1. Differential equations on the unit sphere

The objective of the software is to provide a systematic spherical harmonic method to numerically solve partial differential equations on the two dimensional sphere, $S = \{\mathbf{r} = (x, y, z) : |\mathbf{r}| = x^2 + y^2 + z^2 = 1\}$, or in spherical coordinates, $\mathbf{r} = (x, y, z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, where $0 \le \theta \le \pi$, $0 \le \phi \le 2\pi$. The partial differential equations considered here are of the form

$$\frac{\partial}{\partial t}\psi = F(\mathbf{r}, \boldsymbol{\nabla})\psi, \tag{1}$$

where ψ is a function (for example, the probability distribution function) defined on the sphere. Here $\boldsymbol{\nabla}$ is the gradient operator restricted to the sphere that is defined as

$$\begin{aligned}\boldsymbol{\nabla} &= (\nabla_x, \nabla_y, \nabla_z)\\ &= \left(\cos\theta\cos\phi\frac{\partial}{\partial\theta} - \csc\theta\sin\phi\frac{\partial}{\partial\phi}, \cos\theta\sin\phi\frac{\partial}{\partial\theta} + \csc\theta\cos\phi\frac{\partial}{\partial\phi}, -\sin\theta\frac{\partial}{\partial\theta}\right)\\ &= \left((1-x^2)\frac{\partial}{\partial x} - xy\frac{\partial}{\partial y} - xz\frac{\partial}{\partial z}, -xy\frac{\partial}{\partial x} + (1-y^2)\frac{\partial}{\partial y} - yz\frac{\partial}{\partial z},\right.\\ &\qquad \left. -xz\frac{\partial}{\partial x} - yz\frac{\partial}{\partial y} + (1-z^2)\frac{\partial}{\partial z}\right).\end{aligned} \tag{2}$$

In the above, F is a polynomial in six variables, with the proviso that it matters in which order the terms of each monomial part are written. We believe that this includes many of the published, if not all, of the partial differential equations that describe the evolution of the orientation distribution function for short fiber suspensions.

The spherical harmonic approach converts equation (1) to a system of ordinary differential equations written as

$$\frac{\partial}{\partial t}\hat{\psi}_l^m = \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} c_{l,l'}^{m,m'}\hat{\psi}_{l'}^{m'}, \tag{3}$$

where $\hat{\psi}_l^m$ ($l \ge 0$, $|m| \le l$) are the spherical harmonic coefficients of ψ, defined in equation (14) below, and $c_{l,l'}^{m,m'}$ are the coefficients defined through equation (19).

The software provides a systematic algorithm for calculating the coefficients $c_{l,l'}^{m,m'}$ appearing in equation (3) (and also in equation (19) below). This algorithm makes it possible to readily solve all differential equations on the unit sphere of the form shown in equation (1).

2. Description of the model equations

To illustrate the software, we consider variations of Jeffery's equation [4] which describes the motion of fibers in a moving fluid with vorticity $\mathbf{w}$ and rate of deformation tensor Γ. Jeffery's equation is often written in terms of the fiber orientation distribution function ψ and the fiber aspect ratio parameter $-1 \le \lambda \le 1$ as

$$\frac{\partial}{\partial t}\psi = J\psi := -\tfrac{1}{2}\boldsymbol{\nabla}\cdot(\mathbf{w}\times\mathbf{r}\psi + \lambda(\Gamma\cdot\mathbf{r} - \Gamma : \mathbf{rrr})\psi), \tag{4}$$

where we note that the right hand side is in the form of equation (1). A variation of equation (4) is Jeffery's equation with rotary diffusion as expressed by Bird [1] as

$$\frac{\partial}{\partial t}\psi = J\psi + \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}(D_r\psi), \tag{5}$$

where D_r captures the effect of fiber interaction and depends upon the flow kinetics. Folgar and Tucker [2] selected $D_r = C_I\dot{\gamma}$ where $\dot{\gamma} = \left(\frac{1}{2}\Gamma : \Gamma\right)^{1/2}$ and C_I is a constant that depends upon the volume fraction and aspect ratio of the fibers.

Another example is anisotropic diffusion such as that proposed by Koch [5] in the differential equation

$$\frac{\partial}{\partial t}\psi = J\psi + \boldsymbol{\nabla}\cdot(I - \mathbf{rr})\cdot D_r\cdot\boldsymbol{\nabla}\psi = J\psi + (\boldsymbol{\nabla} - 2\mathbf{r})\cdot D_r\cdot\boldsymbol{\nabla}\psi \tag{6}$$

where the anisotropic diffusion matrix D_r is defined in terms of the model parameters C_1 and C_2 (see Koch [5] for more detail) as

$$D_r = C_1\dot{\gamma}^{-1}(\Gamma : \mathbb{A} : \Gamma)I + C_2\dot{\gamma}^{-1}\Gamma : \mathcal{A} : \Gamma. \tag{7}$$

In the above, the $(I - \mathbf{rr})$ term serves to project vectors onto the surface of the sphere. We note that this term is not explicitly included in Koch's formula in [5], however it's existence is implied in the paragraph following the original introduction.

The anisotropic diffusion matrix D_r defined in equation (7) is written in terms of the 2nd, 4th and 6th order moment tensors of ψ which are, respectively, defined as

$$A := \int_S \psi\mathbf{rr}\,d\mathbf{r}, \qquad \mathbb{A} := \int_S \psi\mathbf{rrrr}\,d\mathbf{r}, \qquad \text{and} \qquad \mathcal{A} := \int_S \psi\mathbf{rrrrrr}\,d\mathbf{r}. \tag{8}$$

In these integrals, we adopt the common definition for the integral of a function $F(\mathbf{r})$ over the surface of the unit sphere as

$$\int_S F(\mathbf{r})\,dr := \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} F(\mathbf{r})\sin\theta\,d\phi\,d\theta, \tag{9}$$

and we note here that the moment tensors A, $\mathbb{A}$, and $\mathcal{A}$ can be expressed in terms of spherical harmonics as shown below in equation (22).

Care must be exercised in not confusing the differential geometry on the surface of the sphere S with the differential geometry in the three dimensional space $\mathbb{R}^3$ it is embedded in. Thus, for example, integration by parts is the slightly unexpected form

$$\int_S \mathbf{f}\cdot\boldsymbol{\nabla}g\,d\mathbf{r} = -\int_S(\boldsymbol{\nabla}\cdot(I - \mathbf{rr})\cdot\mathbf{f})g\,d\mathbf{r} = \int_S((2\mathbf{r} - \boldsymbol{\nabla})\cdot\mathbf{f})g\,d\mathbf{r}, \tag{10}$$

which reduces to the usual integration by parts when $\mathbf{f}$ is tangential to the surface of the sphere. We also recall the so called angular momentum operator

$$\mathbf{L} = -i\mathbf{r}\times\boldsymbol{\nabla} = (L_x, L_y, L_z) = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}, z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}, x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right), \tag{11}$$

where, as usual, i denotes the complex number satisfying $i^2 = -1$. Integration by parts for the angular momentum operator is more straightforward, that is,

$$\int_S \mathbf{f}\cdot\mathbf{L}g\,d\mathbf{r} = -\int_S(\mathbf{L}\cdot\mathbf{f})g\,d\mathbf{r}. \tag{12}$$

Note that $\mathbf{L}\times\mathbf{L} = \boldsymbol{\nabla}\times\boldsymbol{\nabla} = i\mathbf{L}$, and in particular ∇_x, ∇_y and ∇_z do not commute with each other. We also use the formulae $\mathbf{r}\cdot\boldsymbol{\nabla} f = \mathbf{r}\cdot\mathbf{L} f = \mathbf{L}\cdot(\mathbf{r}f) = 0$ and $\boldsymbol{\nabla}\cdot(\mathbf{r}f) = 2f$.

3. Spherical harmonics solutions

Any square integrable function ψ defined on the unit sphere may be written as a Fourier series like representation in terms of the spherical harmonics $Y_l^m(\theta,\phi)$ for $l \geq 0$ and $|m| \leq l$ as

$$\psi = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \hat{\psi}_l^m Y_l^m, \tag{13}$$

where Y_l^m are the spherical harmonic functions as defined in [6]. The coefficients $\hat{\psi}_l^m$ in equation (13) are evaluated from

$$\hat{\psi}_l^m = \int_S \psi \bar{Y}_l^m d\mathbf{r}. \tag{14}$$

To obtain the system of ordinary differential equations (3), we integrate equation (1) against $\bar{Y}_l^m$ over the unit sphere to obtain its adjoint or weak form as

$$\frac{\partial}{\partial t}\int_S \psi \bar{Y}_l^m \, d\mathbf{r} = \int_S \psi F^*(\mathbf{r},\boldsymbol{\nabla})\bar{Y}_l^m \, d\mathbf{r}, \tag{15}$$

where the right hand side follows from integration by parts and the term F^* denotes any polynomial F in which each monomial term is written in reverse order with the substitution of $2\mathbf{r} - \boldsymbol{\nabla}$ for $\boldsymbol{\nabla}$. Therefore, applying equation (15), Jeffery's equation (4) is defined by

$$J^* = \tfrac{1}{2}(\mathbf{w}\cdot(\mathbf{r}\times\boldsymbol{\nabla}) + \lambda\mathbf{r}\cdot\Gamma\cdot\boldsymbol{\nabla}), \tag{16}$$

Similarly, the two extensions of Jeffery's equation that include diffusion appearing in equations (5) and (6) (expressed as $\frac{\partial}{\partial t}\psi = F\psi$), respectively become

$$F^* = J^* + D_r \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}, \tag{17}$$

and

$$F^* = J^* + (\boldsymbol{\nabla} - 2\mathbf{r})\cdot D_r \cdot \boldsymbol{\nabla}. \tag{18}$$

In all cases, we can decompose

$$F^*(\mathbf{r},\boldsymbol{\nabla})\bar{Y}_l^m = \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} c_{l,l'}^{m,m'} \bar{Y}_{l'}^{m'}, \tag{19}$$

and therefore obtain the spherical harmonic representation shown in equation (3) above.

4. The "spherical" program algorithm

An automated algorithm is implemented to compute the coefficients $c_{l,l'}^{m,m'}$ in equation (19) for any differential equation satisfying the criteria given above (and, therefore, the $\mathcal{C}_{l,m}$ in equation (22)). The algorithm is to recursively apply the replacement rules described in equation (20) until no further substitutions can be made. Here "op" denotes any of z, L_z, L_+, or L_- operations, and $\mathcal{Y}$ denotes any linear combination of the $\bar{Y}_l^m$'s.

$$
\begin{aligned}
\operatorname{op}(\mathcal{Y} \pm c\bar{Y}_l^m) &\to \operatorname{op}(\mathcal{Y}) \pm c \operatorname{op}(\bar{Y}_l^m), \\
x\mathcal{Y} &\to ziL_y(\mathcal{Y}) - iL_y(z\mathcal{Y}), \\
y\mathcal{Y} &\to iL_x(z\mathcal{Y}) - ziL_x(\mathcal{Y}), \\
z\bar{Y}_l^m &\to \sqrt{\frac{(l+m)(l-m)}{(2l-1)(2l+1)}}\bar{Y}_{l-1}^m + \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}}\bar{Y}_{l+1}^m, \\
\nabla_x\mathcal{Y} &\to ziL_y(\mathcal{Y}) - yiL_z(\mathcal{Y}), \\
\nabla_y\mathcal{Y} &\to xiL_z(\mathcal{Y}) - ziL_x(\mathcal{Y}), \\
\nabla_z\mathcal{Y} &\to yiL_x(\mathcal{Y}) - xiL_y(\mathcal{Y}), \\
L_x(\mathcal{Y}) &\to \tfrac{1}{2}\left(L_+(\mathcal{Y}) + L_-(\mathcal{Y})\right), \\
L_y(\mathcal{Y}) &\to -\tfrac{i}{2}\left(L_+(\mathcal{Y}) - L_-(\mathcal{Y})\right), \\
L_z\bar{Y}_l^m &\to -m\bar{Y}_l^m, \\
L_+\bar{Y}_l^m &\to -\sqrt{(l+m)(l-m+1)}\bar{Y}_l^{m-1}, \\
L_-\bar{Y}_l^m &\to -\sqrt{(l-m)(l+m+1)}\bar{Y}_l^{m+1}
\end{aligned}
\tag{20}
$$

It is important to note that $x\bar{Y}_l^m$, $y\bar{Y}_l^m$, $z\bar{Y}_l^m$, $\nabla_x\bar{Y}_l^m$, $\nabla_y\bar{Y}_l^m$, and $\nabla_z\bar{Y}_l^m$ involve $\bar{Y}_{l'}^{m'}$ for l' and m' that differ from l and m, respectively, by at most one. The script described in the appendix uses the recursive algorithm in equation (20) to create threaded functions in the programming language C which in turn are used in an iterative procedure for computing the solution to the differential equation in equation (1).

Moment tensors may be computed using this algorithm as well. For example, to compute the 6th order moment tensor $\mathcal{A}$ in equation (8) we simply expand

$$
\mathbf{rrrrrr}\bar{Y}_0^0 = \sum_{l=0}^{6}\sum_{m=-l}^{l} \mathcal{C}_{l,m}\bar{Y}_l^m,
\tag{21}
$$

where $\mathcal{C}_{l,m}$ is the tensor of rank six composed of coefficients calculated by applying x, y and z to $\bar{Y}_0^0$ six times using the algorithm. It follows that since $\bar{Y}_0^0 = 1/\sqrt{4\pi}$, the 6th order orientation tensor becomes

$$
\mathcal{A} = \sqrt{4\pi}\int_S \psi\mathbf{rrrrrr}\bar{Y}_0^0\, d\mathbf{r} = \sqrt{4\pi}\sum_{l=0}^{6}\sum_{m=-l}^{l} \mathcal{C}_{l,m}\hat{\psi}_l^m,
\tag{22}
$$

where the orthogonality of the spherical harmonics are used to simplify the final result.

5. The "spherical" software package

The program developed to implement our spherical harmonics simulation procedure described above which computes the coefficients in equation (3), and then convert these terms into a C program, may be found at `http://www.math.missouri.edu/~stephen/software/spherical`. The program is written in *perl*, and makes use of either the commercial computer algebra system *Mathematica* by Wolfram

Research, or the open-source computer algebra system *Maxima*. The scripts are designed to work in a Unix like environment.

The program that evaluates spherical harmonics coefficients is a *perl* script which applies the rules in (20). It is invoked with the command sequence "perl expand-method.pl". The user may type in an expression involving x, y, z, dx, dy, dz, lx, ly, or lz representing "multiply by x," "multiply by y," "multiply by z," ∇_x, ∇_y, ∇_z, L_x, L_y, or L_z respectively, or any number, including I for i, and any appropriate combination of parentheses, addition and subtraction, and "*" which represents composition of the operators. It outputs a sequence of lines, which when added together, represents the effect of the expression upon $\bar{Y}_l^m$. Each line has three entries separated by semicolons, l';m';c, and represents $c\bar{Y}_{l+l'}^{m+m'}$. The third entry is written in the programming language C, using complex numbers as described in [3]. So, for example, the input

```
%perl expand-method.pl
> -2*I*(dy-y)
```

yields the output

```
-1;-1;((l*sqrt(-1+l+m)*sqrt(l+m))/(sqrt(-1+2*l)*sqrt(1+2*l)))+(0)*I
-1;1;((l*sqrt(-1+l-m)*sqrt(l-m))/(sqrt(-1+2*l)*sqrt(1+2*l)))+(0)*I
1;-1;(((1+l)*sqrt(1+l-m)*sqrt(2+l-m))/(sqrt(1+2*l)*sqrt(3+2*l)))+(0)*I
1;1;(((1+l)*sqrt(1+l+m)*sqrt(2+l+m))/(sqrt(1+2*l)*sqrt(3+2*l)))+(0)*I
```

This result reflects the equation

$$\begin{aligned} -2i(\nabla_y - y)\bar{Y}_l^m = & \frac{l\sqrt{(l+m-1)(l+m)}}{\sqrt{(2l-1)(2l+1)}}\bar{Y}_{l-1}^{m-1} + \frac{l\sqrt{(l-m-1)(l-m)}}{\sqrt{(2l-1)(2l+1)}}\bar{Y}_{l-1}^{m+1} \\ & + \frac{(l+1)\sqrt{(l-m+1)(l-m+2)}}{\sqrt{(2l+1)(2l+3)}}\bar{Y}_{l+1}^{m-1} + \frac{(l+1)\sqrt{(l+m+1)(l+m+2)}}{\sqrt{(2l+1)(2l+3)}}\bar{Y}_{l+1}^{m+1}. \end{aligned}$$

The program "perl expand-method.pl" is called by another script invoked as "perl expand-iterate.pl <filename>" which converts a configuration file into a C program to numerically solve the spherical harmonics differential equation. For example, Jeffery's equation (written here in weak form) with Koch diffusion can be written as below

```
void compute_psidot(complex* psidot, complex* psi,
                    double lambda, double w[3], double g[3][3]) {
  double a4[3][3][3][3], a6[3][3][3][3][3][3], Dr[3][3];

  tensor4(psi,a4); tensor6(psi,a6);
  ... compute Dr from g, a4 and a6 ...

  @spherical_iterate {
    psidot[@index] =
      /* Jeffery's equation */
        w[0]*@method(psi,0.5*y*dz-0.5*z*dy)
      + w[1]*@method(psi,0.5*z*dx-0.5*x*dz)
      + w[2]*@method(psi,0.5*x*dy-0.5*y*dx)
      + lambda*g[0][0]*@method(psi,0.5*x*dx)
      + lambda*g[0][1]*@method(psi,0.5*x*dy+0.5*y*dx)
      + lambda*g[0][2]*@method(psi,0.5*x*dz+0.5*z*dx)
      + lambda*g[1][1]*@method(psi,0.5*y*dy)
```

```
      + lambda*g[1][2]*@method(psi,0.5*y*dz+0.5*z*dy)
      + lambda*g[2][2]*@method(psi,0.5*z*dz)
      /* Koch diffusion */
      + Dr[0][0]*@method(psi,(dx-2*x)*dx)
      + Dr[0][1]*@method(psi,(dx-2*x)*dy+(dy-2*y)*dx)
      + Dr[0][2]*@method(psi,(dx-2*x)*dz+(dz-2*z)*dx)
      + Dr[1][1]*@method(psi,(dy-2*y)*dy)
      + Dr[1][2]*@method(psi,(dy-2*y)*dz+(dz-2*z)*dy)
      + Dr[2][2]*@method(psi,(dz-2*z)*dz);
  }
}
```

To calculate the coefficients for the moment tensors, as in equation (21), if the environmental variable `TENSOR` is set to a non-zero value, then `expand-method.pl` applies the input expression to $\bar{Y}_0^0$, and outputs the answers in floating point format. So, for example the input

```
%env TENSOR=1 perl expand-method.pl
> x*y*z*z
```

yields

```
2;-2;(0)+(-0.026082026547865053022)*I
2;2;(0)+(0.026082026547865053022)*I
4;-2;(0)+(-0.030116930096841707924)*I
4;2;(0)+(0.030116930096841707924)*I
```

This results reflects the 1233 component of 4th order moment tensor

$$\mathbb{A}_{1233} = i\sqrt{4\pi}\left(\tfrac{\sqrt{30}}{210}(\hat{\psi}_2^2 - \hat{\psi}_2^{-2}) + \tfrac{\sqrt{10}}{105}(\hat{\psi}_4^2 - \hat{\psi}_4^{-2})\right).$$

This is used by "`perl make-tensor.pl` n" and "`perl make-reverse-tensor.pl` n", which create C programs to convert, respectively, spherical harmonic coefficients to moment tensors of rank n, and vice-versa.

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