A Multi-scale Parallel Numerical Solver for Modeling of Two-phase Viscoelastic Fluids Based on the OpenFOAM

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***Abstract*—With the rapid development of high performance computing technology, the simulation of viscoelastic fluids has become an extremely important research area and numerous new promising techniques have been proposed over the last decades. In this paper we proposed a numerical algorithm for solving the multi-scale two-fluid model, additionally, based on an open source CFD toolbox, we implemented a parallel solver and verified the algorithms through parallel simulations. The results verified the numerical algorithm and show that the parallel codes of the solver have good parallel efficiency.**

Keywords-numerical simulation; multi-scale; OpenFOAM; parallel computing; viscoelastic fluids

I. INTRODUCTION

Viscoelastiticy refers to the property of materials that exhibit both viscous and elastic characteristics when undergoing deformation. Many natural and synthetic fluids exhibit viscoelastic characteristics; notable examples include blood, DNA solutions, polymer melts and solutions, and fiber suspensions [1-4]. The most challenging part of modeling the viscoelastic fluids is to determine the non-linear coupling between the macroscopic rheological responses and the microscopic evolution of molecular configurations under flow, thus modeling the viscoelastic fluids intrinsically is a multi-scale problem.

As a microscopic approach, the atomistic modeling is limited to the flow geometries of molecular dimensions due to the massive computing resource requirements. Recent years, the coarse-grained molecular kinetic theory gained major devolvement, and numerous constitutive equations derived from the closure approximations of a kinetic theory were proposed [5]. Nevertheless, the approximations such as the pre-averaging or the decoupling involved for a macroscopic constitutive equation significantly impact on the rheological predictions of viscoelastic fluids. The micro-macro methods that couple the macroscopic continuum mechanics with the microscopic coarse-grained molecular kinetic theory plays a much more important role in the simulation of viscoelastic fluids. The Brownian Configuration Field (BCF) method [6] is a new promising micro-macro simulation approach for the complex fluids simulations.

In this paper, we aim to numerically solve a multi-scale two-fluid model based on the BCF approach. The detailed algorithms are described along with the parallel implementation based on an open source CFD toolbox, named OpenFOAM [7]. The main contributions of the paper are as follows:

- Proposed a numerical algorithm for solving the multi-scale two-fluid model;
- Implemented a parallel solver for modeling of two-phase viscoelastic fluids based on the OpenFOAM;
- Verified the numerical solver and the algorithms through parallel simulations.

The remainder of this article is organized as follows: Firstly we give the basic ideas and describe the architecture of the numerical solver in Section II. In Section III the governing equations for modeling the two-phase viscoelastic fluids are presented and followed by the iterative algorithm to solve the model. The simulation results are showed in Section IV. Some related work in viscoelastic fluids simulation is reviewed in Section V. We present our conclusions in Section VI.

II. THE ARCHITECTURE OF THE NUMERICAL SOLVER BASED ON OPENFOAM

To discretize the governing equations and solve the discretized linear systems, we use an Open Source CFD toolbox released by the OpenCFD Ltd, named OpenFOAM. OpenFOAM is a C++ library used to solve the CFD problems. Many typical linear system solvers and discretization schemes are predefined in this library. Appropriate type of solvers and the schemes could be configured through the control dictionary file. The OpenFOAM uses programming languages that is very close to the verbal and mathematical languages used in science and engineering, thus writing a numerical solver based on OpenFOAM becomes significantly easier. The schematic diagram of the architecture for written a numerical solver is shown in Figure I. It forms a four-layer structure to keep the key functions of the numerical solver independent. The iterative numerical algorithms are written in OpenFOAM programming languages in the Multi-scale Numerical solver layer.

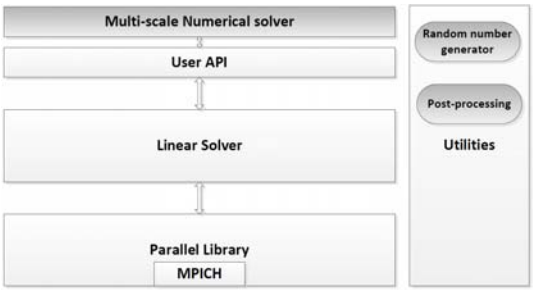


FIGURE I THE SCHEMATIC DIAGRAM OF THE PARALLEL NUMERICAL SOLVER BASED ON OPENFOAM

The User API layer provides all the necessary classes and interfaces to write the equations in C++. At this point, the users do not need to know anything about the linear system solvers and the parallel computing techniques in detail. The application to describe the Algorithm 1 can be written in OpenFOAM programming languages. The Linear solver layer contains numerous most commonly used linear equation algorithms including the conjugate (PCG) and bi-conjugate gradient (PBiCG) methods. The discretization schemes used in the numerical solver are also implemented in this layer and the configurations used in our solver are listed in Table I.

TABLE I THE DISCRETISATION SCHEMES USED IN THE NUMERICAL SOLVER FOR DIFFERENT TERMS

Term	Scheme	Order of accuracy
Temporal term	Euler	First order
Gradient term	Gauss linear	Second order
Divergence term	Gauss linear	Second order
Laplacian term	Gauss linear corrected	Second order
Convection term default	Gauss Minmod	Second order
Convection term for ϕ_A	Gauss vanLeer	First order

In this architecture, the only module related to the parallel communication is the Parallel Library layer. Here the MPICH library is used and the interfaces provided in this layer can enable the leaner solvers communicating with each other while running in parallel.

III. THE NUMERICAL ALGORITHM FOR MODELING TWO-PHASE VISCOELASTIC FLUIDS

A. *The Governing Equations of A Multi-scale Two-fluid Model*

To model the phase transitions of a two-phase viscoelastic fluid, macroscopic constitutive equations are replaced to the BCF approach for calculating the viscoelastic stress tensor. The governing equations for the full model are brought together below.

For isothermal and incompressible viscoelastic fluids with density, the continuity equation and the momentum balance equation can be expressed as

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

and

$$\rho \frac{D\vec{v}}{Dt} = \eta_s \nabla^2 \vec{v} - \vec{\nabla} p - (2\phi_A - 1)\, \vec{\nabla}\mu + \vec{\nabla} \cdot \sigma_{\mathrm{p}}\,(\vec{r}, t) \tag{2}$$

The evolution equation of the composition field A could be written as

$$\frac{D\phi_A(\vec{r},t)}{Dt} = \vec{\nabla} \cdot \left[\frac{\phi_A^2 (1-\phi_A)^2}{\varsigma} \left(\vec{\nabla}\mu - \alpha \vec{\nabla} \cdot \sigma_{\mathrm{p}} \right) \right] \tag{3}$$

The thermodynamic effects in two-fluid framework are described through the chemical potential difference $\mu = \mu_A - \mu_B$, which could be defined as the functional derivative of the mixing free energy with respect to local volume fraction, i.e.,

$$\mu = \frac{\delta \mathcal{F}_{\mathrm{mix}}[\phi_A(\vec{r})]}{\delta \phi_A(\vec{r})} \tag{4}$$

We take a first order approximation of the Flory-Huggins-de-Gennes form for the mixing free energy function F_{mix}.

The viscoelastic stress tensor σ_p is considered on a microscopic viewpoint. To simulating the distribution of the molecular chain, N_f configuration fields $\vec{Q}_i(\vec{r},t)$ are introduced to replace the Fokker-Planck equation, therefore the corresponding stochastic differential equation can be rewritten as [6]

$$d\vec{Q}_i(\vec{r},t) = [-\vec{v}(\vec{r},t) \cdot \nabla \vec{Q}_i(\vec{r},t) + (\nabla \vec{v}(\vec{r},t))^T \cdot \vec{Q}_i(\vec{r},t)) - \frac{F(\vec{Q}_i(\vec{r},t))}{2\lambda(\phi_A)}]dt + \sqrt{\frac{1}{\lambda(\phi_A)}} d\vec{W}_i(t) \tag{5}$$

According to the Kramer's expression, the viscoelastic stress σ_p can be given by [8]

$$\sigma_{\mathrm{p}} = \left(\frac{b+d+2}{b}\right) \frac{\eta_p(\phi_A)}{\lambda(\phi_A)} \left(\left\langle \vec{Q} \otimes F(\vec{Q}) \right\rangle - I \right) \tag{6}$$

and

$$\left\langle \tilde{Q} \otimes F(\tilde{Q}) \right\rangle = \frac{1}{N_f} \sum_{i=1}^{N_f} \tilde{Q}_i(\tilde{r};t) \otimes F(\tilde{Q}_i(\tilde{r};t)) \tag{7}$$

In this representation $d\tilde{W}_i(t)$ only depends on time and essentially are independent Gaussian variables with zero mean and variance dt.

B. *An Iterative Numerical Algorithm Based on OpenFOAM*

To numerically solve the multi-scale model described in Section III, a modified PISO iterative algorithm is adopted. In our previous research, A similar algorithm for solving the macroscopic model has been well tested in a numerical study for the dynamics of polymer solutions in contraction flow [9]. Additionally, the shear-banding flows with a macroscopic two-fluid model have been studied recently [10]. The revised version of the multi-scale numerical algorithm has been presented in Algorithm 1. In this algorithm, steps 4 ~7 solved the microscopic equations to obtain the viscoelastic stress. The modified PISO iterations presented in steps 8~11, then followed by the volume fraction calculations at steps 12 ~14. It should be noted that the correction steps 13 ~14 are added to restrict the volume fraction variables in the range of [0, 1].

Data: Mesh data, initial conditions
Result: $\vec{v}$, p, $\boldsymbol{\sigma}_{\mathbf{p}}$, ϕ_A

1 read the mesh data and the initial conditions;
2 initialization;
3 **while** t^{n+1} *not reach the end of the simulation time* **do**
4 **for** $i = 1$ *to* N_f **do**
5 Solve Eq.(5) to get the configuration field $\vec{Q}_i(\vec{r},t)$ at time t^{n+1} using a semi-implicit Euler method: $(1+\frac{\Delta t^n}{2\lambda(\phi_A^n)(1-|\vec{Q}_i^{n+1}(\vec{r})|^2/b)})\vec{Q}_i^{n+1}(\vec{r}) = \vec{Q}_i^n(\vec{r}) + [-\vec{v}^n(\vec{r})\cdot\nabla\vec{Q}_i^n(\vec{r}) + (\nabla\vec{v}^n(\vec{r}))^T\cdot \vec{Q}_i^n(\vec{r},t))]\Delta t^n + \sqrt{\frac{\Delta t^n}{\lambda(\phi_A^n)}}\vec{N}_i(0,1)$;
6 **end**
7 Compute the polymer stress tensor using Kramers' expression $\boldsymbol{\sigma}_{\mathbf{p}}^{n+1}(\vec{r}) = (\frac{b+d+2}{b})\frac{\eta_p(\phi_A^n)}{\lambda(\phi_A^n)}(\sum_{i=1}^{N_f}\vec{Q}_i^{n+1}(\vec{r})\otimes F(\vec{Q}_i^{n+1}(\vec{r})) - \boldsymbol{I})$;
8 Solve the discretised momentum equation $\frac{\partial\vec{v}}{\partial t}+\vec{v}\cdot\vec{\nabla}\vec{v}-\frac{\eta_s}{\rho}\nabla^2\vec{v}+\frac{(2\phi_A-1)}{\rho}\vec{\nabla}\mu-\frac{\vec{\nabla}\cdot\boldsymbol{\sigma}_{\mathbf{p}}(\vec{r},t)}{\rho} = -\frac{\vec{\nabla}p}{\rho}$ to obtain the estimated components $\vec{U}^{(n+1)*}$;
9 Solve the pressure-correction equation $\nabla\cdot\vec{U}^{n+1} = \nabla\cdot(A^{-1}\nabla[p])^{n+1}$ to obtain the pressure field $p^{(n+1)*}$;
10 Calculate the corrected velocity field $\vec{v}^{(n+1)*}$ by solving $\vec{v}^{n+1} = \vec{U}^{n+1} - A^{-1}\nabla[p]^n$;
11 Repeat the steps $\mathbf{8}\sim\mathbf{10}$ using the corrected $p^{(n+1)*}$,$\vec{v}^{(n+1)*}$ until all corrections are negligibly small for the solutions at the present time $\vec{v}^{n+1}$ and p^{n+1};
12 Solve Eq.(3) using $\boldsymbol{\sigma}_{\mathbf{p}}^{n+1}$ and $\vec{v}^{n+1}$ to obtain the volume fraction ϕ_A^{n+1};
13 Solve the equation for ϕ_B by replacing $\phi_A = 1-\phi_B$ to get ϕ_B^{n+1};
14 Volume fraction correction: $\phi_A = \frac{\phi_A}{\phi_A+\phi_B}$, $\phi_B = 1-\phi_A$;
15 $n \leftarrow n+1$;
16 **end**

Algorithm 1 The iterative algorithm to solve the multi-scale two-fluid model

IV. Simulation Results

The codes of the parallel solver have been investigated in test simulations on a HPC cluster located in the State Key Laboratory of High Performance Computing. Each computing node of this cluster contains 12 Intel Xeon E5-2620 2.10GHz CPU cores and a total main memory of 16GB. The parallel simulations are executed by distributed the processes to the computing nodes with 1 process every CPU core.

The main parameters of the multi-scale model remain constant throughout all of the simulations and are set as shown in Table II. Furthermore, we specify a poiseuille flow in a planar channel as shown in Figure II. In a planar channel, the viscoelastic fluid flows driven by the constant pressure gradient between the inlet and the outlet of the channel.

TABLE II PARAMETERS USED IN SIMULATIONS

Parameter	Value
η_s	0.1
k_BT	1.3
M_A	1.0
M_B	1.0
Γ	1.0
ς	0.1
b	20.0
λ^0	10.0
η_p^0	20.0
$\dot{\gamma}$	1.0

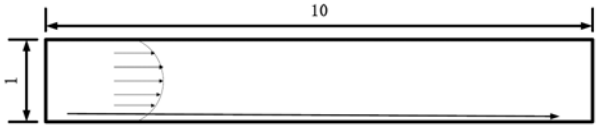
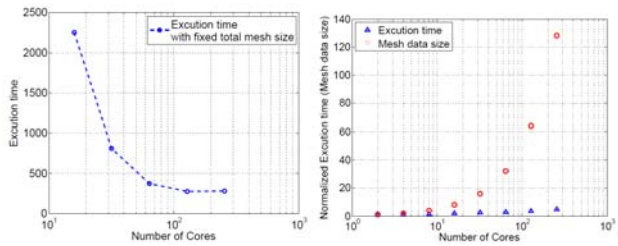


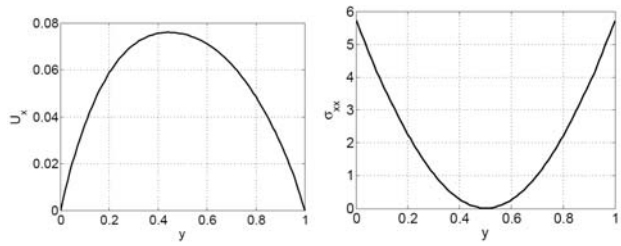
FIGURE II THE POISEUILLE FLOW IN A PLANAR CHANNEL WITH THE LENGTH RATIO $\frac{l_x}{l_y} = 10$. THE FLOW FIELD IS DRIVEN BY OCCURRING CONSTANT PRESSURE GRADIENT IN THE CHANNEL DIRECTION.

The steady-state velocity U_x and the corresponding viscoelastic stress component σ_{xx} are sampled after a long time simulation with $T_{sim} > 100$. At a fixed x-axis x = 5.0, the profiles are plotted in Figure III. The parabolic profiles of the simulation results are consistent with previous research.



(a) (b)

FIGURE III (A) THE STRONG SCALABILITY WITH FIXED TOTAL MESH SIZE 1048576; (B) THE WEAK SCALABILITY FOR FIXED MESH SIZE 8192 PER PROCESSOR CORE



(a) $\vec{v}_x$ (b) σ_{xx}

FIGURE IV THE STEADY-STATE VELOCITY FIELD U_x AND THE VISCOELASTIC STRESS COMPONENT σ_{xx} AT A FIXED X-AXIS X = 5.0

To evaluate the scalability of the parallel codes based on the OpenFOAM, firstly we fixed the problem size with a mesh of 1048576 cells, and the execution times varies with the number of processor cores are plotted in Figure IV(a). From 16 to 128 processor cores, the time cost is significantly reduced as the

parallel scale increasing. Nevertheless, the execution time cannot be decreased as the core number larger than 128. As shown in the plot, the execution time with 128 cores and 256 cores are almost the same. It is found that the optimal number of mesh cells for each processor core may be around 8192. Therefore a fixed mesh size of 8192 cells are distributed to each core in the weak scalability tests as presented in Figure IV(b). As the parallel scale (processor cores) raising, the total problem size measured by the mesh data size increases linearly, however the execution time of the simulations changes little. That means the parallel codes implemented in this paper can be easily scale to more than 256 processor cores.

V. Related Work

With the developing of the high performance computing technology, the simulation of viscoelastic fluids has become an extremely important research area and numerous new promising techniques have been proposed over the last decades. The atomistic modeling is the most detailed approach to describe the rheological behavior in complex fluids, however, considering the massive computer resource requirement, this microscopic approach is limited to flow geometries of molecular dimensions. Thus some micro-macro methods [5] were introduced that coupled the coarse-grained molecular kinetic theory to the macroscopic continuum equations. The Brownian configuration field (BCF) method proposed by Hulsen et al.[6] is a promising new multi-scale approach to model the viscoelastic fluids. The key idea of the BCF method is using Brownian configuration fields instead of tracking discrete particles, and that significantly reduces the drawbacks of the CONNFFESSIT method introduced by Laso and Ottinger[11].

In practice the BCF method works very well and has been applied to simulation of numerous viscoelastic flows, including the flow past a cylinder[6,12], viscoelastic free surface flows[13], contraction and expansion flows[14], Couette flow, Poiseuille flow, lid driven cavity flow[8] and flow between eccentrically rotating cylinders [15]. Due to the spatial smoothness, the BCF method has a considerable increased numerical stability. This advantage was confirmed in previous research and Mangoubi [16] recently gave an in-depth analysis about the origin of the numerical stability of the BCF method.

The numerical solver proposed in this paper is inspired by these previous researches. We expect the research will motivate more progress in large-scale parallel simulation for viscoelastic fluids.

VI. Conclusion

The dynamics under flow of multi-phase viscoelastic fluids plays essential roles in numerous applications ranging from biological systems to the industrial production. As modeling the two-phase viscoelastic fluids is a multi-scale problem, we introduce a macro-micro model that couples the microscopic BCF method into the macroscopic two-fluid framework. In this paper, we give a parallel numerical algorithm to solve this multi-scale two-fluid model, and the basic ideas to implement the solver based on an open source CFD toolbox have been presented in detail. Finally, the parallel codes of the numerical solver have been tested in a HPC cluster. The profile of the simulation results and the parallel scalability are presented. The results verified the numerical algorithm and show that the solver has good parallel efficiency.

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