynolds stress and that significant positive contributions to Reynolds stress come from non-gradient transport processes.

A comprehensive description of the physics of momentum transport in the near wall region can be obtained by the Lagrangian analysis. In particular, it is of interest to better describe the turbulence constitutive equation as well as the reasons of the inadequacies of a linear closure. The insights provided by these analysis may be of considerable benefit in the construction of a non-local Reynolds stress model such as those proposed in Hamba (2005) and Huang (2004) enlightened by the Lagrangian analysis. Many studies (Hinze et al. 1974; Schmitt, 2007a,b) have mentioned the inadequacies of a linear closure for simple shear flow. Our contribution here is to apply the Lagrangian point of view for determining the Knudsen number through which the degree of validity of the scale separation hypothesis can be established.

In the present study, fluid elements are tracked in a turbulent channel flow in pursuit of these objectives. The flow is resolved by DNS. Statistics on particle trajectories which have terminal points on a certain distance  $y_0$  from the wall are computed. With the view afforded by these data a description of the inadequacy of the turbulent constitutive equation emerges through estimations of the turbulent mixing length scale and the Knudsen number. The computed Knudsen number is compared to the Knudsen number in the case of scale separation enabling the detection of flow regions where the turbulence constitutive equation (equation 1) is not verified.

The next section provides background on the method of Lagrangian analysis employed here. It describes how the Reynolds stress is estimated based on the analogy with the kinetic theory of gases. Following this the computational aspects of the approach, including that of channel flow simulation and the particle data sets are given. The chief results concerning the turbulent mixing length scale and the Knud-

sen number are then presented, including the evolution with distance from the wall of the mean and probability density function (PDF) of these quantities. An overall assessment of the inadequacies of the turbulence constitutive equation is then made and some implications of this for the modelling of the Reynolds stress are described. In the last section conclusions are given together with outline of future work.

### ESTIMATES OF THE REYNOLDS STRESS BY ANALOGY WITH THE KINETIC THEORY OF GASES

In the following section we briefly describe how the turbulent constitutive equation is obtained when the mixing length scale is small compared to other macroscopic length scales. Details about this description may be found in Tennekes and Lumley (1972).

Let us consider a steady channel flow homogeneous in the  $x, z$  plane. Here  $x, y$  and  $z$  represent the streamwise, the vertical and the transverse direction, respectively. The corresponding velocity components will be denoted by  $u, v$  and  $w$ . Finally, the total velocity will be given according to the Reynolds averaged decomposition by  $u = \bar{u} + u'$ . The overline will therefore represent a mean value in terms of the Reynolds averaged decomposition.

In the classical kinetic theory of gases (Tennekes and Lumley, 1972)  $-\overline{\rho u'v'}$  is estimated as follows. The mean free path of molecules is denoted by  $y^*$ . A molecule coming from  $y - y^*$  has a positive velocity  $v'$ . On the average, a molecule coming from  $y - y^*$  collides with another molecule at the reference level  $y = y_0$ . As a result of this collision the molecule coming from below adjusts its momentum in the  $x$  direction to that of its new environment. This adjustment takes place by absorption of an amount of momentum equal to  $M = m(\bar{u}(y_0) - \bar{u}(y_0 - y^*))$ . The quantity  $M$  is equal to the amount of momentum lost by the environment at the reference level  $y_0$ . The right-hand side of this equation may be expanded in a Taylor series:

$$M = my^* \frac{\partial \bar{u}}{\partial y} + \frac{1}{2}m(y^*)^2 \frac{\partial^2 \bar{u}}{\partial y^2} + \dots \quad (2)$$

If  $\frac{\partial \bar{u}}{\partial y} \gg \frac{1}{2}y^* \frac{\partial^2 \bar{u}}{\partial y^2}$  the second and higher order terms in the expansion may be neglected. If we define  $l$ , a characteristic length scale as:

$$l = \frac{\frac{\partial \bar{u}}{\partial y}}{\frac{1}{2} \frac{\partial^2 \bar{u}}{\partial y^2}} \quad (3)$$

then the condition expressed above writes as:

$$y^* \ll l \quad (4)$$

If this condition is fulfilled, the momentum  $M$  can be expressed as  $M = my^* \frac{\partial \bar{u}}{\partial y}$ . Considering that per unite area and time there are  $Nv_0$  collisions, with  $v_0$  the average free path velocity, we finally obtain  $-\overline{\rho u'v'} = \rho v_0 y^* \frac{\partial \bar{u}}{\partial y}$ . By denoting the viscosity  $\nu = v_0 y^*$  we obtain the turbulence constitutive equation:

$$-\overline{\rho u'v'} = \rho \nu \frac{\partial \bar{u}}{\partial y} \quad (5)$$

Equation 5 can be applied if the condition expressed in equation 4 is satisfied. This condition may as well be given in terms of a Knudsen number defined by:

$$Kn = \frac{y^*}{l} \quad (6)$$

Table 1: Numerical simulation characteristics.

Reynolds number	Mesh
$Re_\tau = 180$	$192 \times 192 \times 192$
$Re_\tau = 590$	$256 \times 384 \times 384$
Friction velocity	Viscosity
$u_\tau = 0.05m/s$	$\nu = 3 \times 10^{-3}m^2/s$
$u_\tau = 0.05m/s$	$\nu = 8 \times 10^{-5}m^2/s$

In conclusion, the simple gradient turbulence constitutive equation (equation 5) is valid if the Knudsen number is small  $Kn \ll 1$ . Finally, the gradient transport model used for establishing the turbulence constitutive equation rests on the hypothesis that fluid particles essentially maintain their momentum over a small mixing length  $y^*$  before blending in with the surroundings. This assertion requires that the momentum of fluid particles be preserved over  $y^*$  and that  $y^*$  must be less than the distance over which a linear approximation to  $\bar{u}$  is satisfactory. In that case, the Knudsen number is small and scale separation takes place. The extension to which these conditions are fulfilled in channel flow can be explored with the present data. The numerical simulations by which the data are obtained are described in the following section.

### NUMERICAL SIMULATION

Particle paths were computed using DNS of channel flow at two different Reynolds numbers,  $Re_\tau = 180$  and  $Re_\tau = 590$ , based on the friction velocity  $u_\tau$  and the channel half-width  $H$ , or  $Re = 3280$  and  $Re = 12500$  based on the velocity at the center of the channel and  $H$ . Some parameters for both simulations may be found in table 1. In the following the superscript  $+$  will denote quantities normalized by the friction velocity  $u_\tau$  and the viscosity  $\nu$ . For both Reynolds numbers 200,000 fluid elements were tracked. The resolution of the incompressible Navier-Stokes equations for a turbulent channel flow is based on a pseudo-spectral code using a Chebyshev formulation in the wall-normal direction and a Fourier expansion in the periodic directions (Godeferd and Lollini 1999, Laadhari 2002).

Fluid particle trajectories are computed by numerical integration of the equation of particle motion. The Lagrangian velocity is extracted from the nearest grid information using an eight-point Hermite interpolation scheme. Initially, fluid particles are randomly distributed in the flow. The particles are then tracked by continually updating their position using an Adams-Bashforth time advancement scheme.

### ESTIMATION OF THE TURBULENT MIXING LENGTH SCALE

In this section we will describe how we estimate the turbulent mixing length and the Knudsen number for each fluid element tracked in the flow. The estimation of individual turbulent mixing lengths will then lead to a PDF of the turbulent mixing length. The statistical samples for building this PDF will be given by individual turbulent mixing lengths.

We first consider the time series  $Z = u'v'(t)$  for a given fluid element, starting retrospectively from the moment when  $y = y_0$ . As suggested by Bernard et al. (1989), a possible measure of the mixing time relevant to the present objective is the time  $\tau$  at which the autocorrelation function

of  $u'v'(t)$ ,  $C(\tau) = 0$ . Fulfillment of this condition implies an end to the correlation between  $u'$  and  $v'$ . In essence, this time period is that necessary for the correlation of  $u'$  and  $v'$  to evolve out of the prior dynamics of the motion.

The memory associated to the time series  $Z = u'v'(t)$  is therefore obtained throughout the characteristic timescale  $t^*$  of the autocorrelation function  $C(\tau)$ . Here,  $t^*$  will be considered as the first time  $\tau$  for which  $C(\tau) = 0$ . This is illustrated in Figure 1. The characteristic timescale  $t^*$  is the mixing time for each considered trajectory. As shown in Figure 2,  $t^*$  is a variable quantity.

After determining  $t^*$  for each considered fluid element we can build a PDF of  $t^*$  for all particles in the flow ending at  $y = y_0$ .

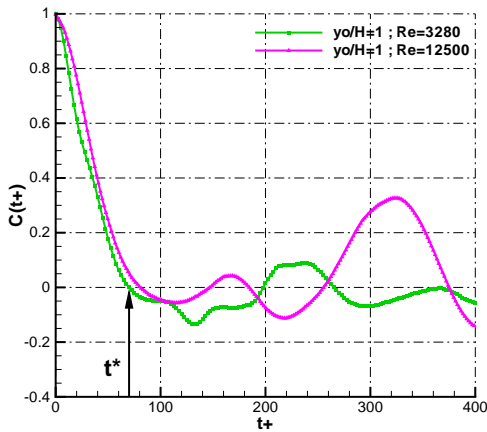


Figure 1: Example of the autocorrelation  $C(\tau)$ , of  $u'v'$  for each particle ending at  $y_0 = H$  for  $Re = 3280$  (green squares) and  $Re = 12500$  (magenta triangles).

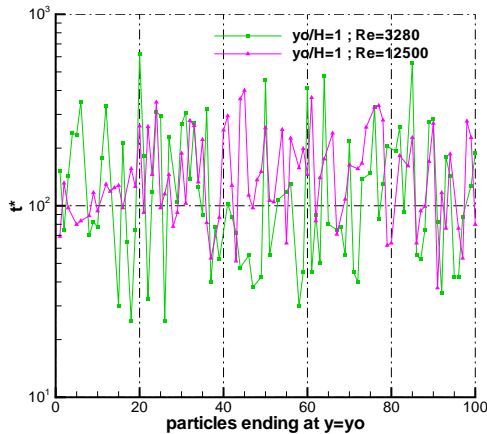


Figure 2: Example of the mixing time  $t^*$  for different fluid elements ending at  $y_0 = H$  for  $Re = 3280$  (green squares) and  $Re = 12500$  (magenta triangles).

The mixing timescale  $t^*$  can also be used for determining the individual mixing length scale  $y^*$  by the following relation:

$$y^* = \sqrt{(y_0 - y(t_0 - t^*))^2 + (x_0 - x(t_0 - t^*))^2} \quad (7)$$

$y^*$  represents the distance that a fluid elements needs to cover before it loses the information about its initial momentum  $u'v'$ . This mixing length scale is determined here for each fluid element ending at  $y = y_0$ . Once again, after obtaining  $y^*$  for all fluid elements ending at  $y = y_0$  a PDF of the mixing length scale can be built. An example of the PDF for the mixing length scale  $y^*$  is presented in Figure 3.

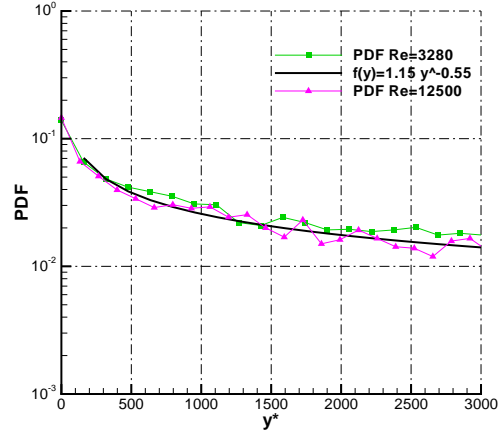


Figure 3: PDF of the mixing length scale  $y^*$  for all fluid elements ending at  $y_0 = H$  for  $Re = 3280$  (green squares) and  $Re = 12500$  (magenta triangles).

### ESTIMATION OF THE KNUDSEN NUMBER

The results described in the previous section can be used for estimating the individual Knudsen number. The Knudsen number is given by the ratio of the turbulent mixing length scale  $y^*$  and a characteristic length scale of the mean gradient denoted by  $l$ . Therefore, the Knudsen number can be written as:

$$Kn = \frac{y^*}{l} \quad (8)$$

Here,  $Kn$  depends on the particle and on the ending position  $y_0$ . The characteristic length scale of mean gradient  $l$  can be obtained from:

$$l = \frac{\frac{d\bar{u}}{dy}}{\frac{d^2\bar{u}}{dy^2}} \quad (9)$$

One has  $l \sim y_0$  in the log-low region. Therefore, for each fluid element ending at  $y = y_0$  the Knudsen number is given by:

$$Kn = \frac{y^*}{y_0} \quad (10)$$

The values of  $Kn$  for different fluid particles ending at  $y = y_0$  are presented in Figure 4. As it was shown in the previous section, the turbulence constitutive equation (equation 1) is valid if the Knudsen number is small  $Kn \ll 1$ . We can see here that for the set of particles chosen for this example, the condition of small Knudsen number is not verified.

### TURBULENT MIXING LENGTH AND THE KNUDSEN NUMBER EVOLUTION WITH WALL DISTANCE

The mean values of the turbulent mixing length scale  $y^*$  and timescale  $t^*$  for fluid particles ending at different

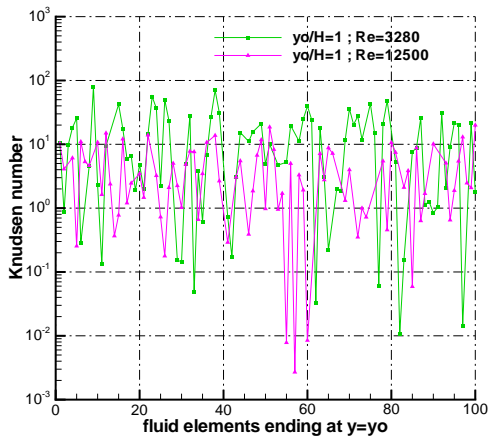


Figure 4: Example of the Knudsen number  $Kn$  for different fluid elements ending at  $y_0 = H$  for  $Re = 3280$  (green squares) and  $Re = 12500$  (magenta triangles).

$y_0$  are presented in figure 5 and 6, respectively. Both the mean turbulent length scale and timescale reach high values for all wall distances. Even though individual mixing length scales and timescales are highly variable quantities, the mean length scale and timescale weakly depend on the distance from the wall. A slight increase in the mean of  $t^*$  can be seen as  $y^+$  increases. In average, a particle whose ending trajectory is far from the wall needs more time for losing the information on  $u'v'$  that it initially contained. This may lead us to think that particles whose ending trajectories are far from the wall come from lower turbulence regions. However, while  $t^*$  increases with  $y^+$ ,  $y^*$  does not present a monotonic evolution and we could say that it remains rather constant. Therefore, in average particles that need more time to lose their initial information do not necessarily travel a longer distance. These particles are contained in regions of the flow with lower velocity and lower turbulence than the average at this distance. Finally, as the Reynolds number increases, mean values of  $t^*$  and  $y^*$  decrease, traducing the fact that turbulence increases and that less time and distance is needed for better mixing.

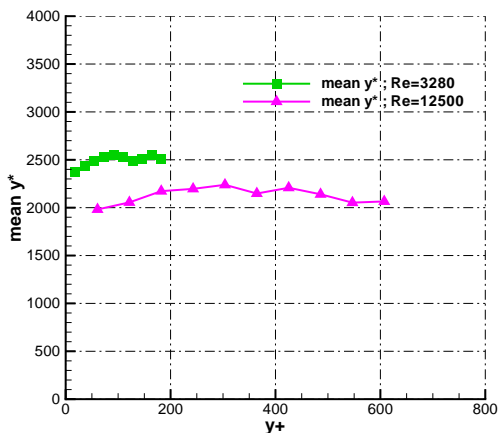


Figure 5: Mean turbulent mixing length scale  $y^*$  evolution with distance from the wall.

Figure 7 illustrates the evolution with wall distance of the

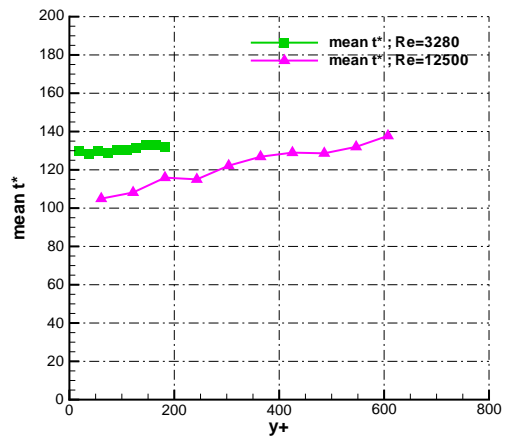


Figure 6: Mean turbulent mixing timescale  $t^*$  evolution with distance from the wall.

average Knudsen number. The Knudsen number remains rather high even far from the wall. Whatever the wall distance, in average fluid particles travel well beyond the region of linear variation in  $\bar{u}$  during this same period. On average the low Knudsen number assumption fails whatever the wall distance.

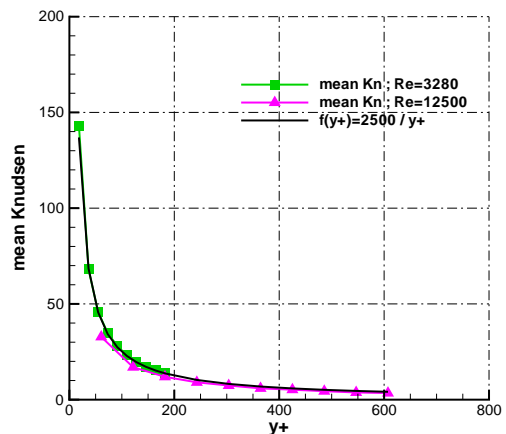


Figure 7: Mean Knudsen number evolution with distance from the wall.

Figures 8 and 9 illustrate the PDF of the turbulent mixing length scale  $y^*$  for different  $y_0$ . The PDF of  $y^*$  has an exponential behaviour for small values of  $y^*$  (Figure 9). The PDF is not a delta function around the mean value of  $y^*$ . The same statement can be made when it comes to the PDF of Knudsen numbers (figures 10 and 11). Therefore, both  $y^*$  and  $Kn$  reach large values far from the mean. This leads to the conclusion that there is no scale separation and that the small Knudsen number hypothesis fails often in this type of flow whatever the wall distance.

**CONCLUSION**

Ensembles of paths arriving at a given distance above the channel wall were used to evaluate a Lagrangian expression of the Reynolds stress. Then the autocorrelation function of the Lagrangian expression of the Reynolds stress was used

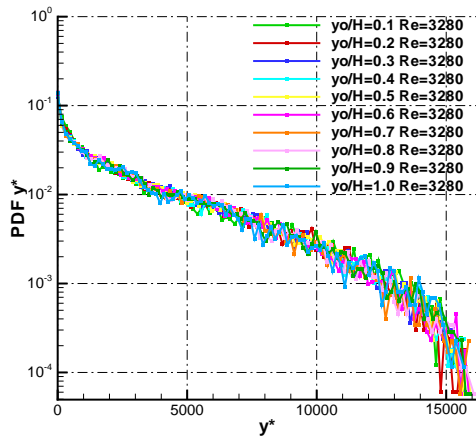


Figure 8: PDF of the turbulent mixing length scale  $y^*$  for different distances from the wall  $y_0$  for  $Re = 3280$ .

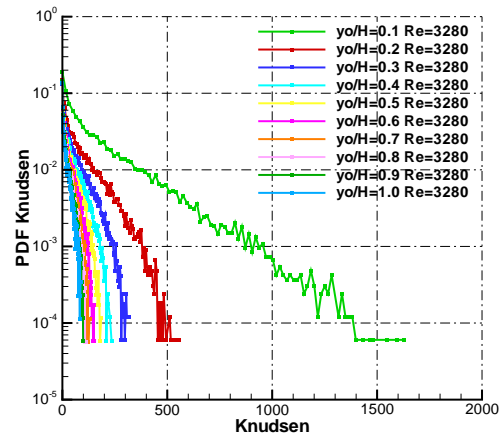


Figure 10: PDF of the Knudsen number  $Kn$  for different distances from the wall  $y_0$  for  $Re = 3280$ .

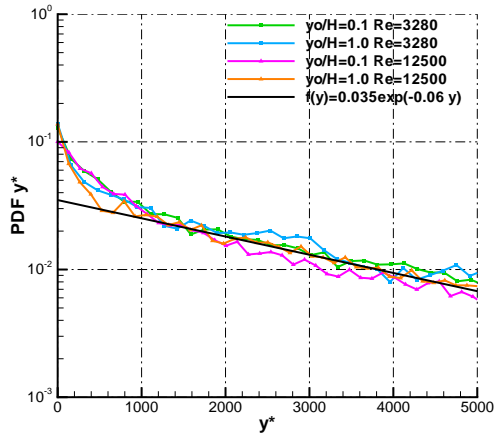


Figure 9:

for determining the turbulent mixing timescale and length scale. Finally, the corresponding Knudsen number was computed.

The values of the computed Knudsen number were compared to the values imposed when establishing the turbulent constitutive equation with the gradient transport model. The PDF of the Knudsen number presents an exponential behaviour for small Knudsen number values, whatever the wall distance. This PDF is not represented by a delta function around a small mean value. Therefore, the computed results show that the small Knudsen number hypothesis fails practically in every region of the flow, whatever the wall distance.

In subsequent studies it is planned to propose a non-local approach for predicting the Reynolds stress and to establish the influence of the Reynolds number and of the flow configuration on the proposed non-local kernels. This expanded database may reveal additional information about the relationship between the Reynolds stress and the Lagrangian paths of fluid elements. In addition to this, it is interesting to develop conditional sampling of particle paths used for obtaining the Reynolds stress. For example, particle paths conditioned by sweeps or ejections may play particularly important roles in the determination of turbulent mixing length

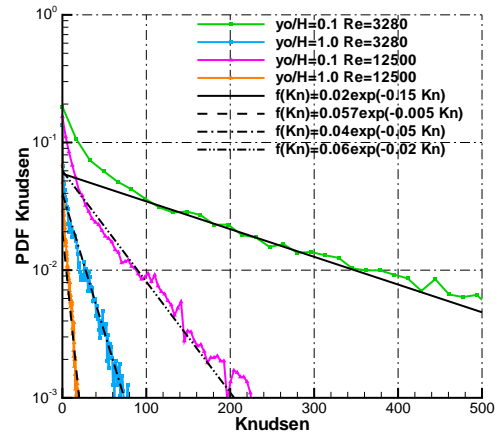


Figure 11: Zoom of PDF for small values of the Knudsen number  $Kn$  with corresponding exponential adjustment, for  $Re = 3280$  (green and blue squares) and  $Re = 12500$  (magenta and orange triangles).

or time scales.

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