Spectral Methods for Jeffrey Orbits v2.0

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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,

$$\frac{\mathrm{d}\mathbf{b}}{\mathrm{d}t} = D_r\mathbf{\Lambda}\mathbf{b} - \dot{\gamma}\mathbf{\Gamma}\mathbf{b} - \dot{\varepsilon}\mathbf{\Omega}\mathbf{b}, \tag{17}$$

where $\mathbf{b} := b_{\ell,m}$, $\mathbf{\Lambda} := \mathrm{diag}[-\ell(\ell+1)]$, $\mathbf{\Gamma} := (\ell', m'|\beta\hat{\Gamma} + \frac{1-\beta}{2}\mathrm{i}\hat{L}_y|\ell, m)$, 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 $0 \leq m \leq \ell$, 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

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

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

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

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

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

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

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.