USING THE FEC SOFTWARE

The `fec` software is invoked by the command

```
fec -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:

```
fec -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 `fec` uses the Fast Exact Closure (FEC) to solve Jeffery's equation [1] with diffusion for the second order moment tensor A:

$$\frac{\partial A}{\partial t} = \tfrac{1}{2}(\Omega \cdot A - A \cdot \Omega + \lambda(\Gamma \cdot A + A \cdot \Gamma) - 2\lambda \mathbb{A} : \Gamma) + D_r(2I - 6A),$$

where Γ is the rate of strain tensor, Ω is the vorticity tensor, and $\mathbb{A}$ is the fourth order moment tensor computed from A using the exact closure.

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 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 four-five Runge-Kutta-Fehlberg method.
- The parameter set as `ode_rk_4=1` will cause the program will use the order four Runge-Kutta method.
- For the Runge-Kutta method, 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 method, the parameter `tol` sets the desired error. 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.
- The parameter set as `do_reset=1` makes the program slightly slower, but slightly more accurate in the case that the eigenvalues of A are sometimes not all distinct.

Output

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

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

where a_{ij} denotes the entries of A. If the command line option `-v` with a number is specified, the program will write this same information to the console. Here a_{ij} are the coefficients of the second moments tensor.

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.

The ARD model of Phelps and Tucker

This "Anisotropic Rotary Diffusion" model is described in [5].

$$\begin{aligned}\frac{\partial A}{\partial t} =& \tfrac{1}{2}(\Omega\cdot A - A\cdot\Omega + \lambda(\Gamma\cdot A + A\cdot\Gamma) - 2\lambda\mathbb{A} : \Gamma)\\ &+ 2D_r - 2(\operatorname{tr} D_r)A - 5(A\cdot D_r + D_r\cdot A) + 10\mathbb{A} : D_r.\end{aligned}$$

Here

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

- 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.

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 [4]. It causes the P.D.E.

$$\frac{\partial A}{\partial t} = F(A),$$

to be replaced by

$$\frac{\partial A}{\partial t} = F(A) - (1-\kappa)\mathbb{M} : F(A),$$

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 [3]. 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.

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References

[1] G.B. Jeffery, The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid, Proceedings of the Royal Society of London A **102**, 161-179, (1923).

[2] F.P. Folgar and C.L. Tucker, Orientation Behavior of Fibers in Concentrated Suspensions, Jn. of Reinforced Plastics and Composites **3**, 98-119 (1984).

[3] C.L. Tucker III, J. Wang, and J.F. O'Gara, Method and article of manufacture for determining a rate of change of orientation of a plurality of fibers disposed in a fluid. U.S. Patent No. 7,266,469 (2007).

[4] Jin Wang, John F. O'Gara, and Charles L. Tucker, III, An objective model for slow orientation kinetics in concentrated fiber suspensions: Theory and rheological evidence, J. Rheology **52**, 1179-1200 (2008).

[5] Jay H. Phelps and Charles L. Tucker III, An anisotropic rotary diffusion model for fiber orientation in short- and long-fiber thermoplastics, Journal of Non-Newtonian Fluid Mechanics, to appear (2008).