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Toward large scale parallel computer simulation of viscoelastic fluid flow: A study of benchmark flow problems ☆

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ABSTRACT

Followed by our previous study, an OpenFOAM-based viscoelastic flow solver has been further validated through simulation of viscoelastic flow past a cylinder. The drag coefficients calculated by the Oldroyd-B model under the creeping flow in a range of Weissenberg (*Wi*) number are in good agreements with those reported in the literature. Using the linear Phan-Thien Tanner (L-PTT) model, time-dependent two-dimensional simulations of flow past cylinder have been carried out in a range of *Wi* number and Reynolds (*Re*) number, and revealed interesting cooperative effects of inertia and elasticity on the structural evolution of the wake behind the cylinder. The details of parallel computing strategy are analysed and discussed. The codes are evaluated for large scale parallel simulation of two-dimensional and three-dimensional contraction flow as well as two-dimensional flow past a cylinder. The key bottlenecks, which affect the scalability of parallel computing, are discussed.
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1. Introduction

Flow around a cylinder is a common benchmark flow problem studied experimentally by Manero and Mena [1], McKinley et al. [2] and Broadbent and Mena [3], and numerically by Bush [4], Liu et al. [5], Oliveira et al. [6], Fan et al. [7], Sun et al. [8], Alves et al. [9], Phan-Thien and Dou [10], Dou and Phan-Thien [11], Kim et al. [12]13, Oliveira and Miranda [14] and Gerritsma [15]. The results are not only of significance to a better understanding of the dynamics of viscoelastic fluids around solid bodies, but also to many industrial processes, including flows through porous media for enhanced oil recovery [2], composite and textile coating [5]. The development of thin stress boundary layers on the cylinder walls and especially the high extensional stress developed along the rear wake centreline imposes a limited value on Weissenberg (*Wi*) number in numerical simulations, results in the so-called high *Wi* number problem, which often occurs in simulation of the upper convective Maxwell model and the Oldroyd-B model.

Sigli and Coutanceau [16] used photographic flow visualisation techniques to study the spatial kinematics of the viscoelastic wake structure in shear-thinning polyethylene oxide (PEO) solutions with moderate concentrations in low *Re* number and *Wi* number flow regime. They observed a secondary recirculation region in the wake of the sphere, downstream very close to the sphere, within which the fluid moves along the same direction as the sphere, however at a distance far from the sphere, the flow reverses and moves away from the sphere. They also found that the increase of sphere-to-tube diameter ratio makes the elastic effect more pronounced. However the inertial effects act to dampen the elastic effects. Hassager [17] found the same type of recirculating region in the wake of rising bubble in a shear-thinning, viscoelastic solution of 1% polyacrylamide (PAAm) in glycerol and named this behaviour as a negative wake.

Maalouf and Sigli [18] observed the existence of such negative wake in flows of various aqueous, shear-thinning, viscoelastic fluids around ellipsoid, ovoid, and cylinder. In their experiments, there are four types of fluid flows: (1) a Newtonian fluid; (2) an inelastic, shear-thinning fluid (3.5% carboxymethylcellulose, CMC, in water); (3) a highly elastic, constant viscosity fluid (PAAm in glucose) and (4) several viscoelastic, shear-thinning solutions (1.5% and 2.5% PEO in water). These results show that negative wakes are only observed in objects falling in fluids exhibiting both elastic and shear-thinning properties, and that the formation of the

☆ This paper is dedicated to Professor Ken Walters, FRS on the occasion of his 80th birthday.

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negative wake is dependent on value of Elasticity (*El*) number, defined as *El* = *Wi*/*Re*.

Computer simulation of flow past a cylinder can be carried out by setting the cylinder in either stationary or free fall in bounded or unbounded flow domains. These two settings are physically equivalent. The formal is more convenient as there is no need for adaptive mesh in simulation. Chilcott and Rallison [19] numerically studied flow of polymer solution past a cylinder, sphere and bubbles, respectively, using FENE-CR model and a finite difference method. Based on the velocity profiles and conformational analysis, they showed that extension of dumbbells near the wake line of sphere is as if action of body force to accelerate fluid away from the sphere; further downstream the dumbbells relax and the fluid decelerates. Compared with the experiment results, the FENE-CR model gives a better prediction of the Boger fluids than those of previous FENE dumbbell models. Phan-Thien and Dou [10] simulated flow of viscoelastic fluids past a confined cylinder using the upper-convected Maxwell (UCM) model, the Oldroyd-B model and the PTT model, respectively, and found the negative wakes behind the cylinder at high *Wi* number flow using the PTT model. In order to improve the numerical accuracy, Alves et al. [9] implemented high order differencing scheme, such as MINMOD and SMART, to the convective terms of the governing equations using a general collocated finite-volume method (FVM) developed by Oliveira et al.[6]. Those schemes were tested under flow past a confined cylinder benchmark flow problem with a blockage ratio of 50% using the UCM model and the Oldroyd-B model. Using highly refined non-orthogonal meshes, they are able to make a critical comparison with the literature results, *e.g*. Liu et al. [5], Fan et al. [7], Sun et al. [8], Phan-Thien and Dou [10] and Kim et al. [20]. The predictions of the drag coefficient up to *Wi* = 0.7 are in good agreement with the results from the finite element method (FEM) simulations of Fan et al. [7]. More recently, Hulsen et al. [21] implemented the log-conformation formulation using FEM for modelling flow of the Oldroyd-B fluid and the Giesekus fluid past a confined cylinder, respectively. They reported an almost unbounded convergence limit for the Giesekus model, whereas for the Oldroyd-B fluid the solution became unsteady at higher *Wi* number flow regime and exhibited symptoms of strong mesh dependency particularly in the stress fields near the cylinder. Coronado et al. [22] used an alternative implementation of the log-conformation formulation in their simulations of the planar Couette flow and flow past a cylinder in a channel, for several viscoelastic fluids. A generalised constitutive equation formulated in terms of the conformation tensor was used to improve the numerical stability in high *Wi* number flow. The maximum achievable *Wi* number in simulation of flow past a confined cylinder was extended to 1.0 as compared to 0.7 if using the standard DEVSS-TG/SUPG method.

Although a lot of experimental results are available, there are very limited numerical studies in flow regime of significantly high *Wi* number and *Re* number, hence a range of (*El*) number. In this paper, the previously proposed OpenFOAM-based viscoelastic flow solver is further validated under flow past a cylinder problem. The interplay of inertia and elasticity on the structural evolution of the wake behind the cylinder is numerically studied using the linear Phan-Thien Tanner (L-PTT) model. Effects on the scalability of parallel computing viscoelastic flow are evaluated and discussed. The paper is arranged as the following. The governing equations and constitutive models for modelling viscoelastic fluid flow are outlined in Section 2. Numerical methods for large scale parallel simulation of viscoelastic fluid flows are illustrated in Section 3 and Appendices. Validation of the numerical methods under flow past a cylinder is reported in Section 4, along with the simulation results of the L-PTT model in a range of *Wi* number and *Re* number. In Section 5, the scalability of parallel viscoelastic flow solver is evaluated and analysed for better understanding the effects of computational scale, constitutive models, decomposition methods and communication modes. Conclusions are drawn in Section 6.

2. Governing equations

The motion of an incompressible, isothermal viscoelastic fluid is governed by the continuity equation,

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

where $\mathbf{v}$ is the velocity, and the momentum balance equation,

$$\rho \frac{D\mathrm{v}}{Dt} = \nabla \cdot \boldsymbol{\tau} - \nabla p \tag{2}$$

where ρ is the fluid density, p is the isotropic pressure, and the stress tensor, $\boldsymbol{\tau}$, is related to the rate of the deformation tensor $\boldsymbol{D}$ by the expression,

$$\boldsymbol{\tau} = 2\eta_s \boldsymbol{D} + \boldsymbol{\tau}_p \tag{3}$$

where $\boldsymbol{D} = \frac{1}{2}\left[\nabla \mathrm{v} + (\nabla \mathrm{v})^T\right]$, η_s is the solvent viscosity, and τ_p is the polymer contribution to the stress tensor, which may be defined by an appropriate constitutive equation.

The Oldroyd-B model is the simplest and most commonly used constitutive model for modelling viscoelastic fluid flow. The time evolution of $\boldsymbol{\tau}_p$ is expressed by,

$$\boldsymbol{\tau}_p + \lambda \overset{\nabla}{\boldsymbol{\tau}}_p = 2\eta_p \boldsymbol{D} \tag{4}$$

where the upper convected time derivative is given by,

$$\overset{\nabla}{\boldsymbol{\tau}}_p = \frac{\partial \boldsymbol{\tau}_p}{\partial t} + \mathbf{v} \cdot \nabla \boldsymbol{\tau}_p - (\nabla \mathbf{v})^T \cdot \boldsymbol{\tau}_p - \boldsymbol{\tau}_p \cdot \nabla \mathbf{v}. \tag{5}$$

The L-PTT model is a well-studied phenomenological constitutive model. It may be written as

$$\boldsymbol{\tau}_p + \lambda \overset{\nabla}{\boldsymbol{\tau}}_p + \frac{\varepsilon \lambda}{\eta_p} tr(\boldsymbol{\tau}_p)\boldsymbol{\tau}_p + \frac{1}{2}\xi\lambda(\boldsymbol{D} \cdot \boldsymbol{\tau}_p + \boldsymbol{\tau}_p \cdot \boldsymbol{D}) = 2\eta_p \boldsymbol{D} \tag{6}$$

where the parameter ξ and ε control shear and extensional viscosity, respectively.

In a generalised FENE model, named as the FENE-CD-JS model [23], the evolution equation for polymer conformation tensor $\boldsymbol{A}$ can be written as

$$\overset{\nabla}{\boldsymbol{A}} + \xi(\boldsymbol{D} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{D}) = -\frac{f[tr(\boldsymbol{A})]}{\lambda}\left(\boldsymbol{A} - \hat{\boldsymbol{\delta}}\right) \tag{7}$$

where $\hat{\delta}$ is the unit tensor. By setting the model parameter $\xi = 0$, the FENE-CD-JS model is reduced for modelling Boger fluids. The non-linear function $f[tr(\boldsymbol{A})]$ is given by

$$f[tr(\boldsymbol{A})] = \frac{L^2}{\left[L^2 - tr(\boldsymbol{A})\right]\left[1 - \kappa + \kappa\sqrt{\frac{1}{2}tr(\boldsymbol{A})}\right]} \tag{8}$$

where κ is a model parameter and L is the fully extended length of polymer chain. From a generalised spring force law, $\boldsymbol{F} = f[tr(\boldsymbol{A})]H\boldsymbol{Q}$, where $\mathbf{Q} = \boldsymbol{r_2} - \boldsymbol{r_1}$ represent the dumbbell end-to-end vector and H is a molecular constant, the polymeric stress tensor can be expressed by

$$\boldsymbol{\tau}_p = N\langle \boldsymbol{FQ} \rangle = \frac{\eta_p}{\lambda} f[tr(\boldsymbol{A})]\langle \boldsymbol{A} \rangle \tag{9}$$

where N is a number of polymer molecules per unit volume. By tuning the parameters ξ and κ, the model can capture the key non-linear rheometric behaviour. The effects of elongational viscosity and its transient characteristics as well as shear thinning on the vortex dynamics of semi-dilute polymer solutions can be studied, as observed in the experimental results [24–26].

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