USING THE SPHERICAL SOFTWARE

The `spherical` software is invoked by the command

```
spherical -p parameter-file.txt
```

where `parameter-file.txt` is a text file that sets various parameters, described below. The command can be invoked with two other command line options, for example:

```
spherical -p parameter-file.txt -o output-file -v10
```

where `output-file` is the output file, which will default to `s.out` if not specified, and `-v` denotes verbose output, and if followed by a number n, will write out to the console every nth time it writes data to the output file.

The program `spherical` uses spherical harmonics to solve Jeffery's equation [1] for $\psi = \psi(\mathbf{r})$:

$$\frac{\partial}{\partial t}\psi = \boldsymbol{\nabla} \cdot \big(-\dot{\mathbf{r}}\psi + \boldsymbol{\nabla}(D_r\psi)\big),$$

where

$$\dot{\mathbf{r}} = \tfrac{1}{2}(\mathbf{w} \times \mathbf{r}) + \lambda\dot{\tilde{\mathbf{r}}}, \quad \dot{\tilde{\mathbf{r}}} = \tfrac{1}{2}(\Gamma \cdot \mathbf{r} - \Gamma : \mathbf{rrr}),$$

where Γ is the rate of strain tensor, and $\mathbf{w}$ is the vorticity. Note that $\boldsymbol{\nabla}$ here denotes the gradient projected tangentially to the sphere, namely $\boldsymbol{\nabla} f = (I - \mathbf{rr}) \cdot (\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z})$.

Basic Parameters

The parameter file consists of a number of lines, each of the form

```
parameter=value
```

The order in which they are written in the parameter file is unimportant.

- The number of threads used by the program is set by `nr_threads`. This can be overridden by the environment variable `NR_THREADS` (using,for example, the `SET` command in the windows command shell, or the `export` or `env` commands in the unix `sh` or `bash` shells.)
- The parameter `max_order` sets the order of spherical harmonics used.
- The start time and stop time are set by parameters `tstart` and `tend`.
- The rate of strain tensor is set by parameters `gamma11`, `gamma12`, `gamma13`, `gamma22`, `gamma23`, `gamma33`.
- The vorticity is set by parameters `w1`, `w2`, `w3`.
- The initial state is $\psi = 1/4\pi$. Later versions of the software may allow this to be different.
- By default the program will solve the differential equations using the order two-three Runge-Kutta-Fehlberg method.
- The parameter set as `ode_rkf_45=1` will cause the program will use the order four-five Runge-Kutta-Fehlberg method.
- The parameter set as `ode_adams_bash_2=1` will cause the program will use the order two Adams-Bashforth multistep method.

- The parameter set as `ode_adams_bash_4=1` will cause the program will use the order four Adams-Bashforth multistep method.
- The parameter set as `ode_rk_4=1` will cause the program will use the order four Runge-Kutta method.
- For fixed timestep methods (Runge-Kutta or Adams-Bashforth), the step size of time is set by the parameter `h`. For adaptive methods, this parameter sets the initial step size of time. This defaults to 10^{-3} if not set.
- For the adaptive Runge-Kutta-Fehlberg methods, the parameter `tol` sets the desired error, which is computed as the maximum of the absolute values of the spherical harmonic coefficients. This defaults to 10^{-3} if it is not set.
- Data will be printed to the output file every `print_every` time steps. This defaults to 1 if it is not set.

Output

The program, by default, will write to the output file a series of lines containing

$$t\ a_{11}\ a_{22}\ a_{33}\ a_{12}$$

This same information is output to the console if the command line option `-v` with a number is specified. Here a_{ij} are the coefficients of the second moments tensor. Similarly a_{ijkl} are the coefficients of the fourth moments tensor, and a_{ijklmn} are the coefficients of the sixth moments tensor.

- The parameter set as `print_aij=1` will cause the lines written to the output file to change to

  $$t\ a_{11}\ a_{12}\ a_{13}\ a_{22}\ a_{23}\ a_{33}$$

  (but the output to the console will remain as before).
- The parameter set as `print_aijkl=1` will add to the end of each line of output the values

  $a_{1111}\ a_{1112}\ a_{1113}\ a_{1122}\ a_{1123}\ a_{1133}\ a_{1222}\ a_{1223}\ a_{1233}\ a_{1333}\ a_{2222}\ a_{2223}\ a_{2233}\ a_{2333}\ a_{3333}$
- The parameter set as `print_aijklmn=1` will add to the end of each line of output the values

  $a_{111111}\ a_{111112}\ a_{111113}\ a_{111122}\ a_{111123}\ a_{111133}\ a_{111222}\ a_{111223}\ a_{111233}\ a_{111333}\ a_{112222}\ a_{112223}\ a_{112233}\ a_{112333}\ a_{113333}\ a_{122222}\ a_{122223}\ a_{122233}\ a_{122333}\ a_{123333}\ a_{133333}\ a_{222222}\ a_{222223}\ a_{222233}\ a_{222333}\ a_{223333}\ a_{233333}\ a_{333333}$
- The parameters `print_daij`, `print_daijkl`, and `print_daijklmn` set to 1 will print out the derivatives with respect to time of, respectively, the second, fourth, and sixth order moment tensors.

Folgar-Tucker model

The program will default to solving Jeffery's equation with the Folgar-Tucker diffusion term [2]. This sets the diffusion term to $D_r = C_I\gamma$. Here, and elsewhere, $\gamma = \left(\frac{1}{2}\Gamma : \Gamma\right)^{1/2}$.

- The parameter `lambda` is the Jeffery's parameter λ.
- The parameter `CI` sets the parameter C_I.

Modified Koch model

This provides an anisotropic diffusion model:

$$\begin{aligned}\frac{\partial}{\partial t}\psi &= -\boldsymbol{\nabla}\cdot(\dot{\mathbf{r}}\psi) + \boldsymbol{\nabla}\cdot(I-\mathbf{rr})\cdot D_r\cdot\boldsymbol{\nabla}\psi \\ &\quad -\mathbf{L}\cdot(I-\mathbf{rr})\cdot E_r\cdot\mathbf{L}\psi \\ &= -\boldsymbol{\nabla}\cdot(\dot{\mathbf{r}}\psi) + (\boldsymbol{\nabla}-2\mathbf{r})\cdot D_r\cdot\boldsymbol{\nabla}\psi - \mathbf{L}\cdot E_r\cdot\mathbf{L}\psi.\end{aligned}$$

Here $(I-\mathbf{rr})$ is the matrix of the projection onto the tangent space of the sphere, and $\mathbf{L} = -i\mathbf{r}\times\boldsymbol{\nabla}$ is the so called angular momentum operator. (Note that the Laplacian operator can be expressed two different ways as $\boldsymbol{\nabla}\cdot\boldsymbol{\nabla} = -\mathbf{L}\cdot\mathbf{L}$.)

Koch [3] defines D_r as the matrix

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

Here A, $\mathbb{A}$, and $\mathcal{A}$ are the tensors of 2nd, 4th and 6th moments, respectively, of ψ. This software has an additional modification in the form of E_r:

$$E_r = C_3\gamma^{-1}\Gamma:\mathcal{A}:\Gamma.$$

- The parameter set as `do_koch=1` will cause the modified Koch diffusion model to be used.
- The parameter `lambda` is the Jeffery's parameter λ.
- The parameters `C1`, `C2` and `C3` are the modified Koch parameters C_1, C_2 and C_3.

Directional diffusion model

This gives values for $D_r = D_r(\mathbf{r})$ that depend upon $\mathbf{r}$, in the diffusion term of Jeffery's equation. The directional diffusion model is described in the Ph.D. thesis of David Jack [4]: and the second directional diffusion model is

$$\begin{aligned}D_r &= C_1\gamma^{-1}\int_{\boldsymbol{\rho}\in S^2}|\boldsymbol{\rho}\cdot(\mathbf{r}\times(\dot{\tilde{\boldsymbol{\rho}}}-\dot{\tilde{\mathbf{r}}}))|^2\psi(\boldsymbol{\rho})\,d\boldsymbol{\rho} + C_2\gamma \\ &= C_1\gamma^{-1}\int_{\boldsymbol{\rho}\in S^2}\big(|\boldsymbol{\rho}\cdot(\mathbf{r}\times\dot{\tilde{\boldsymbol{\rho}}})|^2 + |\boldsymbol{\rho}\cdot(\mathbf{r}\times\dot{\tilde{\mathbf{r}}})|^2\big)\psi(\boldsymbol{\rho})\,d\boldsymbol{\rho} + C_2\gamma.\end{aligned}$$

- The parameter set as `do_dd=1` will cause the directional diffusion model to be used.
- The parameter `lambda` is the Jeffery's parameter λ.
- The parameters `C1` and `C2` are the directional diffusion parameters C_1 and C_2.

The RSC model of Wang, O'Gara and Tucker

This causes an artificial scaled reduction of the evolution of ψ, the "Reduced-Strain Closure" model. This can be used in conjunction with any of the other models. It is described in [6], and the file `rsc.pdf`. It causes the P.D.E.

$$\frac{\partial}{\partial t}\psi(\mathbf{r}) = F(\mathbf{r}),$$

to be replaced by

$$\frac{\partial}{\partial t}\psi(\mathbf{r}) = F(\mathbf{r}) - \tfrac{15}{8\pi}(1-\kappa)(\mathbf{rr}-\tfrac{1}{5}I):\mathbb{M}:\int_{S^2}F(\boldsymbol{\rho})\boldsymbol{\rho}\boldsymbol{\rho}\,d\boldsymbol{\rho},$$

where $\mathbb{M} = \sum_{i=1}^{3} \mathbf{e}_i\mathbf{e}_i\mathbf{e}_i\mathbf{e}_i$, with $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ being the orthonormal eigenvectors of A.

This method has intellectual property restrictions [5]. If you use `do_rsc=1`, the program will interrogate you to see if you comply with this patent. You may switch off the interrogation by setting the environment variable `MAY_USE_PATENT_7266469`.

- The parameter set as `do_rsc=1` causes RSC to take place.
- The parameter `kappa` sets the scale reduction factor κ.

The ARD model of Phelps and Tucker

This "Anisotropic Rotary Diffusion" model is described in [7]. This is the same form as the Koch model, with

$$D_r = b_1\gamma I + b_2\gamma A + b_3\gamma A^2 + \tfrac{1}{2}b_4\Gamma + \tfrac{1}{4}b_5\gamma^{-1}\Gamma^2.$$

- The parameter set as `do_ard=1` causes ARD to be used.
- The parameters `b1`, `b2`, `b3`, `b4` and `b5` set b_1, b_2, b_3, b_4 and b_5.

Variable diffusion and variable lambda models

Define:

$$s = \gamma^{-1}\int_{S^2} \Gamma : \boldsymbol{\rho}\boldsymbol{\rho}\psi(\boldsymbol{\rho})\, d\boldsymbol{\rho} = \gamma^{-1}A : \Gamma.$$

Note that it can be shown that $|s| \le \sqrt{2}$.

The variable diffusion model sets $D_r = \gamma f(s)$, and the variable lambda model sets $\lambda = g(s)$, for functions $f(s)$ and $g(s)$.

- The parameter set as `do_vd`=1 causes variable diffusion to occur.
- The parameter set as `do_vl`=1 causes variable lambda to occur.
- In the case `do_vd`=1, the function $f(s)$ is defined using the parameter `vd_fun`.
- In the case `do_vl`=1, the function $g(s)$ is defined using the parameter `vl_fun`. In this case the parameter `lambda` should NOT be set.

Functions are expressed using formulae involving '`+`', '`-`', '`*`', '`/`', '`^`' (exponentiation), '`m`' (minimum), '`M`' (maximum), parentheses '`(`' and '`)`', and the variable '`s`'. So, for example, '`1-5*(s M(-s)) M 0.2`' denotes $\max\{1 - 5|s|, 0.2\}$.

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