Abstract. In this paper, we propose a deterministic particle-FEM discretization to micro-macro models of dilute polymeric fluids, which combines a finite element discretization to the macroscopic fluid dynamic equation with a variational particle scheme to the microscopic Fokker-Planck equation. The discretization is constructed by a discrete energetic variational approach, and preserves the microscopic variational structure in the semi-discrete level. Numerical examples demonstrate the accuracy and robustness of the proposed numerical scheme for some special external flows with a wide range of flow rates.

1. Introduction. Complex fluids comprise a large class of soft materials, such as polymeric solutions, liquid crystals, ionic solutions, and fiber suspensions. These are fluids with complicated rheological phenomena, arising from different “elastic” effects, such as elasticity of deformable particles, interaction between charged ions and bulk elasticity endowed by polymer molecules [48]. Modeling and simulations of complex fluids have been interesting problems for a couple of decades [8, 41, 43, 44].

Models for complex fluids can be classified as pure macroscopic models [37, 45, 68] and micro-macro models [9, 43]. The macroscopic models utilize an empirical constitutive equation for the stress tensor \( \tau \) to supplement the conservation of mass and momentum [37, 45, 68]. Examples include Oldroyd-B model [57] and FENE-P model [62]. The advantage of this approach is low computational cost, however, the closed-form of the constitutive equation may fail to captures the complicated flow behaviors of complex fluids, such as the hysteresis effects. The idea of micro–macro approaches is to couple the macroscopic conservation laws with a microscopic kinetic theory, which describes the origin of the macroscopic stress tensor [9, 43]. One of the simplest micro-macro models of complex fluids is the dumbbell model for dilute polymeric fluids given by [47]

\[
\begin{cases}
\rho \left( u_t + u \cdot \nabla u \right) + \nabla p = \eta_s \Delta u + \nabla \cdot \tau, \\
\tau = \lambda_p \mathbb{E} (\nabla q \Psi \otimes q) = \lambda_p \int_{\mathbb{R}^d} f \nabla q \Psi \otimes q \, dq, \\
\nabla \cdot u = 0, \\
f_t + u \cdot \nabla f + \nabla q \cdot (u q f) = \frac{2}{\lambda_p} \nabla q \cdot \left( f \nabla \Psi \right) + \frac{2k_B T}{\lambda_p} \Delta_q f.
\end{cases}
\]

In this model, the macroscopic motion of the fluid is described by a Navier–Stokes equation with an elastic stress \( \tau \) depending on the microscopic configuration of polymer chains, where \( u \) denotes the fluid velocity field, \( p \) is the pressure, \( \rho \) is the density of the fluid, and \( \lambda_p \) is a parameter related to the polymer density. On the microscopic level, a polymer chain is modeled by an elastic dumbbell with two beads connected

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by a single spring. The molecular configuration is described by an end-to-end vector $q \in \mathbb{R}^d$ of the dumbbell, see Fig. 1.1, and $\Psi(q)$ is the spring potential. The interactions among polymer chains are neglected due to the dilute assumption. In the case that $\Psi(q) = \frac{H}{2} |q|^2$ ($H > 0$ is the elastic constant), the model is known as the Hookean dumbbell model. While the case that $\Psi(q) = -\frac{H Q_0^2}{2} \ln(1 - \frac{|q|^2}{Q_0^2})$ ($Q_0$ is the maximum dumbbell extension) is known as the FENE (Finite Extensible Nonlinear Elastic) dumbbell model. The microscopic dynamics is described by a Fokker–Planck equation of the number density distribution function $f(x, q, t)$ with a drift term depending on the macroscopic velocity field $u$, where $\zeta$ is a constant related to the polymer relaxation time, $k_B$ is the Boltzmann constant and $T$ is the absolute temperature. Alternatively, the microscopic dynamics can also be described by a stochastic differential equation (SDE), or Langevin dynamics, given by

$$(1.2) \quad dq(x, t) = (u \cdot \nabla q(x, t) + \nabla u q(x, t) - 2\zeta^{-1} \nabla q \Psi(q(x, t))) \, dt + \sqrt{4k_B T \zeta^{-1}} \, dW_t,$$

where $dW_t$ is the standard multidimensional white noise.

Fig. 1.1: Schematic representation of the micro–macro model with microscopic vectors acting as springs in the fine scale and averaged to the macroscopic scale.

Although micro-macro models give an elegant description to the origin of the macroscopic stress tensor, it is a long lasting challenge to simulate micro-macro models directly. During the past decades, various computational techniques have been developed for various micro-macro models. There are mainly two approaches, the Langevin equation based stochastic simulation methods and direct simulation methods based on the Fokker–Planck equation. The CONFFESSIT (Calculation of Non-Newtonian Flow: Finite Elements and Stochastic Simulation Technique) algorithm, was the first Langevin equation based numerical method, which couples a finite element discretization to the macroscopic flow with a numerical solver for the microscopic SDE (1.2). Along this direction, other stochastic approaches, the Lagrangian particle method (LPM) and the Brownian configuration field (BCF) method were proposed in order to reduce the variance and the computational cost of the original CONFFESSIT algorithm. Several extensions of these approaches and the corresponding numerical experiments have been extensively investigated in recent years. Stochastic approaches have been the dominant simulation methods of the micro-macro model. However, such stochastic approaches suffer from several shortcomings, including the high computational cost and the stochastic fluctuations. An alternative approach is the direct simulation of the equivalent Fokker–Planck equation in the configurational space. Examples include Galerkin spectral element technique and the
lattice Boltzmann technique [1, 7]. As pointed out in Ref. [56], the computational cost of Fokker-Planck-based methods increases rapidly for simulations in strong flows (with highly localized distribution function) or involving high dimensional configuration spaces. Besides, there are a huge literature devoted to developing macroscopic closure systems, as an approximation to the original macro-micro model [21, 25, 33]. Although the closure systems are easier to solve, they may not able to capture some flow behaviors, such as hysteresis, of the original micro-macro model [34].

During the past decades, there have been growing interests in solving the Fokker-Planck equation by a deterministic particle method [66, 18, 40, 13, 71]. Compared with the Langevin dynamics based stochastic particle methods, the deterministic particle methods are often computationally cheap and do not suffer from stochastic fluctuations. The main challenge of applying the deterministic particle method to the Fokker-Planck type equation is how to deal with the diffusion term. Various kernel regularization approaches have been developed to overcome this difficulty [13, 18, 40, 66].

The goal of this paper is to develop an efficient numerical method for the micro-macro model (1.1) by coupling a finite element discretization to the macroscopic flow with a deterministic particle discretization to the microscopic Fokker-Planck equation. As pointed out in Ref. [71], applying the kernel regularization to the equation may not preserve variational structure at the particle level. To preserve the variational structure, we apply the particle approximation at the energy-dissipation law level and employ a discrete energetic variational approach [50, 71] to derive a coarse-grained micro-macro model with a particle approximation first. A structure-preserving particle-FEM discretization is developed for the coarse-grained model. Various numerical experiments have been performed to validate the new scheme via several benchmark problems. Despite its simplicity, the deterministic particle method is robust, accurate and able to catch certain complex behaviors of polymeric fluids. The numerical results obtained by our scheme are in excellent agreement with those from the former work. Moreover, the deterministic particle discretization is shown to be more efficient than the stochastic particle approaches, where a large ensemble of realizations of the stochastic process are needed.

The rest of this paper is organized as follows. A formal derivation of the micro-macro model of dilute polymeric fluids by employing the energetic variational approach (EnVarA) will be given in section 2. Then we derive a coarse-grained micro-macro model with the particle approximation and construct a deterministic particle-FEM scheme in Section 3. Numerical simulations to validate our scheme are presented in Section 4.

2. Energetic variational approach to the micro-macro model. In this section, we give a formal derivation to micro-macro models of dilute polymeric fluids by employing the energetic variational approach (EnVarA).

Starting with a prescribed energy-dissipation law and a kinematic (transport) relation, the framework of EnVarA derives the dynamics of a non-equilibrium system through two distinct variational processes: the Least Action Principle (LAP) and the Maximum Dissipation Principle (MDP) [6, 59]. This approach was developed from pioneering works of Rayleigh [64] and Onsager [58, 59], and has been successfully applied to build up many mathematical models in physics, chemical engineering and biology [26, 48, 73, 72]. From a numerical perspective, the EnVarA formulation also provides a guide line to develop structure-preserving numerical schemes for different systems [51, 49, 50].
For an isothermal and closed system, an energy-dissipation law is often given by

\[
\frac{d}{dt}E_{\text{total}}(t) = -\Delta(t) \leq 0,
\]

which comes from the first and second laws of thermodynamics [23, 26]. Here \( E_{\text{total}} \) is the total energy, which is the sum of the Helmholtz free energy \( F \) and the kinetic energy \( K \); \( \Delta(t) \) stands for the rate of energy dissipation, which equals to the entropy production in this case. The LAP states that, the dynamics of the Hamiltonian part of the system can be determined by taking variation of the action functional \( A(x) = \int_0^T K - F \) with respect to \( x \) (the trajectory in Lagrangian coordinates) [2, 26], which derives the conservative force

\[
\delta A = \int \int_{\Omega(t)} (\text{force}_{\text{iner}} - \text{force}_{\text{conv}}) \cdot \delta x dx dt,
\]

where \( \Omega^t \) is the physical domain at time \( t \). For a dissipative system \( (\Delta(t) \geq 0) \), the dissipative force can be obtained by minimizing the Onsager dissipation functional \( D = \frac{1}{2} \Delta(t) \) with respect to the “rate” \( x_t \) in the linear response regime, i.e.,

\[
\delta D = \int_{\Omega(t)} \text{force}_{\text{diss}} \cdot \delta x_t dx.
\]

This principle is known as Onsager’s MDP [26]. Consequently, the force balance condition (Newton’s second law, in which the inertial force plays a role of \( ma \)) results in

\[
\frac{\delta A}{\delta x} = \frac{\delta D}{\delta x_t},
\]

which is the dynamics of the system.

Now we show how to derive the micro-macro model (1.1) formally under the EnVarA framework. As mentioned in the introduction, the polymer molecules are modeled as an elastic dumbbell consisting of two "beads" joined by a one-dimensional spring at the microscopic scale [44, 47]. The microscopic configuration between the two beads is described by an end-to-end vector \( q \in \mathbb{R}^d \). Let \( f(x, q, t) \) be the number density distribution function of finding a molecule with end-to-end vector \( q \) at position \( x \) at time \( t \). To derive the micro-macro model by EnVarA, one needs to introduce Lagrangian descriptions in both micro- and macro- scales. Let \( x(X, t) \) be the flow map at the physical space and \( q(X, Q, t) \) be the flow map at the configurational space, where \( X \) and \( Q \) are Lagrangian coordinates in physical and configurational space respectively. For given flow maps \( x(X, t) \) and \( q(X, Q, t) \), the corresponding macroscopic velocity \( u \) and the microscopic velocity \( V \) satisfy

\[
u(x(X, t), t) = x_t(X, t), \quad V(x(X, t), q(X, Q, t), t) = q_t(X, Q, t).
\]

Moreover, one can define the deformation tensor associated with the flow map \( x(X, t) \) by

\[
\tilde{F}(x(X, t), t) = F(X, t) = \nabla_x x(X, t).
\]

Without ambiguity, in this paper, we will not distinguish \( F \) and \( \tilde{F} \). Obviously, \( F \) carries all the transport information of configurations in the system [46] and satisfies the transport equation in Eulerian coordinates [47]

\[
F_t + u \cdot \nabla F = \nabla u F.
\]
Due to the conservation of mass, the density distribution function \( f(x, q, t) \) satisfies

\[
\frac{d}{dt} \int_{\Omega} \int_{\mathbb{R}^d} f(x, q, t) dq dx = 0,
\]

which can be written as

\[
\partial_t f + \nabla \cdot (fu) + \nabla_q \cdot (fV) = 0
\]
in Eulerian coordinates. Here \( u(x, t) \) and \( V(x, q, t) \) are the macro- and microscopic velocities defined in \((2.5)\).

In the framework of EnVarA, the micro-macro system can be modeled through an energy-dissipation law

\[
\frac{d}{dt} \int_{\Omega} \left( \frac{1}{2} \rho |u|^2 + \lambda_p \int_{\mathbb{R}^d} k_B T f \ln f + \Psi(q) dq \right) dx
\]

\[= - \int_{\Omega} \left( \eta_s \nabla |u|^2 + \int_{\mathbb{R}^d} \frac{\lambda_p \zeta}{2} f |V - \tilde{V}|^2 dq \right) dx,
\]

where \( \rho \) is the constant density of the fluid, \( \lambda_p \) is a constant that represents the polymer density, \( k_B \) is the Boltzmann constant, \( T \) is the absolute temperature, \( \eta_s \) is the solvent viscosity, the constant \( \zeta \) is related to the polymer relaxation time, \( \Psi = \Psi(q) \) is the microscopic elastic potential of the polymer molecules. For Hookean and FENE models, the elastic potential \( \Psi(q) \) is given by

\[\Psi(q) = \frac{1}{2} H |q|^2,\]

and

\[\Psi(q) = - \frac{HQ_0^2}{2} \ln \left( 1 - \left( \frac{|q|}{Q_0} \right)^2 \right),\]

respectively, where \( H > 0 \) is the elastic constant, \( Q_0 \) is the maximum dumbbell extension in FENE models. The second term of the dissipation accounts for the micro-macro coupling with \( \tilde{V} \) being the macroscopic induced velocity. According to the Cauchy-Born rule, \( q = F Q \) at the macroscopic scale, which indicates

\[\tilde{V} = \frac{d}{dt} (FQ) = \left( \frac{d}{dt} F \right) Q = (\nabla u F) Q = \nabla u q.\]

Now we are ready to derive the dynamics of the system. First, we look at the dynamics at the macroscopic scale. Due to the "separation of scale" [26], the second term on the right hand side of the dissipation \((2.9)\) vanishes when deriving the macroscopic force balance. Since \( \det F = 1 \), the action functional can be written as

\[
A(x) = \int_0^T \int_{\Omega_0} \left[ \frac{1}{2} \rho |x|^2 - \lambda_p \int_{\mathbb{R}^d} k_B T f_0 \ln f_0 + \Psi(FQ)f_0 dq \right] dX dt
\]
in Lagrangian coordinates, where \( f_0(X, Q) \) is the initial number distribution function, and \( f(x, FQ, t) = f_0(X, Q) \) due to \( \det F = 1 \). By applying the LAP, i.e., taking variation of \( A(x) \) with respect to \( x \), we get

\[
\frac{\delta A}{\delta x} = -\rho(u + \nabla u) + \lambda_p \nabla \left( \int_{\mathbb{R}^d} f \nabla_q \Psi \otimes dq \right)
\]
in Eulerian coordinates. Indeed, consider a perturbation
\[ x' = x + \epsilon y, \]
where \( y(X,t) = \tilde{y}(x(X,t),t) \) satisfying \( \tilde{y} \cdot n = 0 \). Then
\[
\frac{d}{dt} A(x') \bigg|_{\epsilon = 0} = \int_0^T \int_{\Omega_0} \left[ -\rho x_{tt} \cdot y - \lambda_p \int f_0 \nabla_q \Psi \otimes Q : \nabla X y dQ \right] dX
\]
Push forward to Eulerian coordinates, we have
\[
\frac{d}{dt} A(x') \bigg|_{\epsilon = 0} = \int_0^T \int_{\Omega} \left[ -\rho (u_t + u \cdot \nabla u) \cdot \tilde{y} - \lambda_p \int f \nabla_q \Psi \otimes q : \nabla x \tilde{y} d\mathbf{q} \right] dx
\]
which leads to (2.11).

For the dissipation part, the MDP, i.e., taking variation of \( D \) with respect to \( x_t \), leads to
\[ \frac{\delta D}{\delta x_t} = -\eta_s \Delta u + \nabla p, \]
where \( p \) is the Lagrangian multiplier for the incompressible condition \( \nabla \cdot u = 0 \). Hence, the macroscopic force balance results in the momentum equation
\[ \rho (u_t + u \cdot \nabla u) + \nabla p = \eta_s \Delta u + \nabla \cdot \tau, \]
where
\[ \tau = \lambda_p \int_{\mathbb{R}^d} f \nabla_q \Psi \otimes q d\mathbf{q} \]
is the induced stress from the configuration space, representing the microscopic contributions to the macroscopic level. Here, \( \otimes \) denotes a tensor product and \( u \otimes v \) is a matrix \( (u_i v_j) \) for two vectors \( u \) and \( v \).

On the microscopic scale, by taking variations with respect to \( q(X,Q,t) \) and \( V(X,Q,t) \), we obtain
\[ \frac{\zeta}{2} (V - \nabla u q) = -\nabla_q (k_B T \ln f + 1 + \Psi). \]
Then combining with Eq. (2.8), we get the equation on the microscopic scale:
\[ f_t + \nabla \cdot (uf) + \nabla_q \cdot (\nabla u q f) = \frac{2}{\zeta} \nabla_q \cdot (f \nabla_q \Psi) + \frac{2 k_B T}{\zeta} \Delta_q f. \]

And thus, the final coupled system reads as follows,
\[
\begin{align*}
\rho (u_t + u \cdot \nabla u) + \nabla p &= \eta_s \Delta u + \nabla \cdot \tau, \\
\tau &= \lambda_p \int_{\mathbb{R}^d} f \nabla_q \Psi \otimes q d\mathbf{q}, \\
\nabla \cdot u &= 0, \\
\quad f_t + \nabla \cdot (uf) + \nabla_q \cdot (\nabla u q f) &= \frac{2}{\zeta} \nabla_q \cdot (f \nabla_q \Psi) + \frac{2 k_B T}{\zeta} \Delta_q f,
\end{align*}
\]
subject to a suitable boundary condition. For the sake of simplicity, in this paper, we consider Dirichlet boundary conditions for the velocity and non-flux boundary condition for \( f(x, q, t) \) with respect to \( x \).
3. Numerical Methods. In this section, we propose a numerical scheme to solve the micro-macro model by combining a finite element discretization for the macroscopic fluid dynamic equation [4, 5, 16] with a deterministic particle method for the microscopic Fokker-Planck equation [71].

To preserve the variational structure after a particle discretization, we first derive a coarse-grained micro-macro system with a deterministic particle approximation in the configurational space by a discrete energetic variational approach [50]. The discrete energetic variational approach follows the idea of “Approximation-then-Variation”, which first applies particle approximation to the continuous energy dissipation law and derives a coarse-grained model by variational procedures. As an advantage, the derived equations of particles preserve the variational structure at the particle level [71].

For simplicity, we assume that

\[
\int_{\mathbb{R}^d} f(x, q, t) dq = 1, \quad \forall x, 
\]

which means that the number density of polymer chains is spatially homogeneous. Thus, for fixed \( x \), \( f(x, q, t) \) can be approximated by

\[
f(x, q, t) \approx f_N(x, q, t) = \sum_{i=1}^{N} \omega_i(x, t) \delta(q - q_i(x, t)), \quad \forall x
\]

with a particle approximation at the microscopic level. Here \( N \) is the number of particles at \( x \) and time \( t \), \( \{q_i(x, t)\}_{i=1}^{N} \) is a set of representative particles at \( x \) at time \( t \), \( \omega_i(x, t) \) is the weight of the corresponding particle satisfying \( \sum_{i=1}^{N} \omega_i(x, t) = 1 \). In the current work, we fix \( \omega_i(x, t) = \frac{1}{N} \), i.e., all the particles are equally weighted.

Remark 3.1. \( \{q_i(x, t)\}_{i=1}^{N} \) can be viewed as representative particles that represent information of the number density distribution \( f(x, q, t) \) at \( x \). Since only \( q_i(x, t) \) needs to be computed at each time-step, the computational cost can be largely reduced. It is more like an Eulerian approach, rather than a Lagrangian approach.

Substitute the approximation (3.2) into the continuous energy-dissipation law (2.9), we can obtain a discrete energy-dissipation law in terms of \( q_i(x, t) \) and the macroscopic flow. Notice that the term \( \ln f_N(x, q, t) \) can not be defined in a proper way, we introduce a kernel regularization, i.e., replacing \( \ln f_N \) by \( \ln(K_h \ast f_N) \), where \( K_h \) is a kernel function and

\[
K_h \ast f_N(\cdot, q, \cdot) = \int K_h(q - p)f_N(\cdot, p, \cdot) dp = \frac{1}{N} \sum_{j=1}^{N} K_h(q - q_j(x, t)).
\]

A typical choice of \( K_h \) is the Gaussian kernel, given by

\[
K_h(q_1, q_2) = \frac{1}{(\sqrt{2\pi}h_p)^d} \exp \left( -\frac{|q_1 - q_2|^2}{2h_p^2} \right).
\]

Here \( h_p \) is the bandwidth which controls the inter-particle distances and \( d \) is the dimension of the space. We take \( h_p \) as a constant for simplicity. The values of \( h_p \) will affect the numerical results. We’ll discuss the choices of \( h_p \) in the next section.

Within the kernel regularization, the discrete energy can be written as

\[
\mathcal{F}_h \left[ \{q_i\}_{i=1}^{N}, x \right] = \int_{\Omega} \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{1}{N} \sum_{i=1}^{N} \left[ k_B T \ln \left( \frac{1}{N} \sum_{j=1}^{N} K_h(q_i - q_j) \right) + \Psi(q_i) \right] dx,
\]
and the discrete dissipation is

\begin{equation}
(3.4) \quad -2D_h \{ (q_i)_{i=1}^N, (\dot{q}_i)_{i=1}^N, x, u \} = - \int_{\Omega} \eta_i |\nabla u|^2 + \frac{\lambda_p \zeta}{N} \sum_{i=1}^N \dot{q}_i - \nabla u q_i^2 \, dx,
\end{equation}

where \( \dot{q}_i = \partial_t q_i + u \cdot \nabla q_i \) is the material derivative of \( q_i \).

The differential equations of \( q_i \) can be derived via the discrete energetic variational approach \[50\], i.e., performing the EnVarA in terms of \( q_i \) and \( \dot{q}_i \), which leads to

\[
\frac{\delta D_h}{\delta q_i} = - \frac{\delta F_h}{\delta q_i}.
\]

By direct computation we get the equation for \( q_i \),

\begin{equation}
\dot{q}_i = (\nabla u)q_i - \frac{2}{\kappa} \left[ k_B T \left( \sum_{j=1}^N \nabla q_j K_h(q_i, q_j) \right) + \sum_{k=1}^N \sum_{j=1}^N K_h(q_k, q_j) q_i^2 \right] + \nabla_q \Psi(q_i),
\end{equation}

where \( \dot{q}_i = \partial_t q_i + u \cdot \nabla q_i \) in Eulerian coordinates. Here we denote \( K_h(q_i, q_j) \) by \( K_h(q_i, q_j) \) for convenience. As an advantage of the “approximation-then-variation” approach, it can be noticed that Eq. (3.5) is a gradient flow with respect to \( \{ q_i \} \) in absence of the flow, i.e. \( u = 0 \) \( \forall x \).

The variational procedure for the macroscopic flow is almost the same as that in the continuous case, shown in section 2. The final micro-macro system with particle approximation is given by

\begin{equation}
\begin{cases}
\rho(u_i + u \cdot \nabla u) + \nabla p = \eta_s \Delta u + \nabla \cdot \tau, \\
\tau(x, t) = \lambda_p \frac{1}{N} \sum_{i=1}^N \nabla_q \Psi(q_i(x, t)) \otimes q_i(x, t), \\
\nabla \cdot u = 0,
\end{cases}
\end{equation}

where \( q_i(x, t) \) satisfies (3.5).

One can view the macroscopic flow equation (3.6) along with the microscopic evolution equation (3.5) as a coarse-grained model for the original micro-macro model (2.17). To solve the system numerically, it is a natural idea to apply some decoupled schemes at each step. Precisely, we apply the following algorithm for the temporal discretization:

- **Step 1:** Solve the equation (3.6) by a finite element method to obtain updated values for the velocity and pressure by treating the viscoelastic stress field \( \tau^n \) as a known term obtained from the last time step.

- **Step 2:** Using the updated velocity field \( u^{n+1} \), solve the equation of \( q_i \). Update the values of the viscoelastic stress at each node, and project them into the finite element space of \( \tau \).

In the present work, we adopt the finite element method developed in \[5, 16\] for Step 1. For more detail, let \( \Omega \) be the bounded computational domain, and \( T_h \) be the triangulation of \( \Omega \). \( T_h \) consists of a set of simplexes \( \{ \kappa_e | e = 1, ..., M \} \) and a set of nodal points \( N_h = \{ x_1, x_2, ..., x_{N_e} \} \). For a nonnegative integer \( r \), denote \( P_r(\kappa) \) as the space of polynomial functions of degree less than or equal to \( r \) on the simplex \( \kappa \). We can construct finite-dimensional subspaces \( S_h \subset H^1(\Omega) \), \( M_h \subset L^2_0(\Omega) \) and \( S_h^0 \subset H^1_0(\Omega) \) as
follows,
\[ S_h = \{ g \in C^0(\Omega) : g|_{\kappa} \in P_1(\kappa) \}, \quad S_h^0 = \{ g \in S_h : g|_{\partial\Omega} = 0 \}, \]
\[ M_h = \{ h \in L_0^2(\Omega) : h|_{\kappa} \in P_1(\kappa) \}, \]
where \( L_0^2(\Omega) = \{ q \in L^2(\Omega), \int_\Omega q dx = 0 \} \).

Let the finite element spaces for the velocity and the stress tensor be \( V_{u_h} = (S_h^0)^d \) and \( V_p = (S_h)^d \) respectively, where \( d \) is the dimension of space. Then the equation (3.6) can be solved by a standard velocity-correction projection method [28]. The advantage of using the \( P_1 - P_1 \) element for the velocity and pressure is that it avoids an inf-sup condition [10].

Next we discuss how to solve equation (3.5) with a given flow field \( u \). The numerical difficulties arise from the fact that \( q_i \) is a function of \( x \) and \( t \) due to the convection term \( u \cdot \nabla q_i(x, t) \). Many earlier numerical studies based on CONNFFEST algorithms either focus on the shear flows in which the convection term vanishes or ignore the convection term [36, 60]. To deal with the convection term in stochastic SIT algorithms either focus on the shear flows in which the convection term vanishes [21, 61, 75]. Another way is to use a Lagrangian viewpoint to compute the convection term [29]. In the current study, we use the idea of the second approach, and use an operator splitting approach to solve (3.5). Initially, we assign ensemble of particles \( \{ q_{x_\alpha,i} \}_{i=1}^{N_\alpha} \) to each node \( x_\alpha \) (\( \alpha = 1, 2, \ldots, N_x \)). We assume that \( f(x, q, 0) \) is spatially homogeneous, and use the same ensemble of initial samples at all \( x_\alpha \). Within the values \( u_{h}^{n+1} \), we solve the microscopic equation (3.5) by the following two steps:

**Step 1**: At each node \( x_\alpha \), solve (3.5) without the convection term \( u_{n+1} \cdot \nabla q \) by

\[
\frac{1}{N} \Delta t q_i^{n+1,*} - q_i^n = -\frac{\delta F_h}{\delta q_i} (\{ q_i^{n+1,*} \}_{i=1}^N),
\]
\[
q^{n+1,**} = (I + (\nabla u^n) \Delta t) q^{n+1,*}.
\]

**Step 2**: To deal with the convention term, we view each node \( x_\alpha \) as a Lagrangian particle, and update it according to the Eulerian velocity field \( u_{n+1} \) at each node

\[
\dot{x}_\alpha = x_\alpha + \Delta t (u_{n+1}|_{x_\alpha}), \quad \alpha = 1, 2, \ldots, N_x.
\]

Hence, \( \{ q_{a,i}^{n+1,**} \} \) is an ensemble of samples at the new point \( \tilde{x}_\alpha \). To obtain \( q_{a,i}^{n+1} \) at \( x_\alpha \), we use some interpolation to get \( q_{a,i}^{n+1} \) (at mesh with \( \{ x_\alpha \} \) being the set of node) from \( q_{a,i}^{n+1,**} \) (at mesh with \( \{ \tilde{x}_\alpha \} \) being node) for each \( i \).

**Remark 3.2.** An advantage of the above update-and-projection approach is that it doesn’t require a spatial discretization on \( q_i(x, t) \).

**Remark 3.3.** The operator splitting approach has been widely used in many previous Fokker-Planck based numerical approaches [30]. One important reason is that the system admits a variational structure without the convention terms. In addition, by treating the convention part separately, we treat the particles at each physical location independently, which largely saves the computational cost.

Since the first step in (3.7) admits a variational structure, the implicit Euler discretization can be reformulated as an optimization problem. In more detail, we define

\[
J_n(\{ q_i \}_{i=1}^N) = \frac{1}{N} \sum_{i=1}^N \left( \frac{1}{2 \Delta t} | q_i - q_i^n |^2 \right) + F_h.
\]
In this case, the first step of (3.7) is the gradient of $J_n(\{q_i\}_{i=1}^N)$ with respect to $\{q_i\}_{i=1}^N$. Hence, we can solve the nonlinear system by solving the optimization problem

$$\{q_i^{n+1,*}\}_{i=1}^N = \arg \min_{\{q_i\}_{i=1}^N} J_n(\{q_i\}_{i=1}^N).$$

An advantage of this reformulation is that we can prove the existence of the $q_i^{n+1,*}$. More precisely, we have the following result.

**Proposition 3.1.** For any given $\{q_i^n\}_{i=1}^N$, there exists at least one minimal solution of (3.9) $\{q_i^{n+1}\}_{i=1}^N$ that also satisfies

$$\frac{F_h(\{q_i^{n+1}\}_{i=1}^N) - F_h(\{q_i^n\}_{i=1}^N)}{\Delta t} \leq -\frac{1}{2N\Delta t^2} \sum_{i=1}^N |q_i^{n+1} - q_i^n|^2.$$

**Proof.** Let $X \in \mathbb{R}^D (D = N \times d)$ be vectorized $\{q_i\}_{i=1}^N$, namely,

$$X = (q_{1,1}, \ldots, q_{N,1}, q_{1,2}, \ldots, q_{N,2}, \ldots, q_{N,d}).$$

Denote $F_h(\{q_i\}_{i=1}^N)$ and $J_n(\{q_i\}_{i=1}^N)$ as $F_h(X)$ and $J_n(X)$ respectively. For given $X^n = \{q_i^n\}_{i=1}^N$, we define

$$S = \{J_n(X) \leq J_n(X^n)\}$$

be the admissible set. Obviously, $S$ is non-empty and closed, since $X^n \in S$ and $J_n(X)$ is continuous. Moreover, it’s easy to prove that $F_h(X)$ is bounded from below, since

$$\ln \left( \frac{1}{N} \sum_{j=1}^N K_h(q_i^n, q_j^n) \right) \geq \ln \left( \frac{1}{N} \frac{1}{(\sqrt{2\pi h})^d} \right) \quad \text{and} \quad \Psi(q_t) \geq 0.$$

And thus, $J_n(X)$ is coercive and $S$ is a bounded set. Hence, $J_n(X)$ admits a global minimizer $X^{n+1}$ in $S$. And thus, we have

$$\frac{1}{N} \sum_{i=1}^N \left( \frac{1}{2\Delta t} |q_i^{n+1} - q_i^n|^2 \right) + F_h(X^{n+1}) \leq F_h(X^n),$$

which is equivalent to Eq. (3.10).

The full discretization scheme can be summarized as follows. Given the time step size $\Delta t$, the initial conditions $\{q_i^0\}_{i=1}^N$, $u^0 \in V_{u_h}$, and $p^0 \in M_h$, having computed for $\{q_i^n\}_{i=1}^N$, $u^n \in V_{u_h}$, $\tau^n \in V_T$ and $p^n \in M_h$ for $n > 0$, we compute $\{q_i^{n+1}\}_{i=1}^N$, $u^{n+1}$, and $p^{n+1}$ by the following algorithm:

**Step 1:** Treat the stress tensor explicitly and solve the macroscopic flow equation

$$\rho \left( \frac{u^{n+1} - u^n}{\Delta t} + u^n \cdot \nabla u^{n+1} \right) + \nabla p^{n+1} = \eta_h \Delta u^{n+1} + \nabla \cdot \tau^n,$$

$$\nabla \cdot u^{n+1} = 0.$$

The equation (3.12) can be solved by the following two steps:

- **Step 1.1:** Find $u_{h}^{n+1} \in V_{u_h}$, such that for any $v \in V_{u_h}$,

$$\rho \left( \frac{1}{\Delta t} u_{h}^{n+1} + u_{h}^n \cdot \nabla u_{h}^{n+1}, v \right) + (\eta_h \nabla u_{h}^{n+1}, \nabla v) + (\nabla \cdot \tau_{h}^n, v) + (\nabla \cdot \tau_{h}^n, v).$$

10
Step 1.2: Find $p_h^{n+1} \in M_h$, such that for any $\psi \in M_h$,

$$(\nabla(p_h^{n+1} - p_h^n), \nabla \psi) = \frac{1}{\Delta t}(\nabla \cdot \tilde{u}_h^{n+1}, \psi).$$

Then we obtain

$$u_h^{n+1} = \tilde{u}_h^n - \Delta t \nabla (p_h^{n+1} - p_h^n).$$

**Step 2:** Within the values $u_h^{n+1}$, we solve the microscopic equation (3.5) by the update-and-project approach. Within the ensemble of particles $\{q_{x_\alpha}^{n+1}\}_{\alpha=1}^{N_x}$ on each node $x_\alpha$, the updated values of the viscoelastic stress $\tau^{n+1}$ at each node, denoted as $\{\tau^{n+1}_{x_\alpha,l,k}\}_{\alpha=1}^{N_x}$, can be obtained through the second equation of Eq. (3.6). And then project them into the finite element space of $\tau$, i.e. $V$. To this end, we choose the projection operator $I$, such that, for each component of the stress $\tau^{n+1}_{x_\alpha,l,k}$ with $l, k = 1, \ldots, d$, $I(\{\tau^{n+1}_{x_\alpha,l,k}\}_{\alpha=1}^{N_x}) := \sum_{\alpha=1}^{N_x} \tau^{n+1}_{x_\alpha,l,k} \phi_{x_\alpha}$, where $\{\phi_{x_\alpha} : \alpha = 1, \ldots, N_x\} \subset S_h$ denotes the nodal basis for $S_h$.

**Remark 3.4.** In the previous numerical scheme, we estimate the macroscopic stress tensor by taking microscopic distribution function as the empirical measure for the finite number of particles $\{q_i\}_{i=1}^N$. More advanced techniques can be applied to this stage to obtain a more accurate estimation to the stress tensor, such as the maximum-entropy based algorithm developed in Ref. [3] and Ref. [65] that reconstructs basis functions from particles. We'll explore this perspective in future works.

4. Numerical Experiments. In this section, we perform various numerical experiments to validate the proposed numerical scheme by studying various well-known benchmark problems for the micro-macro models [32, 42, 60]. For all the numerical experiments carried out in this section, we suppose that the flow is two-dimensional and the dumbbells lie in the plane of the flow, namely, the configuration vector $q$ is also two-dimensional. At each node, we use the same initial ensemble of $N$ particles, sampled from the 2-dimensional standard normal distribution.

4.1. Hookean case: the accuracy test. We first consider the Hookean model in a simple shear flow [12, 42], where the fluid is enclosed between two parallel planes of infinite length separated by a distance $L$. At $t = 0$, the lower plane starts to move in the positive $x$-direction with a constant velocity $U$, as shown in Fig. 4.1. We consider the no-slip boundary conditions at the walls. In this case, the velocity is in the $x$-direction, and only depends on the $y$-variable, namely, the velocity $u(x,t) = (u(y,t),0)$ with $x = (x,y)$. Obviously, the velocity field automatically satisfies the incompressible condition $\nabla \cdot u = 0$. Moreover, we assume that $q$ also only depends on $y$, so $u \cdot \nabla q = 0$.

Since the micro-macro model (2.17) with the Hookean potential $\Psi(q) = \frac{1}{2}H|q|^2$ is equivalent to a macroscopic viscoelastic model, the Oldroyd–B model. We can compare the simulation results for the micro-macro model and the corresponding Oldroyd–B model, as an accuracy test for the proposed numerical scheme. In this subsection, we take the parameters as follows,

$$\rho = 1; \quad \eta_s = 1; \quad \zeta = 4; \quad k_B T = 1; \quad \lambda_p = 1; \quad H = 1; \quad \Delta t = 10^{-3}.$$  

(4.1)

Such parameters might not be physically reasonable, and we use them primarily to illustrate our numerical scheme. When the parameters are set as Eq. (4.1), the
The corresponding Oldroyd-B model can be written as follows [36],

\[
\begin{align*}
\frac{\partial u(y,t)}{\partial t} &= \frac{\partial^2 u(y,t)}{\partial y^2} + \frac{\partial \tau_{12}(y,t)}{\partial y}, \\
\frac{\partial \tau_{12}(y,t)}{\partial t} + \tau_{12}(y,t) &= \frac{\partial u(y,t)}{\partial y}.
\end{align*}
\]

Here, \(\tau_{12}\) denotes the \((x,y)\) component of the stress \(\tau\). In this work, these equations are solved sequentially in a segregated manner [24, 63]. Namely, for \(0 \leq n \leq \tilde{N}\), having computed \(u^n\) and \(\tau_{12}^n\), we compute \(u^{n+1}\) and \(\tau_{12}^{n+1}\) as follows,

\[
\begin{align*}
\frac{u^{n+1} - u^n}{\Delta t} &= \frac{\partial^2 u^{n+1}}{\partial y^2} + \frac{\partial \tau_{12}^n}{\partial y}, \\
\frac{\tau_{12}^{n+1} - \tau_{12}^n}{\Delta t} + x_{12}^{n+1} &= \frac{\partial u^{n+1}}{\partial y}.
\end{align*}
\]

For the spatial discretization, we use the same finite element method mentioned in Section 3 to simulate the Oldroyd-B model. For both models, we set the number of elements \(M = 40\) and \(\Delta t = 10^{-3}\). The kernel bandwidth \(h_p = \text{med}^2 / \log N\) [53], where med is the median of the pairwise distance between the particles \(\{q_i^n\}_{i=1}^{N}\).

We first study the influence of number of particles. Fig. 4.2(a) presents the time evolution of \(\tau_{12}\) at \(y = 0.5\) with different numbers of particles (\(N = 50, 100\) and \(200\)). The lines in Fig. 4.2(a) stand for the mean values of 10 independent runs, in which we set the same parameters and use different sets of \(N\) particles (sampled from the standard normal distribution). The shaded regions stand for the standard errors. It reveals that when the particle number gets larger, the standard deviations get smaller and the mean values get closer to the results of the Oldroyd-B model. We set \(N = 200\) for all the following numerical experiments.

Fig.4.2(b)-(c) show the time evolutions of the simulated stress \(\tau_{12}\) and the velocity \(u\) at \(y = 0.25, 0.5\) and \(0.75\) for the micro-macro model (a single trail) and the Oldroyd-B model. Fig. 4.2(d) shows relative errors of the velocity with respect to time at different locations. The numerical results obtained by the particle scheme are in excellent agreement with numerical results of the Oldroyd-B model, especially for the velocity field, which validates the numerical scheme.

**Remark 4.1.** Since we are mainly interested in the macroscopic flow behavior of the micro-macro model, it is not necessary to solve the microscopic Fokker-Planck...
Fig. 4.2: Time evolution of the stress at \( y = 0.5 \) with different numbers of particles (a). Comparison with the Hookean case and the Oldroyd-B model (b-d): the stress with respect to time at different locations (b); comparison of the velocity of the Hookean case (marker) and the Oldroyd-B model (continued line) with respect to time at different locations (c); the relative error of velocity with respect to time at different locations (d).

equation in high accuracy. The above simulation results indicate that such a simple particle approximation can lead to an accurate estimate to \( \nabla \cdot \tau \), although a detailed numerical analysis is required to justify this, which will be studied in future works.

4.2. FENE models: Hysteresis behavior in simple extensional flows. The FENE models take the finite extensibility of polymer chains into account and has nonlinear features. One of the key features of FENE models is hysteresis behavior, which can be observed using the normal stress/the elongational viscosity versus the mean-square extension in simple extensional flow during a relaxation \([20, 45]\).

In this subsection, we validate our variational particle scheme by studying the hysteresis behavior of a FENE model. We consider an elongational velocity gradient given by

\[
\nabla u = \varepsilon(t) \text{diag}(1, -1),
\]

where \( \varepsilon(t) \) is the strain rate and \( \text{diag}(1, -1) \) is the \( 2 \times 2 \) diagonal matrix with diagonal entries being 1 and \(-1\). Two cases of \( \varepsilon(t) \) will be considered, the start-up case with

\[
\varepsilon(t) = \begin{cases} r, & 0 \leq t \leq \frac{9}{r}, \\ 0, & \text{otherwise}, \end{cases}
\]

and the constant-gradient velocity case with

\[
\varepsilon(t) = r.
\]
Throughout this subsection, the initial data of particles is sampled from the 2-dimensional standard normal distribution and other parameters are set as follows,

\[ h_p = 0.01; \quad \zeta = 4; \quad k_B T = 1; \quad \lambda_p = 1; \quad Q_0 = \sqrt{50}; \quad H = 1; \quad \Delta t = 10^{-3}. \]

As stated in Section 4.1, we set \( h_p = \text{med}^2 / \log N \) for Hookean models, where \( \text{med} \) is the median of the pairwise distance between the particles \( \{q_{ni}^p\}_{i=1}^N \). However, this approach is not suitable for the FENE potential, as the equilibrium distributions are no longer Gaussian type and the median of the pairwise distance can become very large. Numerical experiments show that taking \( h_p = 0.01 \) produces a good result. Hence, for all the numerical experiments of the FENE case below, we set the kernel bandwidth \( h_p = 0.01 \).

For the start-up case, the numerical results are shown in Figs. 4.3 and 4.4 for different extensional rates. The time evolution of normal stress \( \tau_{11} - \tau_{22} \) and the plot of the normal stress versus the mean-square extension \( \langle q^2 \rangle / Q_0^2 \) in the start-up case are plotted in Fig. 4.3 (left). The comparison of hysteresis behavior of the FENE model for different extensional rates (\( r = 4, 5, 6 \)) is shown in Fig. 4.3 (right). It is observed that when the strength of velocity gradient is getting smaller, the hysteresis behavior becomes narrower. The numerical results are consistent with those obtained in the former work [32].

As discussed in Ref. [32], to catch the hysteresis of the original FENE model, a coarse grained model should be able to catch the spike like behaviors of the probability density in the FENE model in large extensional effect of the flow field. The peak positions of the probability distribution function (PDF) distribution of the FENE model depend on the macroscopic flow field and change in time under the large macroscopic flow effects [34]. Fig. 4.4 shows the distribution of the particles (up to a constant) obtained by the kernel density estimation at different times in the start-up case and the constant-gradient velocity case with \( r = 4 \), respectively. It reveals that the distribution of particles captures the \( \delta \)-function like spikes and the time evolution results of the particles apparently show a separation into two peaks in the two cases.

In the start-up case, the distribution splits into two spikes and then shows gradual
centralized behavior. Eventually, it forms a single peak in the center, as shown in Fig. 4.4 (a). Notice that the numerical results in the equilibrium state are consistent with the equilibrium solution of the Fokker-Planck equation with zero flow rate. We can conclude that our numerical results are reasonable, since the velocity rate turns to be zero when $t$ is big enough ($t > 9/r$). In the constant-gradient velocity case, the particles show two regions of higher concentration near the boundary of the configuration domain at the equilibrium state (i.e., with stable double spikes), as shown in Fig. 4.4 (b). This is a good agreement to the feature of the FENE model.

It has been well-known that, for the FENE model, there exists several closure approximation approaches to obtain the corresponding macroscopic closure systems, such as FENE-P, FENE-S and FENE-D [20, 32, 45, 68]. Even though some macroscopic closure models show good agreement to macroscopic induced stresses, they are not able to catch the hysteresis and $\delta$-function behaviors [32, 68]. From the numerical results shown in this section, we could conclude that the variational particle scheme can catch the hysteretic and peak phenomenon, showing good agreement to track the

![Fig. 4.4: The particle and corresponding PDF (obtained by kernel density estimation) at different times. (a) Start-up case with $r = 4$: the position of particles (left) and the distribution of particles (middle and right) at $t = 3$ (the first row) and $t = 8$ (the second row). (b) The constant-gradient velocity case with $r = 4$: the position of particles (left) and the distribution of particles (middle and right) at $t = 3$ (the first row) and $t = 8$ (the second row).]
dynamic behaviors of FENE dumbbells.

![Fig. 4.5](image)

**Fig. 4.5:** For the FENE model: the velocity \( u \) with respect to location \( y \) at different times (a); the time evolution of the velocity \( u \) at different locations (b); the time evolution of the shear stress (c) and normal stress difference (d) at location \( y = 0.2, y = 0.5, y = 0.8, y = 1 \).

### 4.3. FENE case: the pure shear flow.

In this section, we consider the case with the FENE potential in the simple shear flow as stated in Section 4.1, where the microscopic particle equations are coupled with the incompressible Navier-Stokes equation on the macroscopic level.

In this case, we set \( L = 1, M = 20, \Delta t = 10^{-3} \) and the same boundary conditions as those in Section 2. The parameters are set as those in Ref. [42]:

\[
\rho = 1.2757; \quad \eta_s = 0.0521; \quad \zeta = 2; \quad k_B T = 1; \quad H = 0.01; \quad \lambda_p = 1.91; \quad Q_0 = \sqrt{50}.
\]

Fig. 4.5 (a) presents the evolution of the velocity with respect to location \( y \) at different times. It reveals the phenomenon of velocity overshoot for the FENE model, which is the typical property of viscoelastic fluids. Fig. 4.5 (b) displays the evolution of the velocity with respect to time \( t \) at three locations \( y = 0.2, y = 0.5 \) and \( y = 0.8 \). It can be seen that the velocity overshoot occurs sooner in fluid layers nearer to the moving plane.

Fig. 4.5 (c-d) show the temporal evolution of the shear stress and the normal stress difference at different locations \( y = 0.2, y = 0.5, y = 0.8 \) and \( y = 1 \). As it can be seen, the stress response is sharper in fluid layers nearer to the moving plane, which is consistent with the behavior of velocity overshoot. We notice that there exists delay of the maximum of the normal stress with respect to that of the shear stress. Precisely, the shear stress of the FENE model reaches the maximum at around \( t = 6 \), but the maximum of the normal stress is reached at about \( t = 10 \). The numerical results are in excellent agreement with the former work [42, 75], indicating the accuracy of our numerical scheme in the FENE case. Moreover, small oscillations occur in the
former work [75], which is the stochastic noise due to the stochastic nature of the microscopic stress calculation. It should be noted that, compared with the former work, there exists few oscillations in our numerical results obtained by the variational particle scheme.

4.4. FENE models: the lid driven cavity flow. In this section, we consider a more complicated case, known as the lid driven cavity flow. In this case, the polymeric fluid is bounded in a two dimensional square box of width $L$ and the fluid motion is induced by the translation of the upper wall at a velocity $U$. The width of cavity is set to be $L = 1$ and the velocity $u = (u, v)$, where the horizontal velocity of the lid $u(x) = U = 1$. The three other walls are stationary and the boundary conditions applied to them are no slip and impermeability, i.e., $u = 0$ (see Fig. 4.6 for an illustration). It is well-known that such idealized lid driven cavity problem possesses a geometric singularity at the edges of the lid. To avoid the numerical difficulty arising from the corner singularity, we consider a regularized boundary condition [69], given by

$$u(x) = 16U(x/L)^2(1 - x/L)^2.$$  

Fig. 4.6: Geometry for the lid driven cavity flow.

Since there are no quantitative results for the lid driven cavity flow with FENE dumbbell models, in order to validate our scheme, we make a comparison with the former work [75], which solves the same model by combining the Brownian configuration field method with an SPH simulation for the macroscopic flow. We consider a dimensionless version of the micro-macro system Eq. (3.5)-(3.6), which reads

$$\begin{aligned}
\text{Re}(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) + \nabla p &= \tilde{\eta}_s \Delta \mathbf{u} + \nabla \cdot \mathbf{\tau}, \\
\mathbf{\tau} &= \frac{\epsilon_p}{\text{We}} \frac{1}{N} \sum_{i=1}^{N} \nabla q_i \Psi(q_i(t)) \otimes q_i(t), \\
\nabla \cdot \mathbf{u} &= 0,
\end{aligned}$$  

with $q_i(t)$ satisfying

$$q_i - (\nabla u)q_i = - \frac{1}{2\text{We}} \left( \frac{\sum_{j=1}^{N} \nabla q_i K_h(q_i, q_j)}{\sum_{j=1}^{N} K_h(q_i, q_j)} + \sum_{k=1}^{N} \frac{\nabla q_i K_h(q_k, q_i)}{\sum_{j=1}^{N} K_h(q_k, q_j)} + \nabla q_i \Psi(q_i) \right).$$
Here, the nondimensionalized parameters are defined as

\[ Re = \frac{\rho \tilde{U} \tilde{L}}{\eta}, \quad We = \frac{\lambda \tilde{U}}{\tilde{L}}, \quad \tilde{\eta}_s = \frac{\eta_s}{\eta}, \quad \epsilon_p = \frac{\eta_p}{\eta}, \quad \lambda = \frac{\zeta}{4H}, \]

where \( \tilde{L} = \sqrt{\frac{k_B T}{\eta}} \) is the characteristic length scale, \( \tilde{U} \) is the characteristic velocity, \( \eta_p = \lambda_p k_B T \lambda \) is related to the polymer viscosity, \( \eta \) is the total fluid viscosity and \( \eta = \eta_s + \eta_p \). After the non-dimensionalization, the FENE potential and its gradient become

\[ \Psi(q) = -\frac{b}{2} \ln(1 - |q|^2/b), \quad \nabla_q \Psi = \frac{q}{1 - |q|^2/b}, \]

where \( b = HQ_0^2/k_B T \).

Fig. 4.7: (a)-(b): The streamlines of the lid driven cavity flow in the FENE case: with We = 0.1 (a) and We = 1 (b). (c)-(d): The profile of \( u \)-velocity on \( x = 0.5 \): We = 0.1 (c) and We = 1 (d). (e)-(f): The profile of \( v \)-velocity on \( y = 0.5 \): We = 0.1 (e) and We = 1 (f).
In numerical experiments, we use a uniform triangular mesh in $(0,1) \times (0,1)$ with $M = 5000$ and take the time step size $\Delta t = 10^{-3}$. Unlike the shear flow cases, the convection term $u \cdot \nabla q$ is non-zero, which is dealt with by a Lagrangian particle approach as introduced in Section 3. Other parameters in the numerical experiments are set as follows: $Re = 1$; $\dot{\gamma} = 0.11$; $\epsilon_p = 0.889$; $b = \sqrt{50}$. Fig. 4.7(a)-(b) show the streamlines for the lid driven cavity flow with $We = 0.1$ and $We = 1$, respectively. It is seen that the vortex shifts progressively upward as the We number increases. Figs. 4.7(c)-(d) and 4.7(e)-(f) describe the $u$-velocity profile on $x = 0.5$ and the $v$-velocity profile on $y = 0.5$ for the cavity flow with $We = 0.1$ and $We = 1$, respectively. The simulation results are consistent with those in the former work [75], which validate our numerical scheme in the 2D lid driven cavity flow case.

5. Conclusion. In this paper, we propose a deterministic particle-FEM discretization to micro-macro models of dilute polymeric fluids. The proposed scheme relies on a coupled numerical solution for the macro- and microscopic scales: a finite element method for the fluid flow equation and a variational particle scheme for the kinetic viscoelastic model. Via a discrete energy variational approach, the derived coarse-grained model of particles preserves the variational structure at the particle level. The validity of the proposed scheme has been shown through some benchmark problems in the steady flow, shear flow and 2D lid driven cavity flow. The idea can be applied to other complex fluid models, such as the Doi-Onsager model for liquid crystal polymer [19], the multi-bead spring model [76] and a two species model for wormlike micellar solution [52, 74], which involves a reaction in the microscopic equation.

Although the deterministic particle method performs well for the current model, it may not be suitable for the multi-bead spring models with a high dimensional Fokker-Planck equation. Another direction for future works is to combine the deterministic particle method with some model reduction techniques, such as the proper orthogonal decomposition (POD) and the proper generalized decomposition (PGD) [17], to reduce the degrees of freedom and therefore the computational cost.

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