Numerical simulations of a minimal model for the fluid dynamics of dense bacterial suspensions

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Abstract. Collective behavior is a fascinating phenomenon and ubiquitous in nature. A large variety of complex dynamic structures from swarming to turbulence arise in active particle systems. In recent investigations a set of minimal continuum equations was proposed to model mesoscale bacterial turbulence. Numerical solutions are validated with experimental data of *Bacillus subtilis* bacteria. In this short paper we present a recently used pseudo-spectral operator splitting method that directly solves the nonlinear equations in the turbulent regime. In two and three spatial dimensions we show the resulting typical velocity and vorticity fields as well as energy spectra to highlight the strong difference between turbulence in ordinary fluids and in bacterial suspensions.

1. Introduction

Swimming bacteria, fish schools, moving algae or artificial microswimmers are intriguing examples of self-propelled particle systems. Such active particles are capable to convert ambient or stored energy into directed motion and often show coordinated collective behavior. The related phenomena range from large scale vortex structures, clustering, giant number fluctuations to mesoscale turbulence [1, 2, 3, 4]. Mesoscale turbulence was observed in dense suspensions of Bacillus subtilis and is characterized by self-sustained complex flow pattern. Recently, a phenomenological equation was proposed to model self-sustained turbulence [5]. The model combines properties from the Navier-Stokes equation with a pattern-forming instability mechanism closely related to the one in the Swift-Hohenberg equation. This instability drives the flow even when no external forces are applied. Surprisingly, this simple model could explain turbulent structures which are found in experiments of Bacillus subtilis suspensions in two and three dimensions quantitatively [3, 6]. In this article we will briefly introduce the phenomenological equation and describe in detail the numerical algorithm employed for simulations. Furthermore, we show snap-shots of two and three dimensional self-sustained turbulence and discuss the difference to turbulence of Navier-Stokes type on the basis of energy spectra.

2. Governing equations and numerical scheme

Dense bacterial suspensions of Bacillus subtilis or E-coli show an irregular flow behavior at mesoscales.

Recently, a continuum equation based on the effective velocity $\mathbf{v}$ was introduced to model the dynamics of the dense suspensions of the bacteria [5] ,i.e.,

$$(\partial_t + \lambda_0 \mathbf{v} \cdot \nabla)\mathbf{v} \quad = \quad -\nabla p + \lambda_1 \nabla v^2 - \beta(v^2 - v_0^2)\mathbf{v} + \Gamma_0 \Delta \mathbf{v} - \Gamma_2 \Delta^2 \mathbf{v} \tag{1}$$

$$\nabla \cdot \mathbf{v} = 0. \tag{2}$$

Here, $\lambda_i, \beta, \Gamma_i, v_0^2$ are phenomenological coefficients, p is the hydrodynamical pressure and Δ specifies the Laplace operator. For the parameter values $\lambda_0 = 1$, $\lambda_1 = \beta = \Gamma_2 = 0$ and $\Gamma_0 > 0$ the Navier-Stokes equation is obtained.

A similar theory for flocking of animals was introduced by Toner and Tu. The constant density limit of the Toner-Tu theory is obtained when $\Gamma_0 > 0, \Gamma_2 = 0$. However, a positive Γ_0 stabilizes a polar state and does not exhibit the characteristic vortex structures observed for swimming bacteria. When negative values are allowed the disordered state is exhibiting a Turing like irregular, turbulence like flow pattern appear in simulations even in the absence of external forces that usually causes turbulence in fluid flows. In the following we will explain how the nonlinear partial differential equaitons (1) are solved. Furthermore, we discuss some specific features of bacterial turbulence.

To solve the equations for the bulk flow, we used a pseudo-spectral algorithm with periodic boundary conditions and an operator splitting to treat the time integration of the linear part exactly. The nonlinear part is integrated by a simple Euler scheme. In particular, the algorithm consists of the following steps:

- A Fast Fourier transformation of Eq. (1); treatment of the convection term by forward and backward transformation, i.e., $F[\mathbf{v} \cdot F^{-1}[-i\mathbf{k}F[\mathbf{v}]]]$
- Application of anti-aliasing 2/3 rule to suppress oscillation effects due truncated Fourier series of nonlinear terms
- Splitting of the resulting terms into linear and nonlinear parts
- Exact integration of the linear part (see [7])
- Explicit Euler integration of the remaining equation
- Pressure correction routine to ensure incompressibility
- Inverse Fourier transform; store results

In the next section we will discuss results for simulations of the continuum equation Eq. (1) in two and three dimensions.

3. Results

For simulations, we used a grid resolution of 256×256 points in 2D and 256^3 in 3D, respectively. Initially we generated a random flow field. Eq. (1) are scaled according to Refs. [3, 6]. We used time steps of $\Delta t = 0.1$ for 2D and $\Delta t = 0.05$ for 3D. After a relaxation time of $t = 10$ time units we saved velocity fields for generating snap-shots and for calculating spectra. The final simulation time was between $t = 500$ and 2000 time units which corresponds to a maximum time of about one minute.

Fig. 1 shows representative snap-shots for simulations in two and three dimensions. In the three dimensional case the figure depicts a two dimensional slice from the middle of the simulation box. In both snap-shots the flow pattern are irregular and show vortex structures. Remarkably, the flow is different from that found for inertial turbulence described by the Navier-Stokes equation. The reason is the emergence of vortices of a typical size in contrast to decaying vortices that occur for inertial turbulence found in the classical Navier-Stokes equation.

The key is that the typical vortex size in bacterial turbulence introduces a characteristic length scale into the system. In contrast simple fluids without boundaries are scale invariant. The energy spectra of the two dimensional bacterial turbulence pattern for different values of the parameter λ_0 are shown in Fig.2 (calculated according to [5]). For large values of λ_0 changes of the energy spectra are small.

The spectra of bacterial turbulence differs qualitatively from that obtained for inertial turbulence (see Fig. 2b) for a sketch). Two dimensional initial turbulence is characterized by an upper energy and a lower enstrophy cascade. For bacterial turbulence, the energy injection happens at small scales by the individual swimmer; followed by an upward cascade up to a specific maximum. From the maximum to larger scales we observe a downward cascade. It is the maximum in the energy spectrum that corresponds

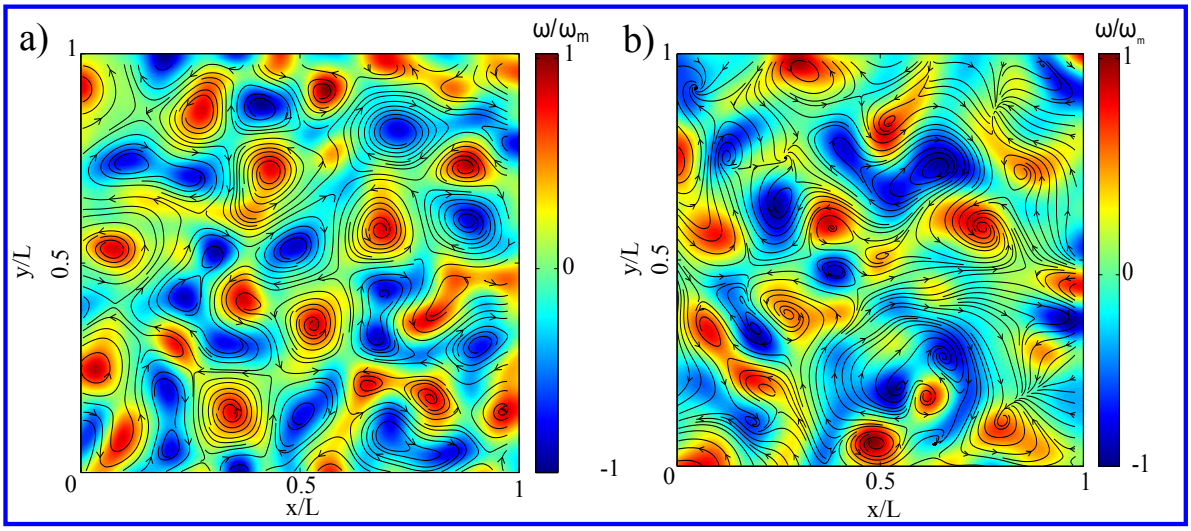

Figure 1. Snapshots of bacterial turbulent states. The color bar encodes vorticity strength and the box length corresponds to $200\mu m$ and $300\mu m$ for 2D and 3D, respectively. a) Two dimensional simulations at parameter values $\Gamma_0 = -1, \Gamma_2 = 1\lambda_0 = 5, \lambda_1 = 2, L = 48 * \pi, \beta = 1, v_0^2 = 0.2$. b) Two dimensional slice of three dimensional simulations. The used parameter values are $\Gamma_0 = -0.9, \Gamma_2 = 0.9\lambda_0 = 1.7, \lambda_1 = 0.35, L = 24 * \pi, \beta = 0.1, v_0^2 = 0.1$.

to the typical length scales of vortices. The typical length scale is encoded in the phenomenological parameters Γ_0 and Γ_2, i.e.,

$$\Lambda = 2\pi\sqrt{\Gamma_2/(-\Gamma_0)}. \tag{3}$$

Typically values for Bacillus subtillis suspensions are $30\mu m$ to $50\mu m$. Unfortunately, there is still no microscopic derivation of the phenomenological equations and the microscopic meaning of the length scale as well as the mechanism that selects the scale remains unknown.

For the three-dimensional case, calculations are challenging and we have simulated the flow pattern, but not yet spectra. The stream lines of the two-dimensional slice of a three-dimensional flow Fig. 1b) show spirals rather than vortices. Here, bacteria are swimming in cycles with a velocity component orthogonal to the plane. The resulting collective motion looks like a twister. Fig. 3b, c) show a three dimensional plot of that flow structure. Fig. 3b) shows a cut perpendicular to a twister and Fig. 3c) the overall shape. In the turbulence regime such twister like structures spontaneously emerge and disappear all the time. The overall flow structure in the simulation box shows isotropic turbulence seen in the iso-energy surface plot in Fig. 3a).

In this article, we introduced phenomenological equations to model the collective flow of active particle suspensions. We presented the numerical scheme and discussed results from two and three dimensional simulation of the bulk flow. Bacterial turbulence is different from inertial turbulence of the Navier-Stokes type due to a typical vortex length. A fingerprint of that vortex size can be found in energy spectra which is also different from inertial turbulence. Finally, we discussed a new type of flow structure that we have found in three dimensional bacterial turbulence; collective twister motion.

In further work we plan to investigate the influence of confinement to the turbulent flow structures. There is experimental evidence that in the presence of boundaries turbulent structures are suppressed in favor to a single vortex [9]. Furthermore, we plan to study rheological properties of the continuum model and compare it to more complex descriptions where higher order parameters are included [8].

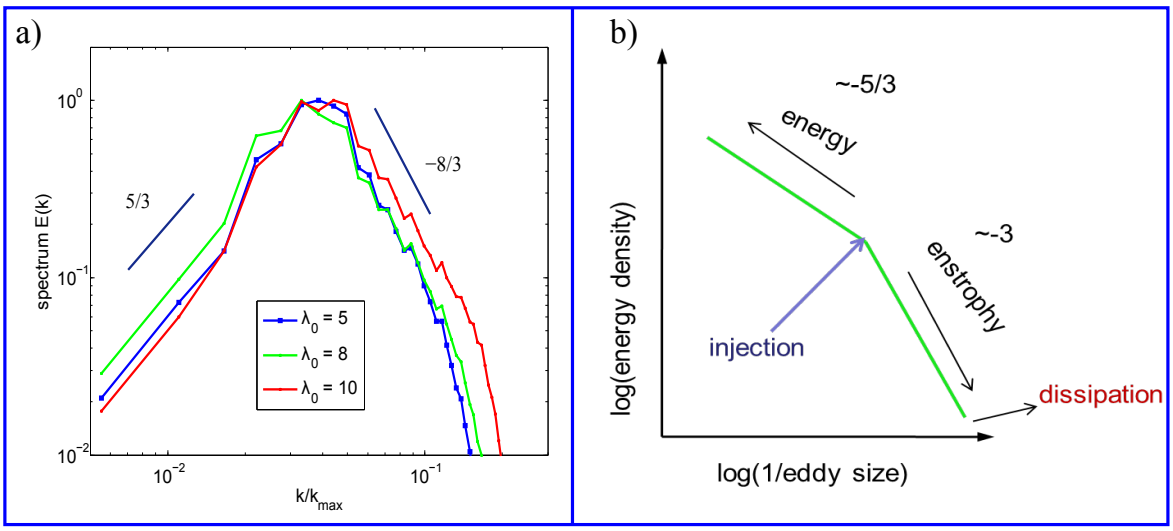

Figure 2. a) Energy spectra of two dimensional bacterial turbulence simulations for different parameter values λ_0. The remaining parameters are the same as in Fig. 1. Energy is injected at the length scale of microswimmer (k_{max}) b) Sketch of a spectrum of inertial turbulence.

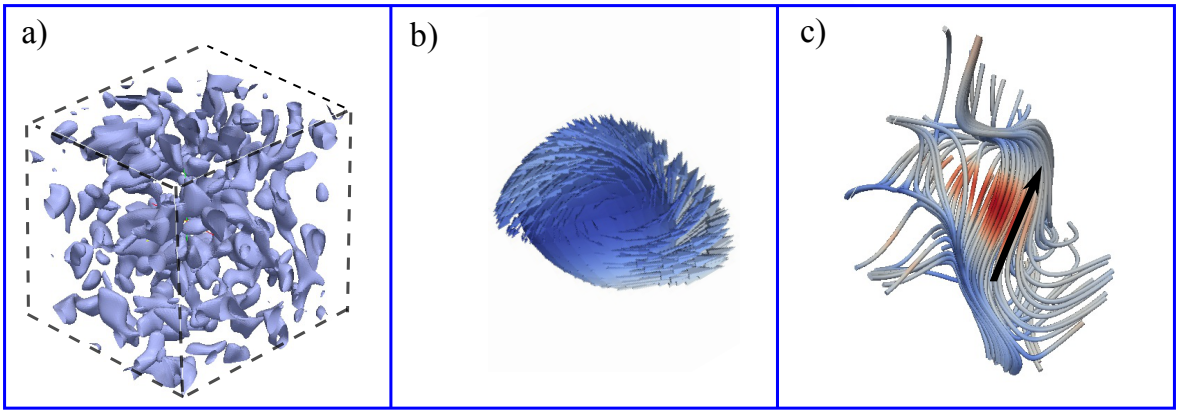

Figure 3. Illustration of three dimensional mesoscale turbulence using Paraview. Parameter values are the same as in Fig. 1. a) Iso-energy surface plot. b) Velocity field of a three dimensional vortex. c) Tube graph of velocity stream lines. The twister like structure shows complex 3D collective bacterial motion.

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References

[1] Sumino Y, Nagai K H, Shitaka Y, Tanaka D, Yoshikawa K, Chaté H and Oiwa K 2012 *Nature* **483** 448
[2] Schaller V, Weber C, Semmrich C, Frey E, Bausch A R 2010 *Nature* **467** 73
[3] Wensink H H, Dunkel J, Heidenreich S, Drescher K, Goldstein R E, Löwen H and Yeomans J M 2012 *Proc. Nat. Acad. Sci. USA* **109** 14308
[4] Peruani F, Starruß J, Jakovljevic V, Sogaard-Anderson L, Deutsch A, and Bär M 2012 *Phys. Rev. Lett.* **108** 098102

[5] Dunkel J, Heidenreich S, Bär M and Goldstein R E 2013 *New J. Phys.* **15** 045016
[6] Dunkel J, Heidenreich S, Drescher K, Wensink H H, Bär M and Goldstein R E 2013 *Phys. Rev. Lett.* **110** 228102
[7] Pedrosa J, Hoyuelos M, and Martel C, *Eur. Phys. J. B* **66** 525
[8] Heidenreich S , Hess S, Klapp S H L 2011 *Phys. Rev. E* **83** 011907
[9] Wioland H, Woodhouse F G, J. Dunkel J, Kessler J O, Goldstein R E 2013 *Phys. Rev. Lett.* **110** 268102