

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 n th time it writes data to the output file.

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

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

where

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

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

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.

- Step size of time is set by the parameter `h`. By default, the program uses 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.
- Data will be printed to the output file every `print_every` time steps.
- 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.

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_aj=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_ajkl=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_ajklmn=1` will add to the end of each line of output the values

$$a_{111111} \ a_{111112} \ a_{111113} \ a_{111122} \ a_{111123} \ a_{111133} \ a_{111222} \ a_{111223} \ a_{111233} \ a_{111333} \ a_{112222} \ a_{112223} \ a_{112233} \ a_{112333} \ a_{113333} \ a_{122222} \ a_{122223} \ a_{122233} \ a_{122333} \ a_{123333} \ a_{133333} \ a_{222222} \ a_{222223} \ a_{222233} \ a_{222333} \ a_{223333} \ a_{233333} \ a_{333333}$$

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, $\gamma = (\frac{1}{2} \Gamma : \Gamma)^{1/2}$.

- 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:

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

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

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 MODELS

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

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

and the second directional diffusion model is

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

- The parameter set as `do_dd=1` will cause the first directional diffusion model to be used.
- The parameter set as `do_dd_2=1` will cause the second 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 .

VARIABLE DIFFUSION MODELS

Define s_ν for $\nu = 1, 2$:

$$s_1 = \left| \int_{S^2} \Gamma : \boldsymbol{\rho} \boldsymbol{\rho} \psi(\boldsymbol{\rho}) d\boldsymbol{\rho} \right| = |\mathbb{A} : \Gamma|,$$

$$s_2 = \left(\int_{S^2} |\Gamma : \boldsymbol{\rho} \boldsymbol{\rho}|^2 \psi(\boldsymbol{\rho}) d\boldsymbol{\rho} \right)^{1/2} = (\Gamma : \mathbb{A} : \Gamma)^{1/2}.$$

The variable diffusion model sets the diffusion term in Jeffery's equation to $D_r = C_1 s_\nu$.

- The parameter `do_vd` can take the values 1 or 2, and will cause the variable diffusion model to be used with the appropriate value of ν .
- The parameter `lambda` is the Jeffery's parameter λ .
- The parameter `C1` is the parameter C_1 .

VARIABLE LAMBDA MODELS

The Jeffery's parameter is allowed to vary as $\lambda = \lambda_1 - \lambda_2 \gamma^{-1} s_\nu$. This can be used in conjunction with any of the diffusion models.

- The parameter `do_vl` can take the values 1 or 2, and will cause the variable lambda model to be used with the appropriate value of ν .
- The parameters `lambda1` and `lambda2` replace the parameter `lambda`.

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

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

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

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

- 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 .

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