Multiscale modelling strategy using the lattice Boltzmann method for polymer dynamics in a turbulent flow

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Abstract

Polymer dynamics in a turbulent flow is a problem spanning several orders of magnitude of length and time scales. A microscopic simulation covering all those scales from the polymer segment to the inertial scale of turbulence seems impossible within the foreseeable future. We propose a multiscale simulation strategy to enhance the spatio-temporal resolution of local Lagrangian turbulent flow by matching two different simulation techniques, i.e. direct numerical simulation for the flow as a whole, and the lattice Boltzmann method coupled to polymer dynamics at the Kolmogorov dissipation scale. Local turbulent flows sampled by Lagrangian tracer particles in the direct numerical simulation are reproduced in the lattice Boltzmann model with a finer resolution, by supplying the latter with both the correct initial condition as well as the correct time-dependent boundary condition, sampled from the former. When combined with a Molecular Dynamics simulation of a polymer chain in the lattice Boltzmann model, it provides a strategy to simulate the passive dynamics of a polymer chain in a turbulent flow covering all those scales. While this approach allows for a fairly realistic model of the macromolecule, the back-coupling to the flow on the large scales is missing.

Key words: Polymer dynamics, turbulent flow, lattice Boltzmann, drag reduction

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1. Introduction

By adding long chain molecules in a concentration as minute as $10^{-5}$ in weight, the frictional drag in a turbulent flow through a pipe can be significantly reduced [1]. This phenomenon of drag reduction in turbulent flow by polymer additives has been known for more than half a century [2], and numerous experimental and theoretical studies have been executed [3]. However, it is widely acknowledged that the theoretical understanding of the mechanism behind this phenomenon has not yet gone beyond the tentative level [4, 5, 6], and is under current debate. Amongst others, not even the question whether drag reduction exists in homogeneous turbulence [7, 8] has been conclusively resolved yet.

It is obvious that the flexibility of the polymer chains must play a crucial role for this phenomenon, given the fact that the addition of non-flexible colloidal particles does not result in such a dramatic effect at such a dilution. In thermal equilibrium, a polymer chain assumes a random coiled shape, and a convenient measure of its size is the root mean square radius of gyration $R_g$ [9]. In a strong flow, however, a polymer chain may be stretched up to its contour length, which, under such conditions, becomes the characteristic size of the macromolecule. This can easily be orders of magnitude larger than $R_g$ for a chain with a large degree of polymerization. In the stretched state, the elongational viscosity increases by factors of $\sim 10^4$ for large molecules [10].

An important attempt to understand the turbulent drag reduction in pipe flow based on this coil-stretch transition [11] and corresponding viscosity variation was made by Lumley [4]. Among other theories for drag reduction, the argument by Tabor and de Gennes is based on the entropic elasticity of polymer chains [5]. They thought that the coil-stretch transition would not occur under randomly fluctuating strains, and the moderately stretched state would prevail, which would not modify the viscosity drastically. They argued that the elastic energy stored within the molecule would interfere with the cascading turbulent energy at some length scale larger than the Kolmogorov dissipation scale ($\eta$), where the crossover from turbulent to laminar behavior occurs. So far, however, the experimental difficulties in observing details of molecular motion in a turbulent flow have prevented us from obtaining a decisive and direct evidence for existing theories and hypotheses.

The main difficulty in the theoretical, experimental or computational
analysis of the drag reduction problem is the strong disparity of the relevant length scales. The energy injection scale of the largest eddy is usually orders of magnitude larger than the energy dissipation Kolmogorov scale ($\eta$) of the smallest eddy. In a turbulent flow with polymer additives, non-linear interactions strongly couple different scales by transferring excitations from the injection scale all the way down to $\eta$, which is coupled with the scales of polymers. In a fully developed homogeneous turbulence, $\eta$ corresponds to $\sim L/Re^{3/4}$, where $L$ is the external scale of flow and $Re$ is the Reynolds number. A textbook Kolmogorovian turbulent flow with clear scale separations among relevant scales requires a relatively large $Re$, which renders negligible $\eta/L$. Even in state-of-the-art Direct Numerical Simulations (DNS) of turbulent flow in a three-dimensional periodic simulation box of $1024^3$ grid points using supercomputers, $\eta$ becomes as long as only a few grid spacings. Considering that $R_g$ in typical experiments is about two orders of magnitude smaller than $\eta$, even for systems with very high molecular weight and large Reynolds numbers [12], it becomes obvious that the details of the polymer conformational degrees of freedom are completely out of the available resolution of DNS. In other words, a first-principles simulation, which covers all these length scales down to the monomer length scale, and, simultaneously, all the corresponding time scales, would need such a fine resolution that it is unfeasible, even on the most advanced supercomputers.

Existing computational studies regarding polymer-flow interaction have relied on simplification either of the turbulence model or of the polymer model, or of both. One approach covers the scale around and above the Kolmogorov scale. The turbulent flow can be simulated with realistic coupling between eddies, but the polymer models used are as simple as variations of the Hookean dumbbell model, which gives only an extremely crude picture of the intricate interplay between the flow and the molecule, whose frictional properties and relaxation time spectrum depend very strongly on the conformation [13, 14, 17, 16]. The other approach focuses on the purely dissipative sub-Kolmogorov scale. Realistic chain models for the polymers can be used, but the flow environment is over-simplified without interaction with larger scales [17, 18, 19]. A numerical simulation of such dynamics with a realistic polymer model and a realistic turbulent flow has so far not yet been done. Hence it is generally acknowledged that a multiscale approach is necessary.

In this paper, we present such a multiscale simulation strategy to simulate the dynamics of a linear polymer chain in a homogeneous turbulent flow.
Essentially, we achieve feasibility by splitting the problem up into two stages that correspond to the large and small scales, respectively. This comes at the price of losing some realism concerning the consistent coupling of the scales: There is only a “top-down” coupling from the large to the small scales, but no corresponding “bottom-up” back-coupling from the latter to the former.

The large scales are therefore handled by just running a standard DNS of turbulent flow, down to the Kolmogorov scale, by a spectral code. The idea is that this is probably the best available source of information about the fluctuating flow field which the polymer chains experience on a finer scale. Certainly it is more realistic than just a simple shear or elongational flow, or a flow just produced by a random number generator. From this simulation, we extract small-scale Lagrangian flow data, and supply these to a lattice Boltzmann (LB) model to simulate the flow on scales finer than the Kolmogorov scale. The LB fluid is then coupled to a bead-spring chain polymer model, thus providing a fairly realistic description of both the macromolecule as well as of the surrounding turbulent flow — with the big caveat that the input from the large scales is taken from the behavior of a Newtonian fluid, i.e. from data that, per construction, lack the influence of the polymeric stress. For this reason, our approach is hampered by a similar lack of realism as are all the other existing simulation studies. Therefore, the method should not be viewed as necessarily superior to previous research, but rather as complementary. Another caveat is that, even within the restricted setting of the present approach, it turns out that it is very difficult, if not practically impossible, within the limitations of existing computational resources, to match all relevant dimensionless parameters to experimentally realistic values. This will be the subject of future publications.

In our opinion, there is no fundamental reason for using a spectral code for the large scales and LB for the smaller ones. Rather, this choice was dictated by simple considerations of convenience: The project is a collaboration between researchers with complementary expertise in turbulence and polymer solution dynamics, respectively. In previous studies, turbulent flows had been simulated by the spectral method [20], while the equilibrium dynamics of polymers in a solvent had been tackled by a hybrid LB-Molecular Dynamics method [21, 22], where the coupling between polymer and solvent was introduced via a Stokes friction coefficient of the beads. For a detailed description and analysis of this method, we refer the reader to a recent review, Ref. [23]. Since the coupling between the two scales was just done via data on a disk, we saw no reason to not simply continue to run the respective
parts with their corresponding well-tested codes.

In the present paper, we wish to outline (Sec. 2) the essential features of our multiscale strategy. One important aspect is that the simulations on the large and small scales should be mutually consistent, in other words, that the LB solver on the small scales produces the same flow field as that which is known from the DNS on the large scales. This will be the content of Sec. 3, while actual simulation data with polymer chains, which are currently not yet available with sufficient accuracy, are deferred to future publications. Finally, Sec. 4 summarizes our conclusions.

2. Modelling strategy

The main task is to construct the flow field for the LB-polymer simulation from the standard DNS of the turbulent flow, where the latter is done with a strict incompressibility constraint. To this end, we make use of a passive tracer particle co-moving with the DNS flow. The tracer particle keeps track of the local environment. Consider a tracer particle moving with a velocity \( v(t) \) during the DNS in a periodic volume of size \( L^3 \). A cubic sub-volume of size \( l^3 \), of order of the Kolmogorov scale, comoving with the tracer, is defined around the tracer particle, such that the tracer is always located at the center of mass of the sub-volume. The velocity field in the sub-volume, \( u(r, t) \), is stored during the DNS run. This local flow field in the sub-volume is to be transplanted into the LB model to provide the hydrodynamic stress field for the single polymer chain.

As a first step, \( u(r, t) \) needs to be Galilei transformed into the co-moving accelerated frame of the tracer particle, so that there is no net flux of mass nor of momentum out of the sub-volume, and the polymer chain, placed at the tracer position, would only interact with the flow without net translational momentum. The transformed velocity field, \( w(r, t) = u(r, t) - v(t) \), is a solution of the same Navier-Stokes equation with an additional external force density, which is the mass density \( \rho \) times the negative acceleration of the tracer, \( -dv/dt \). The resulting local flow field, \( w(r, t) \), is then linearly interpolated and copied into an LB model in a much finer resolution; the LB flow, \( \tilde{w}(\tilde{r}, \tilde{t}) \), will be a zoomed-in flow field of \( w \) below the scale of the sub-volume \( l^3 \) of DNS. The LB resolution needs to be fine enough to model the conformational polymer degrees of freedom.

Therefore, \( \tilde{w}(\tilde{r}, \tilde{t}) \) is already completely determined or prescribed by \( w(r, t) \). However, in this study, we do not prescribe \( \tilde{w}(\tilde{r}, \tilde{t}) \) on every mesh.
point $\hat{\mathbf{r}}$ of the LB lattice. Rather, we prescribe $\mathbf{w}(\hat{\mathbf{r}})$ on all sites only at the initial time $t = 0$. At later times, we prescribe it only on the boundaries of the sub-volume. Since the Reynolds number at the scale of the sub-volume is small (recall $l \sim \eta$), one must expect that the Navier-Stokes equation, together with initial and boundary conditions, has one unique solution. Therefore, the flow generated by the LB solver with these initial and boundary conditions must be identical to the input flow. In the following section, we will show that this is indeed the case, within the intrinsic and unavoidable errors, which mainly come from the enhanced spatio-temporal resolution of the LB dynamics, and to a certain extent also from the fact that the LB simulation works at finite Mach number, while the DNS code imposes strict incompressibility.

The reason why the information about $\mathbf{w}(\hat{\mathbf{r}}, \hat{t})$ is confined to the boundary is twofold. On the one hand, we wish to avoid over-constraining the LB solver as such, which, as discussed, produces a slightly different solution than the DNS. More importantly, however, we need to allow an immersed polymer chain to modify the flow field as much as possible. We thus arrive at a problem that is, at least in principle, mathematically well-defined: We study the motion of a polymer chain in a solvent, where the whole system is subject to some time-dependent boundary conditions, and where in our case these boundary conditions happen to be derived from the DNS.

Technically, we implemented a rather simplistic approach to enforce the supplied initial and boundary conditions, by just setting the LB populations at the pertinent sites to their local equilibrium values. For the simulations with polymer, we need to avoid that it is “washed” out of the simulation box during the course of the simulation. For this reason, we impose one further constraint, which is to fix the polymer center of mass at the tracer (the point where $\mathbf{w}$ is zero, per construction).

3. Validation of the strategy

In this section, an actual application of the proposed strategy is introduced and discussed. The DNS of a homogeneous isotropic turbulent flow was performed in an independent study [20]. In what follows, we focus on the parameters (in DNS units) used in the run number 4 of Ref. [20]: $\nu = 1/400$ is the kinematic viscosity, $\bar{\varepsilon} = 0.1$ is the mean energy dissipation rate, $R_\lambda = \sqrt{5/(3\varepsilon\nu)u_{\text{rms}}^2} = 65$ is the Taylor-microscale Reynolds number, where $u_{\text{rms}}$ is the root mean squared speed of the flow. The large
scale Reynolds number, \( Re = \frac{u_{\text{rms}}L}{\nu} \), is 2243, where the box size \( L = 2\pi \). \( M = 1024 \) is the number of grid points in each direction of the simulation box. The Kolmogorov length \( \eta = \nu^{3/4} \varepsilon^{-1/4} \), becomes 0.0199 in the length unit of DNS, which corresponds to 3.26\( \Delta \), where \( \Delta \) is the grid spacing. The Kolmogorov time, \( \tau_\eta = \sqrt{\nu/\varepsilon} \), is 0.158.

A set of 100 tracer particles is used during the DNS. A sub-volume of \( l^3 = (20\Delta)^3 \simeq (6\eta)^3 \) is defined around each tracer. The flow field in the sub-volume is monitored at every \( \Delta t = 0.05\tau_\eta \) for 81\( \tau_\eta \). Figure 1 shows one example of the flow field sampled by a tracer. The magnitude of the vorticity vector, \( \omega(r,t) = \nabla \times \mathbf{w}(r,t) \), shows strong time dependence during the 81\( \tau_\eta \) of DNS run. The flow field shows a noticeable spatial inhomogeneity as the two lines of different control volumes are not identical.

The standard D3Q19 model \[23\] is used for the LB simulations. In order to parameterize the increased spatial resolution, we define a “zooming factor” via \( z = \Delta/a \), where \( a \) is the grid spacing of our LB model. The Kolmogorov length in the LB model is thus \( \tilde{\eta} = 3.26z\Delta \). Together with the kinematic viscosity of the LB model \( \tilde{\nu} \), the Kolmogorov time in LB units becomes
\[ \tau_\eta = \tilde{\eta}^2 / \tilde{\nu}. \]

In prescribing the velocity boundary condition of LB, we match the reduced velocity between LB and DNS:

\[ \tilde{\mathbf{w}} \left( \frac{\mathbf{r}_b}{\tilde{\eta}}, \frac{\tilde{t}}{\tilde{\tau}_\eta} \right) \frac{\tilde{\tau}_\eta}{\tilde{\eta}} = \mathbf{w} \left( \frac{\mathbf{r}_b}{\eta}, \frac{t}{\tau_\eta} \right) \frac{\tau_\eta}{\eta}, \tag{1} \]

where \( \mathbf{r}_b \) is the position vector for boundary meshes of the sampled sub-volume in DNS. \( \tilde{\mathbf{w}} \) has finer resolution than \( \mathbf{w} \) both in space and time; bilinear interpolation is used between neighboring grid points and time steps.

In Fig. 2 the flow field of LB (\( \tilde{\mathbf{w}} \)) is compared with the flow field of DNS (\( \mathbf{w} \)) for the same tracer used for Fig. 1. A zoom factor \( z = 6 \) is used: The mesh size of the sub-volume around the tracer is \( (20\Delta)^3 \) in DNS, while it is \( (120a)^3 \) in the LB model. The magnitude of the vorticity field over the total sub-volume around the tracer shows a very good quantitative agreement.
between DNS and LB, as Fig. 2(a) shows. However, we are particularly interested in whether the LB field, generated only by the boundary condition, would recover the DNS result in the center region close to the tracer position. In Fig. 2(b), the velocity field is compared over a much smaller region around the center. In general, the LB flow field shows good agreement with the DNS result even in the region far from the boundary. However, the LB flow cannot exactly follow sudden changes of the DNS flow as shown in the time region around $30\tau_{\eta}$.

Averaged over all the flow fields sampled by 100 tracers, the difference between the LB flow field and the original DNS flow field is less than 5% in magnitude compared to the original DNS field. We believe that the error depends on various parameters of the model, especially on the Mach number $Ma = \tilde{\eta}/(\tilde{\tau}_{\eta}c_s)$, where $c_s$ is the speed of sound of the LB model. The Mach number is $1.49 \times 10^{-2}$ for the presented case study. However, given the fact that for our parameters the agreement is quite satisfactory, we did not investigate this issue in a systematic way.

4. Summary and outlook

A multiscale simulation strategy to increase the resolution of a local Lagrangian turbulent flow is proposed. The local Lagrangian flow fields around and below the Kolmogorov scale are sampled by passive tracers in a standard DNS of turbulent flow. The LB model is used to regenerate the sampled flow field in a much finer spatio-temporal resolution.

The strategy proposed in this paper provides a way to generate the local Lagrangian turbulent flow field for the hybrid Molecular Dynamics–lattice Boltzmann method of polymer dynamics in flow [21, 22, 23]. The whole procedure provides an unique opportunity to simulate polymer dynamics in a fairly realistic turbulent flow.

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