A LINEARIZED, DECOUPLED AND UNCONDITIONALLY STABLE BDF2 FEM FOR THE ACTIVE FLUID MODEL

YUXING ZHANG AND BO WANG*

Abstract. In this paper, we develop a linear and decoupled fully discrete mixed finite element scheme for the active fluid model. The scheme employs an auxiliary variable to reformulate the fourth-order derivative term, an implicit-explicit treatment to deal with the nonlinear terms and the second-order pressure-projection method to split the velocity and pressure. Through rigorous theoretical analysis, the unique solvability, unconditional stability and error estimates of the numerical scheme are obtained. Then, several numerical experiments are presented to verify the efficiency and accuracy of the proposed scheme. Finally, the comparison of simulation results with laboratory results, including the motion direction of active fluid changes from disorder to order and reversal in 2D and 3D, demonstrate that the scheme can accurately capture and handle the complex dynamics of active fluid motion.

Key words. Active fluid, error estimates, auxiliary variable, BDF2, pressure-projection.

1. Introduction

The active fluid refers to a collection of particles, macro-molecules or cells that are commonly found suspended in a viscous fluid. Examples abound in the natural world, ranging from liquid-crystal-like arrangements and microbial suspensions to the coherent macro-scale dynamics exhibited by schools of fish and flocks of birds [3,7,15,17,28,42,46]. The active fluid can absorb energy from their surroundings and convert it into kinetic energy, it exhibits sought-after properties such as collective and organized motion that set it apart from classical complex fluid [25,31]. These characteristics have attracted considerable interest from researchers in the fields of materials science, biology, medicine and other related disciplines.

For investigating the collective and organized motion of active fluid, many researchers studied active fluid in the laboratory [10,14,18,23,25,34,36,38,39,45,53]. Nédélec et al. [23] studied the extend and characteristics of self-organization using microtubules and molecular motors, and obtained a variety of self-organization structures. In [38], Schaller et al. investigated the phenomenon of collective motion in highly concentrated actin filaments. The obtained results demonstrate that, beyond a critical density threshold, the actin filaments undergo self-organization, forming coherent structures characterized by persistent density modulations. Guillaume et al. reported the observation of four distinct spatial instabilities within a specific cytoskeletal active gel in [35]. Their findings reveal that these instabilities are controlled by the concentrations of Adenosine triphosphate and depletion agent. However, it is difficult to culture active fluid in the laboratory, which limits the study of active fluid.

As we all know, mathematical models can help to understand the collective and organized motion of active fluid, which can capture the dynamics of active system qualitatively or quantitatively [22, 37, 40, 41, 43, 44]. Toner et al. derived a nonequilibrium continuum dynamical model based on symmetry considerations

Received by the editors on September 28, 2023 and, accepted on September 2, 2024. 2000 Mathematics Subject Classification. 65M12, 65M15, 65M60.

^{*}Corresponding author.

to explore the dynamics of "flocking" behavior among living things in [40]. In [37], Simha and Ramaswamy constructed the equations of motion for small, long-wavelength disturbances in suspensions of self-propelled particles that exhibit polar and apolar ordering, utilizing symmetry principles and conservation laws. Based on the interaction and feedback between the swimming Bacillus subtilis and the fluid, Wolgemuth presented a two-phase model for the bacterial/fluid mixture [43]. But above-mentioned models ignore Pascal's law or the extremely effective suppression of density fluctuations by isotropic pressure, which is essential for the ordered state of active system. In addition, these models focus on the couplings with two or more order-parameters and typically involve a large number of parameters, making it is very difficult to compare with experimental data. Subsequently, Wensink et al. [44] derived an active fluid model based on the non-equilibrium free energy of active particle motion combined with general transport laws. The basic governing equations read as follows

(1a)
$$\mathbf{u}_t - \mu \Delta \mathbf{u} + \gamma \Delta^2 \mathbf{u} + \nu (\mathbf{u} \cdot \nabla) \mathbf{u} + \alpha \mathbf{u} + \beta |\mathbf{u}|^2 \mathbf{u} + \nabla p = \mathbf{f}$$
, in $\Omega \times (0, T]$,

(1b)
$$\nabla \cdot \boldsymbol{u} = 0$$
, in $\Omega \times (0, T]$,

$$(1c) \quad \boldsymbol{u}|_{t=0} = \boldsymbol{u}_0(\boldsymbol{x}), \qquad \text{in } \Omega,$$

(1d)
$$u|_{\partial\Omega} = \frac{\partial u}{\partial n}|_{\partial\Omega} = 0$$
,

where Ω is a smooth, bounded and connected domain in \mathbb{R}^d (d=2 or 3), T is the final time and \boldsymbol{n} denotes the unit outer normal vector on $\partial\Omega$. The prescribed function $\boldsymbol{u}(\boldsymbol{x},t)$, $p(\boldsymbol{x},t)$, $f(\boldsymbol{x},t)$ and $\boldsymbol{u}_0(\boldsymbol{x})$ respectively represent the velocity, pressure, external body force and initial velocity with $\nabla \cdot \boldsymbol{u}_0 = 0$. The model parameters μ , γ and ν represent the viscosity coefficient, the generic stability coefficient and the density coefficient, which are positive. The (α,β) -terms denote a quartic Landau velocity potential, where $\beta > 0$ is positive, and α is allowed to take positive or negative values. For $\alpha > 0$, the potential is mono-stable and the fluid is damped towards a disordered state with $\boldsymbol{u} = \boldsymbol{0}$. For $\alpha < 0$, equation describes a sombrero potential with fixed points $|\boldsymbol{u}| = \sqrt{|\alpha|/\beta}$ corresponding to global polar order [7,16,44]. This paper mainly focuses on the self-organization of active fluid to the global polar order state. Due to the presence of fourth-order derivative term and strong nonlinear terms in the active fluid model, analytical solution is unattainable, necessitating the use of numerical methods for solving the system.

Now, we review some works that have been done for the active fluid model (1). Dunkel et al. in [8] showed that the model effectively captures the experimental characteristics of self-sustained active turbulence, encompassing the suppression of density fluctuations and the occurrence of continuous phase transformations. James et al. [16] numerically simulated the model using pseudo-spectral codes combined with the second-order Runge-Kutta method and found a highly ordered lattice states in an extensive turbulent transient. In [29], Reinken et al. employed the pseudo-spectral method to solve the model and demonstrated how arrays of small pillars, with minimal geometrical constraints, stabilize complex vortex lattices within a turbulent bacterial suspension. It should be noted that the above research mainly focus on numerical simulations of the active fluid model and lack the numerical analysis. Motivated by this, the primary objective of this paper is to develop a highly efficient fully discrete numerical scheme for the active fluid model and conduct a numerical analysis.

To accomplish the aforementioned aim for active fluid system, several proven methods are assembled. First, an auxiliary variable $\mathbf{w} = -\Delta \mathbf{u}$ is used to transform