Spectral Methods for Jeffrey Orbits v3.0

Fabian Hillebrand

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Abstract

We present a Galerkin spectral method to solve the Fokker-Planck equation for Jeffrey orbits. The fluid is assumed to be dilute, but can be either monodisperse or polydisperse. The method allows for simple shear and/or planar extensional flow in the same xz-plane. We use the prior results for simple shear and provide the necessary integral values for planar extensional flow.

1 Governing Equations

The governing equation of the orientation distribution ψ is given by the Fokker-Planck equation:

$$\frac{\partial \psi}{\partial t} = \vec{\nabla} \cdot \left(\mathbf{D_r} \vec{\nabla} \psi - \dot{\mathbf{\Omega}} \psi \right), \tag{1}$$

which we simplify by assuming a homogeneous rotational diffusion coefficient D_r and for a dilute system we take as a constant. Under these assumptions, Eq. (1) simplifies to

$$\frac{\partial \psi}{\partial t} = D_r \nabla^2 \psi - \vec{\nabla} \cdot \left(\dot{\mathbf{\Omega}} \psi \right). \tag{2}$$

The above equations hold for both monodisperse system with orientation distribution $\psi(\chi, \theta \,|\, l)$ and polydisperse system with orientation distribution $\psi(\chi, \theta, l) = \psi(\chi, \theta \,|\, l) f(l)$, where l is the rod length and $f(l)$ the appropriate distribution for polydispersity. In general, it is not clear which distribution is appropriate for polydispersity and instead depends on the measurement.

Under the assumption of a dilute system, we can separate the polydisperse system and solve separately Eq. (2) with $D_r(l)$ for each rod length l. The full orientation distribution is obtained using the definition of conditional probability distributions.

In the equations above, $\dot{\mathbf{\Omega}} = [\dot{\chi}\sin\theta, \dot{\theta}]^{\mathsf{T}}$ captures the force imposed on the flow. Its value connects to the evolution equation of the rod orientation $\mathbf{q}$

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathbf{W}\mathbf{q} + \beta\left(\mathbf{E}\mathbf{q} - (\mathbf{q}\cdot\mathbf{E}\mathbf{q})\,\mathbf{q}\right) \tag{3}$$

where $\mathbf{q} = [\sin(\theta)\cos(\chi), \sin(\theta)\sin(\chi), \cos(\theta)]^{\mathsf{T}}$, β is the Bretherton parameter, $\mathbf{W}$ is the skew-symmetric component and $\mathbf{E}$ the symmetric component of the flow velocity gradient $\vec{\nabla}\mathbf{u}$. Here, we assume that the flow only includes shear with shear rate $\dot{\gamma}$ and planar extension with extension rate $\dot{\varepsilon}$, both within the xz-plane.

$$\dot{\mathbf{\Omega}} = \dot{\gamma}\begin{bmatrix} -\frac{1+\beta}{2}\cos(\theta)\sin(\chi) \\ \frac{1}{2}\cos(\chi) + \frac{\beta}{2}\cos(2\theta)\cos(\chi) \end{bmatrix} + \dot{\varepsilon}\begin{bmatrix} -\beta\cos(\chi)\sin(\chi)\sin(\theta) \\ \frac{\beta}{4}(3+\cos(2\chi))\sin(2\theta) \end{bmatrix}. \tag{4}$$

When the forcing is zero, we recognize that Eq. (2) is the Laplace equation on the sphere and solved exactly by the real spherical harmonics $Y_{\ell,m}$. Our goal is to expand the orientation distribution ψ in terms of the real spherical harmonics $Y_{\ell,m}$ and unknown coefficients $b_{\ell,m}$. As pointed out by Talbot *et al.* [1], symmetries in the problem for shear lead to no contributions from odd ℓ and negative m. We will see that this also applies to planar extensional flows. The expansion is given by

$$\psi(\chi, \theta \,|\, l) = \sum_{\ell\in 2\mathbb{N}_0}\sum_{m=0}^{\ell} b_{\ell,m} Y_{\ell,m}(\chi, \theta), \tag{5}$$

where we drop for ease-of-reading the dependency of rod lengths l and time t on the coefficients $b_{\ell,m}$. Due to numerical limitations, we must choose a maximum $\ell_{\max}$ which corresponds to the numerical discretization.

At this point, we can make a number of observations. First, the real spherical harmonics are orthonormal, which will make many calculations much simpler. Second, under flow cessation Eq. (2) simplifies to a decoupled set of ordinary differential equations because the real spherical harmonics are the eigenfunctions of the Laplace operator with eigenvalue $-\ell(\ell+1)$. Thus, each coefficient decays exponentially with rate $\ell(\ell+1)D_r$. The slowest decaying mode is $6D_r$ and corresponds to $\ell = 2$. Third, we note that $\ell = 0$ does not decay and instead accounts for the normalization. Its value is $b_{0,0} = 1/\sqrt{4\pi}$, where we use the orthonormality of the real spherical harmonics.

Next, we briefly mention quantities of interest. The most common value is the second moment of orientation:

$$\mathbf{Q} = \left\langle \mathbf{q} \otimes \mathbf{q} - \frac{1}{3}\mathbf{I} \right\rangle . \tag{6}$$

The pre-averaged term can be expressed in real spherical harmonics, making the evaluation trivial. We obtain:

$$\mathbf{Q} = \sqrt{\frac{4\pi}{15}} \int_0^\infty \begin{bmatrix} \left(b_{2,2} - \frac{1}{\sqrt{3}} b_{2,0}\right) & 0 & -b_{2,1} \\ 0 & -\left(b_{2,2} + \frac{1}{\sqrt{3}} b_{2,0}\right) & 0 \\ -b_{2,1} & 0 & \frac{2}{\sqrt{3}} b_{2,0} \end{bmatrix} \mathrm{d}l. \tag{7}$$

This is used for the order parameter $S = \sqrt{\langle q_x^2 - q_z^2 \rangle^2 - \langle 2 q_x q_z \rangle^2}$ and extinction angle $\tan(2\chi_e) = \langle 2 q_x q_z \rangle / \langle q_x^2 - q_z^2 \rangle$. Clearly, the order parameter decays with rate $6D_r$ for any monodisperse system, while in a polydisperse system the different $D_r(l)$ values lead to a non-exponential decay.

Another common quantity appears to be the fourth moment of orientation. This will also couple $b_{4,m}$ coefficients but is not discussed further here at this moment.

2 Galerkin Spectral Method

The Galerkin spectral method uses the expansion (5) in Eq. (2) followed by integrating with test functions $Y_{\ell',m'}$. It is now useful to introduce a new notation, following Doi and Edwards [2], where $Y_{\ell,m}$ is written as $|\ell, m)$ and integration as $(\ell', m'|\hat{A}|\ell, m)$ with operator $\hat{A}$ acting on $|\ell, m)$. This follows the standard notation in quantum mechanics, where we will make use of the complex spherical harmonics Y_ℓ^m, typically written as $|\ell, m\rangle$, and results involving them. The complex and real spherical harmonics are related:

$$|\ell, m) = \begin{cases} \frac{\mathrm{i}}{\sqrt{2}}(|\ell, m\rangle - (-1)^m |\ell, -m\rangle) & m < 0 \\ |\ell, 0\rangle & m = 0 \\ \frac{1}{\sqrt{2}}(|\ell, -m\rangle + (-1)^m |\ell, m\rangle) & m > 0 \end{cases} . \tag{8}$$

To make full use of our new notation, we rewrite $\vec{\nabla}\cdot(\dot{\mathbf{\Omega}}\psi)$ in terms of a shear operator $\hat{\Gamma}$ and a planar extension operator $\hat{\Omega}$. To this end, we use the angular momentum operators $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ and spherical harmonics Y_ℓ^m. The angular momentum operators are explicitly given by

$$\begin{aligned}
\mathrm{i}\hat{L}_x &= -\sin\chi\frac{\partial}{\partial\theta} - \cot(\theta)\cos(\chi)\frac{\partial}{\partial\chi},\\
\mathrm{i}\hat{L}_y &= \cos\chi\frac{\partial}{\partial\theta} - \cot(\theta)\sin(\chi)\frac{\partial}{\partial\chi},\\
\mathrm{i}\hat{L}_z &= \frac{\partial}{\partial\chi},
\end{aligned}$$

and have well known effects when acting on $|\ell,m\rangle$:

$$\hat{L}_z|\ell,m\rangle = m|\ell,m\rangle, \tag{9}$$

$$\hat{L}^2|\ell,m\rangle = \ell(\ell+1)|\ell,m\rangle, \tag{10}$$

$$\hat{L}_+|\ell,m\rangle = \sqrt{(\ell-m)(\ell+m+1)}|\ell,m+1\rangle, \tag{11}$$

$$\hat{L}_-|\ell,m\rangle = \sqrt{(\ell+m)(\ell-m+1)}|\ell,m-1\rangle, \tag{12}$$

with ladder operators $\hat{L}_+ = \hat{L}_x + \mathrm{i}\hat{L}_y$ and $\hat{L}_- = \hat{L}_x - \mathrm{i}\hat{L}_y$, and $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$. The shear operator is given by Doi and Edwards [2][1]:

$$\hat{\Gamma} = \left(\sqrt{\frac{16\pi}{45}}Y_2^0 + \frac{1}{3}\right)\mathrm{i}\hat{L}_y + \sqrt{\frac{2\pi}{15}}\left(Y_2^1 + Y_2^{-1}\right)\hat{L}_z + 3\sqrt{\frac{2\pi}{15}}\left(Y_2^1 - Y_2^{-1}\right), \tag{13}$$

and for $\beta \neq 1$ by Talbot *et al.* [1] as $\beta\hat{\Gamma} + \frac{1-\beta}{2}\mathrm{i}\hat{L}_y$. With some simple manipulations, we obtain a similar result for the planar extension part:

$$\begin{aligned}
\hat{\Omega} = 2\sqrt{\frac{\pi}{15}}\Bigg(&3\left(\sqrt{3}Y_2^0 - \frac{1}{\sqrt{2}}\left(Y_2^{-2} + Y_2^2\right)\right) + \frac{1}{\sqrt{2}}\left(Y_2^{-2} - Y_2^2\right)\hat{L}_z\\
&+ \frac{2}{\sqrt{2}}\left(Y_2^{-1} - Y_2^1\right)\mathrm{i}\hat{L}_y + \frac{1}{\sqrt{2}}\left(Y_2^{-1} + Y_2^1\right)\hat{L}_x\Bigg).
\end{aligned} \tag{14}$$

Alternatively, we can write both operators using real spherical harmonics to be more compact:

$$\hat{\Gamma} = 2\sqrt{\frac{\pi}{15}}\left(-3\sqrt{3}Y_{2,1} - Y_{2,-1}\mathrm{i}\hat{L}_z + \left(\sqrt{\frac{4}{3}}Y_{2,0} + \sqrt{\frac{5}{12\pi}}\right)\mathrm{i}\hat{L}_y\right),$$

[1] Following the notation of Talbot *et al.* [1].

$$\hat{\Omega} = 2\sqrt{\frac{\pi}{15}}\left(3\left(\sqrt{3}Y_{2,0} - Y_{2,2}\right) - Y_{2,-2}\mathrm{i}\hat{L}_z + 2Y_{2,1}\mathrm{i}\hat{L}_y - Y_{2,-1}\mathrm{i}\hat{L}_x\right).$$

Finally, we rewrite Eq. (2) in terms of these operators:

$$\frac{\partial \psi}{\partial t} = -D_r \hat{L}^2 \psi - \left(\dot{\gamma}\left(\beta\hat{\Gamma} + \frac{1-\beta}{2}\mathrm{i}\hat{L}_y\right) + \dot{\varepsilon}\beta\hat{\Omega}\right)\psi. \tag{15}$$

For the spectral method, we apply the Galerkin procedure to Eq. (15) to obtain a linear system of equations:

$$\begin{aligned} \delta_{\ell',\ell}\delta_{m',m}\frac{\mathrm{d}b_{\ell,m}}{\mathrm{d}t} =& -\ell(\ell+1)D_r\delta_{\ell',\ell}\delta_{m',m}b_{\ell,m} \\ &-\left(\ell',m'\middle|\dot{\gamma}\left(\beta\hat{\Gamma} + \frac{1-\beta}{2}\mathrm{i}\hat{L}_y\right) + \dot{\varepsilon}\hat{\Omega}\middle|\ell,m\right)b_{\ell,m}, \end{aligned} \tag{16}$$

or, vectorized,

$$\frac{\mathrm{d}\mathbf{b}}{\mathrm{d}t} = -D_r\mathbf{L^2}\mathbf{b} - \dot{\gamma}\beta\mathbf{\Gamma}\mathbf{b} - \dot{\gamma}\frac{1-\beta}{2}\mathbf{L_y} - \dot{\varepsilon}\beta\mathbf{\Omega}\mathbf{b}, \tag{17}$$

where $\mathbf{b} := b_{\ell,m}$, $\mathbf{L^2} := \mathrm{diag}[\ell(\ell+1)]$, $\mathbf{\Gamma} := (\ell', m'|\hat{\Gamma}|\ell, m)$, $\mathbf{L_y} := (\ell', m'|\mathrm{i}\hat{L}_y|\ell, m)$, and $\mathbf{\Omega} := (\ell', m'|\hat{\Omega}|\ell, m)$. To solve the integrals, we can make use of Eqs. (8), (9)-(12) and the Wigner's 3-j symbols:

$$\langle \ell', m'|Y_p^q|\ell, m\rangle = (-1)^m\sqrt{\frac{(2\ell+1)(2\ell'+1)(2p+1)}{4\pi}}\begin{pmatrix}\ell' & p & \ell \\ -m' & q & m\end{pmatrix}\begin{pmatrix}\ell' & p & \ell \\ 0 & 0 & 0\end{pmatrix}.$$

A number of observations are in order. Wigner's 3-j symbols are zero unless $|\ell' - p| \le \ell \le \ell' + p$. Moreover, they are zero unless the sum $\ell' + p + \ell$ is even, due to the second 3-j symbol. Therefore, with $p = 2$ throughout, we immediately see that only terms $\ell' \in \{\ell - 2, \ell, \ell + 2\}$ are non-zero. The system thus decouples into two subsystems with even and odd ℓ, which for odd ℓ leads to the trivial solution. As expected from the symmetry, we indeed only need to consider even ℓ. Wigner's 3-j symbols are also zero unless $-m' + q + m = 0$. This implies for shear only $m' = \pm m$ and for planar extension only $m' \in \{m - 2, m, m + 2\}$ result in non-zero integrals. For pure planar extensional flow, the system decouples into even and odd m, with trivial solution for odd m. Therefore, for pure planar extensional flow, all $b_{\ell,m}$ with odd m are zero, simplifying some quantities of interest. This does not apply to mixed flows.

The integrals for shear can be found in [2] or [1] (the latter with a typo). We similarly define the function $g_0 = \sqrt{2}$ and otherwise $g_m = 1$. Considering only $\ell \in 2\mathbb{N}_0$ and $0 \le m \le \ell$, we find for planar extensional flow:

$$(\ell, m|\hat{\Omega}|\ell, m) = F_0(\ell, m), \tag{18}$$
$$(\ell, m|\hat{\Omega}|\ell, m+2) = g_m F_1(\ell, m), \tag{19}$$
$$(\ell, m+2|\hat{\Omega}|\ell, m) = g_m F_1(\ell, m), \tag{20}$$
$$(\ell, m|\hat{\Omega}|\ell+2, m) = -F_2(\ell, m), \tag{21}$$
$$(\ell+2, m|\hat{\Omega}|\ell, m) = F_3(\ell, m), \tag{22}$$
$$(\ell, m|\hat{\Omega}|\ell+2, m+2) = g_m F_4(\ell, m), \tag{23}$$
$$(\ell, m+2|\hat{\Omega}|\ell+2, m) = g_m F_4(\ell, -m-2), \tag{24}$$
$$(\ell+2, m+2|\hat{\Omega}|\ell, m) = -g_m F_5(\ell, m), \tag{25}$$
$$(\ell+2, m|\hat{\Omega}|\ell, m+2) = -g_m F_5(\ell, -m-2), \tag{26}$$

where

$$F_0(\ell, m) = \begin{cases} \frac{3}{4}\frac{(\ell+\ell^2-6)}{(2\ell-1)(2\ell+3)} & m=1 \\ \frac{3}{2}\frac{(\ell+\ell^2-3m^2)}{(2\ell-1)(2\ell+3)} & \text{else} \end{cases},$$

$$F_1(\ell, m) = \frac{3}{4(2\ell-1)(2\ell+3)}\sqrt{(\ell-1-m)(\ell-m)(\ell+1+m)(\ell+2+m)},$$

$$F_2(\ell, m) = \begin{cases} \frac{7\ell}{4(2\ell+3)}\sqrt{\frac{\ell(\ell+1)(\ell+2)(\ell+3)}{(2\ell+1)(2\ell+5)}} & m=1 \\ \frac{3\ell}{2(2\ell+3)}\sqrt{\frac{(\ell+1-m)(\ell+2-m)(\ell+1+m)(\ell+2+m)}{(2\ell+1)(2\ell+5)}} & \text{else} \end{cases},$$

$$F_3(\ell, m) = \begin{cases} \frac{7(\ell+3)}{4(2\ell+3)}\sqrt{\frac{\ell(\ell+1)(\ell+2)(\ell+3)}{(2\ell+1)(2\ell+5)}} & m=1 \\ \frac{3(\ell+3)}{2(2\ell+3)}\sqrt{\frac{(\ell+1-m)(\ell+2-m)(\ell+1+m)(\ell+2+m)}{(2\ell+1)(2\ell+5)}} & \text{else} \end{cases},$$

$$F_4(\ell, m) = \frac{\ell}{4(2\ell+3)}\sqrt{\frac{(\ell+1+m)(\ell+2+m)(\ell+3+m)(\ell+4+m)}{(2\ell+1)(2\ell+5)}},$$

$$F_5(\ell, m) = \frac{\ell+3}{4(2\ell+3)}\sqrt{\frac{(\ell+1+m)(\ell+2+m)(\ell+3+m)(\ell+4+m)}{(2\ell+1)(2\ell+5)}}.$$

3 Code Details

3.1 Version History Overview

3.1.1 v1.0 Shear flow: Basic functionality based on literature results

The initial version provides a spectral solver for simple shear flow based on the works of Doi and Edwards [2] and Talbot *et al.* [1]. The system contains two non-dimensional control parameters in form of the Péclet number $Pe := \frac{\dot{\gamma}}{D_r}$ and the Bretherton parameter $\beta := \frac{r_p-1}{r_p+1}$ based on the aspect ratio $r_p = \frac{l}{d}$. Internally, the steady state is solved in non-dimensional form while it is easier to solve the unsteady state in dimensional form. In addition to monodisperse systems, the solver also allows for polydisperse systems. Here, the polydispersity in length typically results in varying D_r, i.e. several local Pe_{loc} and potentially varying β values. The code uses a simple trapezoidal rule to integrate the provided polydispersity distribution. A rule of thumb is used to adjust `Lmax` if set to zero.

3.1.2 v2.0 Planar extensional flow: Newly evaluated operator and integrals for planar extensional flow

Version 2.0 adds the option for planar extensional flow in the same plane as the shear flow. The flow types can be combined. The operator and integrals were evaluated as described above. The planar extensional flow introduces a third non-dimensional control parameter with an additional Péclet number $Pe_{\text{ex}} := \frac{\dot{\epsilon}}{D_r}$ to the shear Péclet number $Pe_{\text{sh}} = \frac{\dot{\gamma}}{D_r}$. I acknowledge that a more suitable definition would include a factor 2, such that both shear and planar extension coincide at low Pe, which a future version may correct or remove entirely, leaving only dimensional solvers. Note that planar extensional flow requires greater values for `Lmax` to achieve accurate results. As such, only smaller values for Pe_{ex} compared to Pe_{sh} can be achieved. The additional symmetry in pure planar extensional flows is not exploited.

3.1.3 v3.0 Efficiency improvements: Pre-compute matrices

Starting with version 3.0, the matrices discussed above are pre-computed making use of their independence on physical parameters. This is augmented with an adaptive method, which uses sub-blocks of the large pre-computed matrices to estimate the error and provide additional efficiency. Note that the error is estimated only based on $b_{2,m}$ and compares a size $L_{\max,i}$ with $L_{\max,i}/2$. In the adaptive case, the Lmax argument specifies the maximal size of the numerical discretization. An warning is shown if this size cannot achieve the specified threshold threshold. Larger Lmax will lead to slower simulations but provide greater accuracy. I do not recommend setting a value larger than Lmax > 2048, because the system size scales $N = \mathcal{O}(L_{\max}^2)$.

References

[1] Julian Talbot, Charles Antoine, Philippe Claudin, Ellák Somfai, and Tamás Börzsönyi. Exploring noisy jeffery orbits: A combined fokker-planck and langevin analysis in two and three dimensions. *Phys. Rev. E*, 110:044143, 2024.

[2] Masao Doi and Samuel F. Edwards. Dynamics of rod-like macromolecules in concentrated solution. Part 2. *J. Chem. Soc., Faraday Trans. 2*, 74:918–932, 1978.