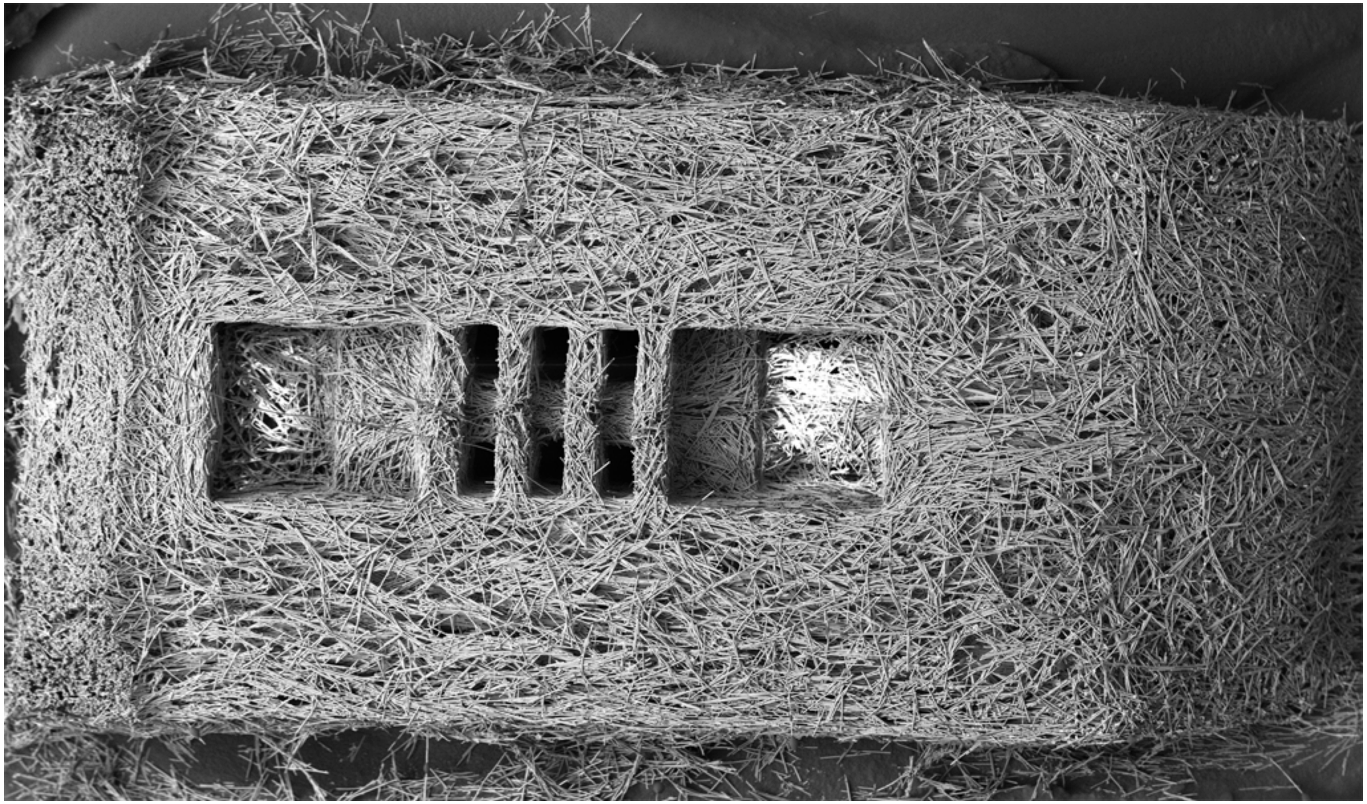
Modeling of fiber orientation in fiber filled thermoplastics

29-03-2010



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Layout

- Introduction.
- Application.
- Models.
- Test cases.
- Conclusions and recommendations

Introduction

Project

- Master student mechanical engineering.
- Final project of mechanical engineering study.
- Carried out at DSM, a Dutch multinational Life Sciences and Materials Sciences company.

Interest

DSM is interested in simulating the production process *injection molding*.

Objective

Implementation of a model to gain insight in the *fiber orientation* development during *injection molding*.

Contribution

- Reproduction of literature material.
- Implementation of models.
- Interpretation of output.
- Comparison of quality of approximations.
- Instruction of implementation.
- Integration of all of the former in a report.

Application

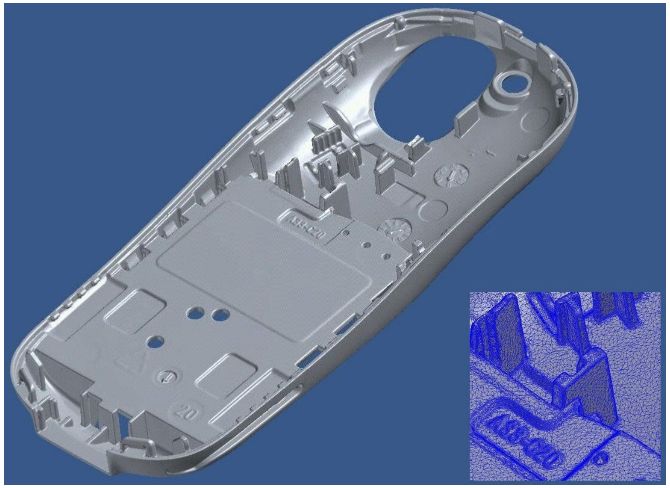
Thermoplastic products

Focus of the project is on *thermoplastic products*.

In our daily lives, we encounter *thermoplastic products*.

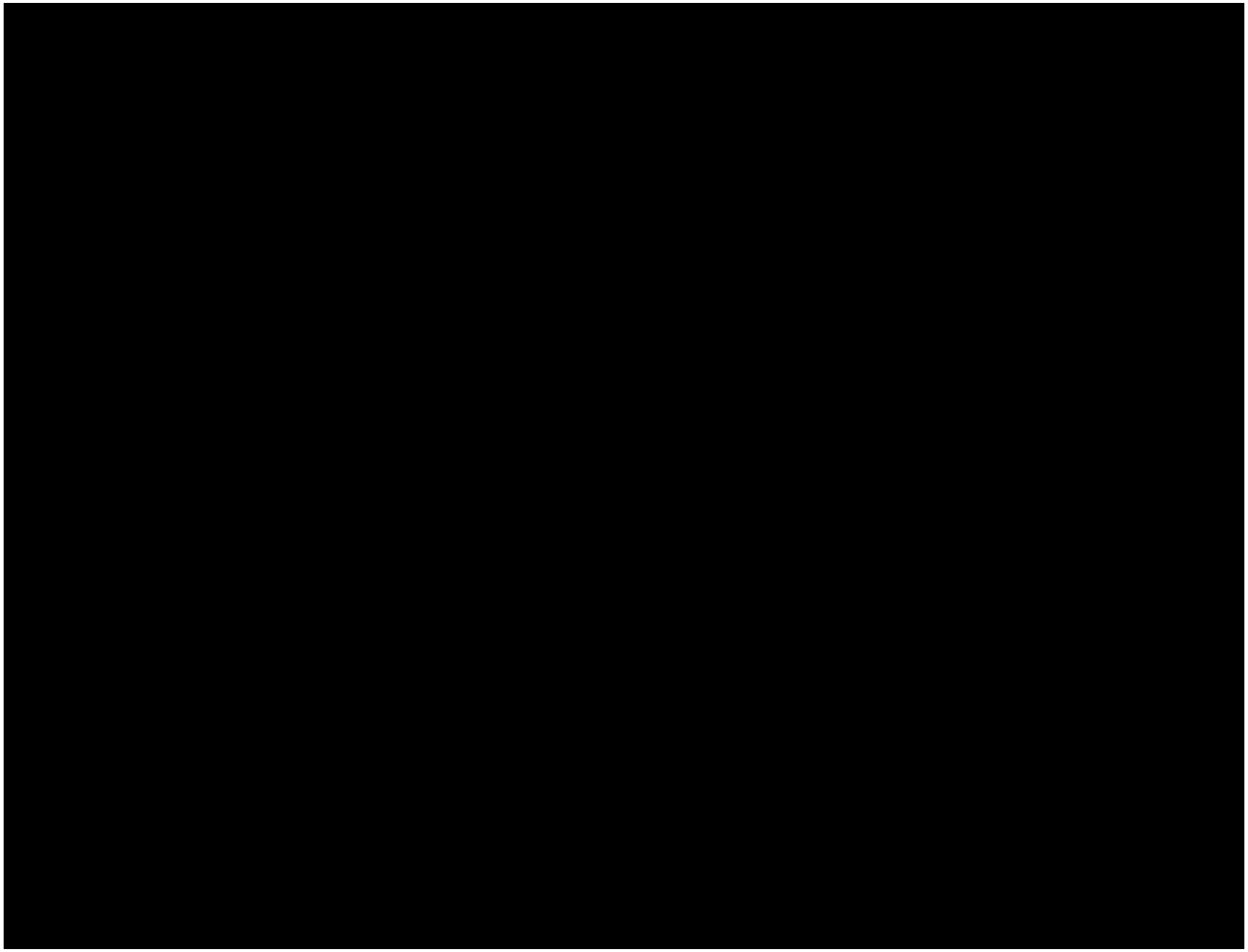
Thermoplastic products

Examples



Used materials in *granules* or *pellets* form.

Injection molding



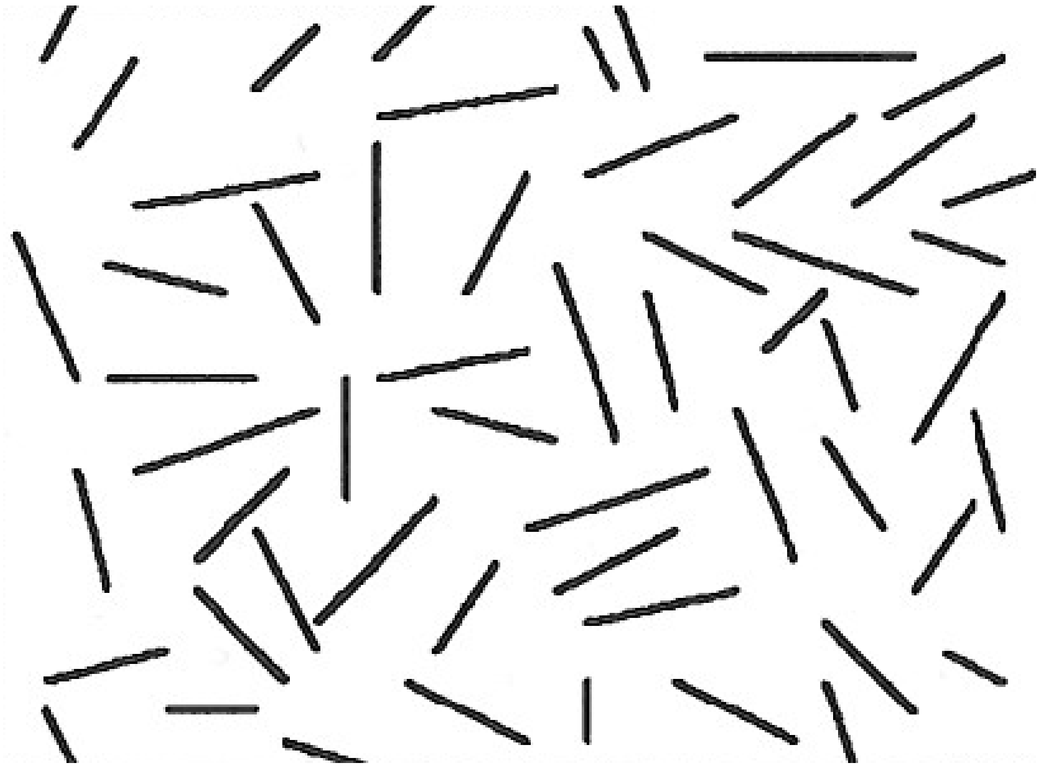
Material

Used materials in *granules* or *pellets* form.

Add *discontinuous fibers* to improve the quality of the final product. Glass or carbon fibers, for instance.

Influences:

- viscosity,
- stiffness,
- thermal conductivity and
- electrical conductivity.

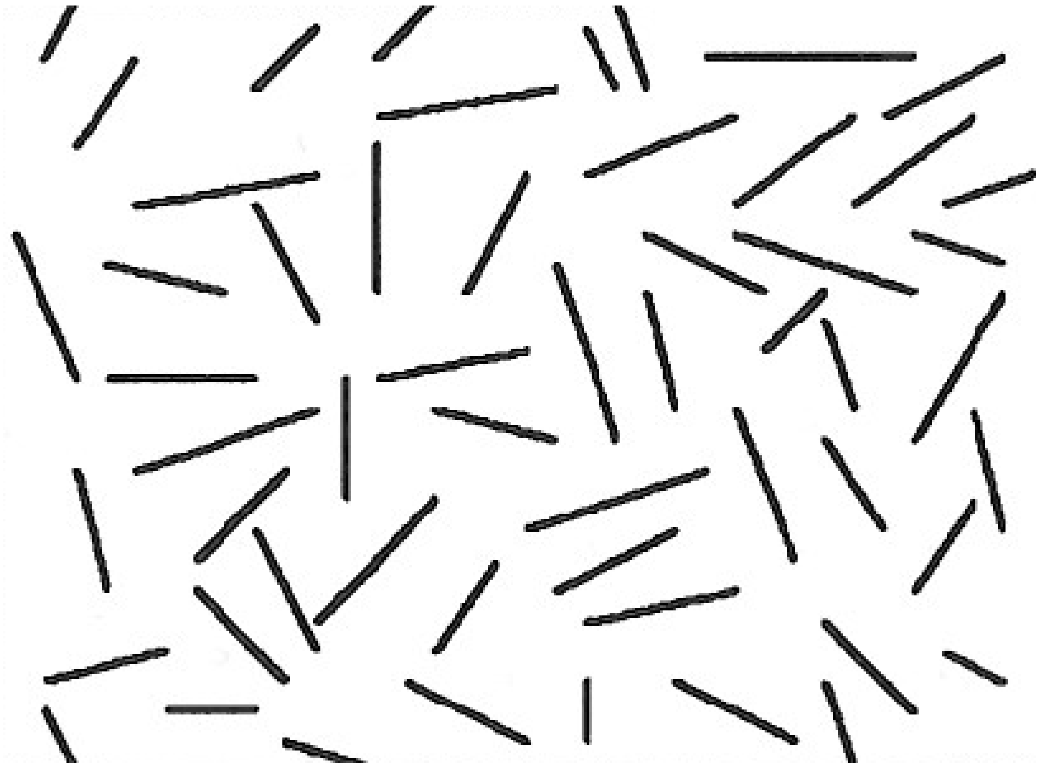


DSM wants to control these properties.

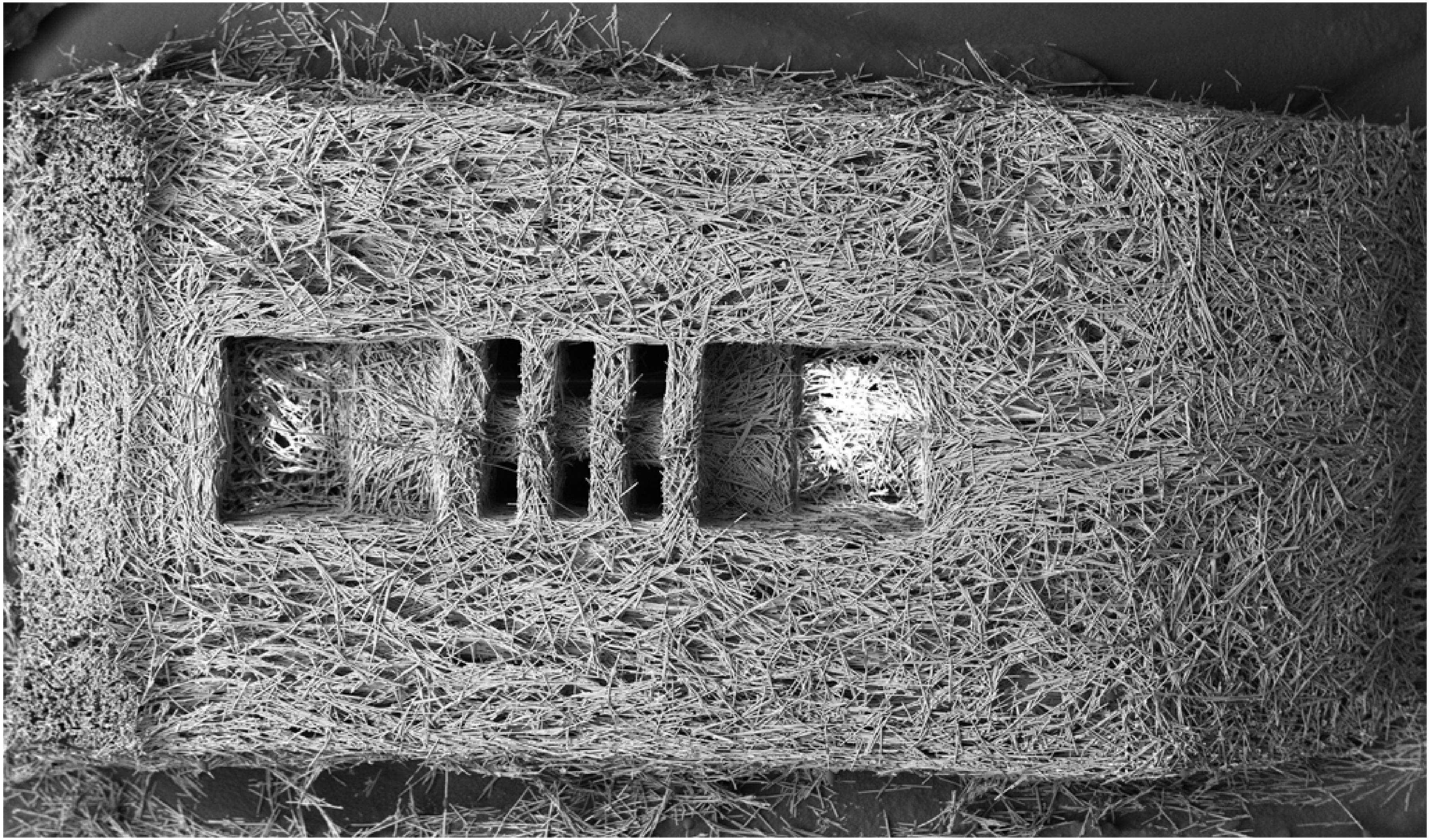
Material

- Typical volume fractions are 8-30%.
- Typical weight fractions 15-60%.
- Typical average final lengths 200-300 [μm].
- Typical diameter 10 [μm].

Average human hair is 100 [μm].



Configuration of the fibers.



Configuration of the fibers

How is the configuration of the fibers controlled?

We want to control the production process.

Control

Configuration of the fibers can be controlled by

•processing settings on the injection molding machine and

•mold geometry (**expensive!**).

Simulations are preferred.

Software

DSM already uses the commercial software

- Moldflow and
- Moldex3D

to simulate injection molding processes.

Problems encountered by DSM:

- results warpage (kromtrekking) analyses not good,
- results fiber orientation analyses not good,
- ‘company secrecy’ response concerning the code,
- models not up to date.

Project

DSM wants implementations of the latest *fiber orientation* models.

Fiber orientation

How can the configuration of the fibers be described?

- Location of the fibers.
- *Orientation of the fibers*.

It is reasonable to assume that the concentration of the fibers in the final product is uniform by approximation.

The orientation of the fibers influences the material properties the most.

We will focus on the modeling of the orientation.

Models

Physics behind fiber orientation

What are the physics behind the *fiber orientation*? What are the characteristics?

- Inertia forces are negligible <-> low Reynolds number.
- Viscous forces <-> lift and drag.
- Stiffness of the fibers <-> internal stresses.
- Fiber-fiber interaction <-> fibers ‘hit’ each other.
- Fibers influence surrounding flow field <-> coupling of orientation and velocity.

Order of increasing complexity of the models.

Models are constructed for *incompressible homogeneous flows*. Such flows are characterized by velocities whereof the change in space is constant.

$$\boldsymbol{\nabla} \otimes \boldsymbol{v} = \boldsymbol{K} \quad \text{or} \quad \forall i, j \in \{1, 2, 3\} \quad \frac{\partial v_j}{\partial x_i} = K_{ji}$$

The velocity can be described as

$$\boldsymbol{v} = \boldsymbol{K} \cdot \boldsymbol{x} + \boldsymbol{c}$$

Incompressibility demands that

$$\mathrm{tr}\left(\boldsymbol{K}\right) = \sum_i \left(\left(\boldsymbol{\nabla} \boldsymbol{v}\right)^T\right)_{ii} = \boldsymbol{\nabla} \cdot \boldsymbol{v} = 0.$$

Incompressible homogeneous flow fields

Examples are

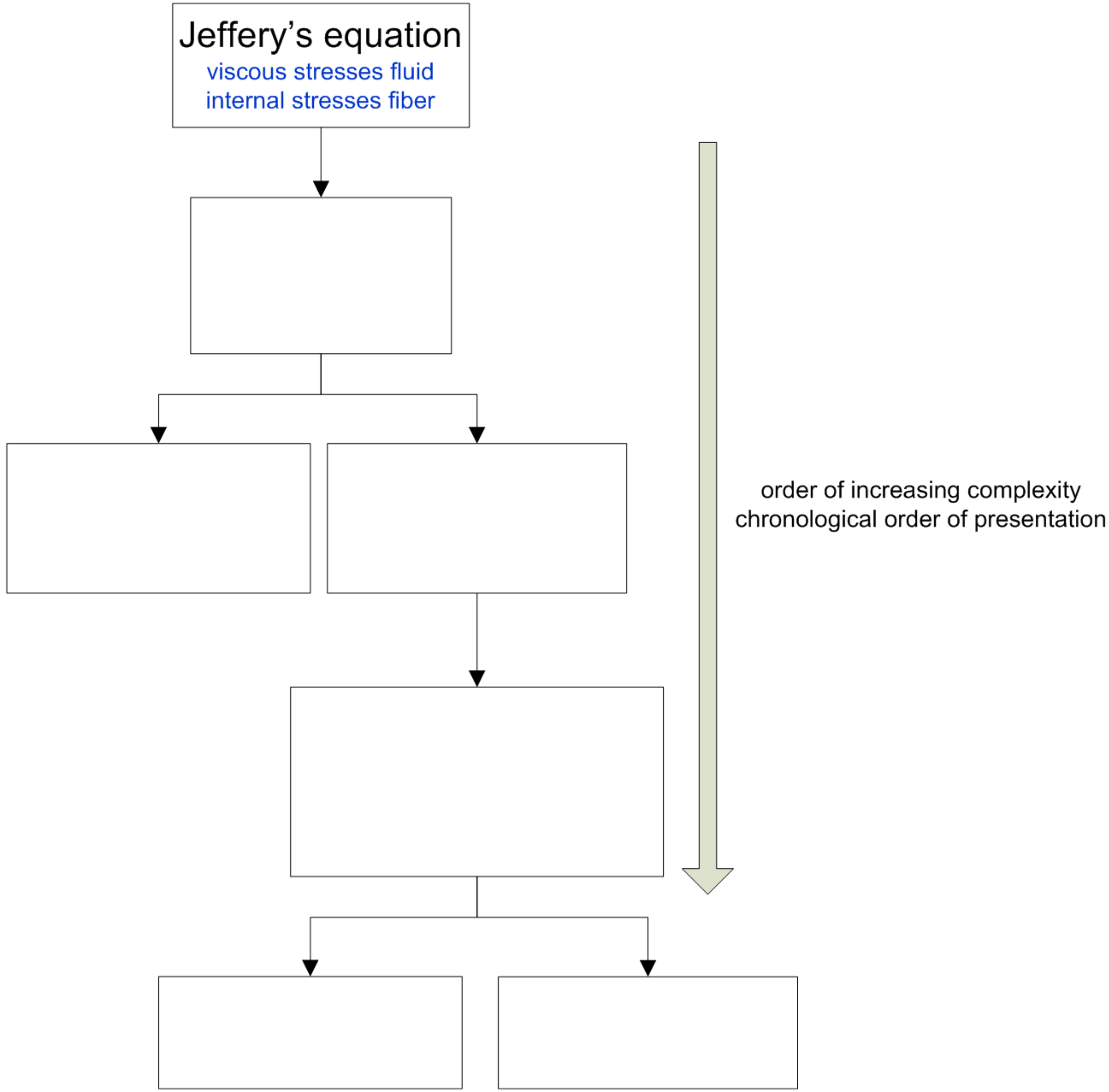
•the *simple shear* flow field

$$\boldsymbol{v} = \begin{bmatrix} 0 & G & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot \boldsymbol{x} = \begin{bmatrix} Gx_2 \\ 0 \\ 0 \end{bmatrix}$$

•the *uniaxial elongational* flow field

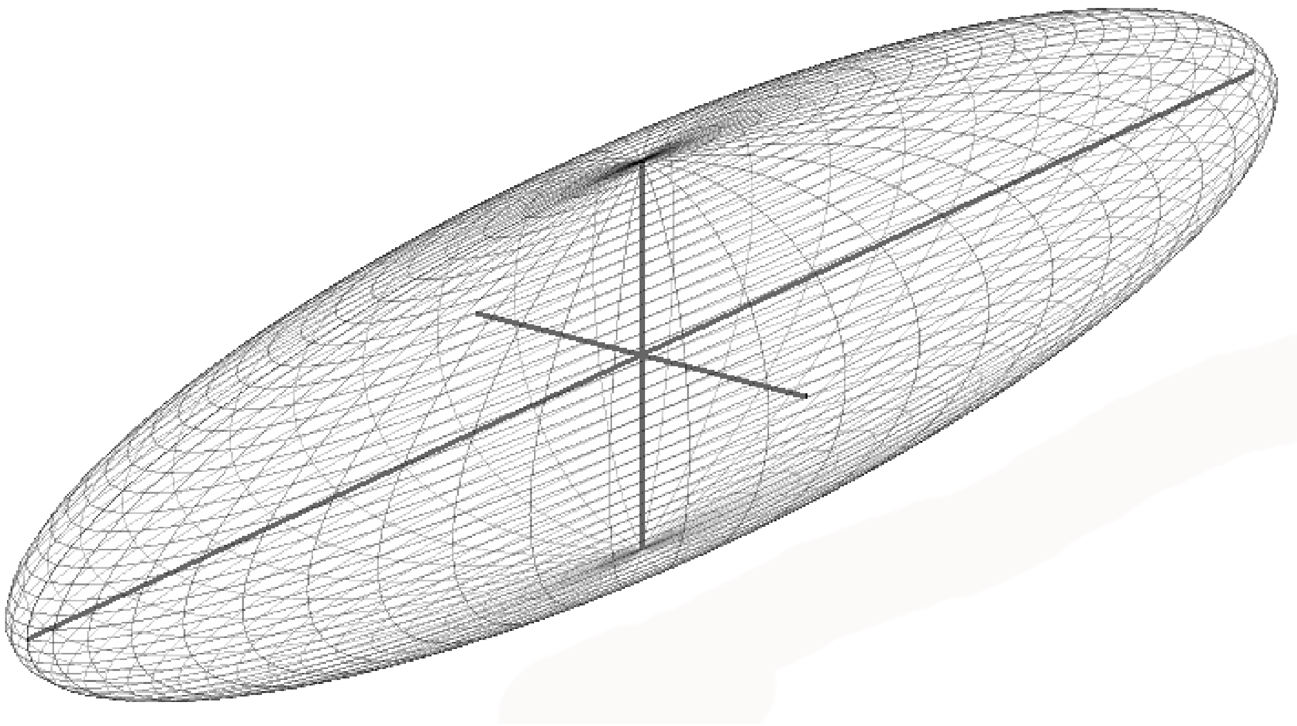
$$\boldsymbol{v} = \begin{bmatrix} 2E & 0 & 0 \\ 0 & -E & 0 \\ 0 & 0 & -E \end{bmatrix} \cdot \boldsymbol{x} = \begin{bmatrix} 2Ex_1 \\ -Ex_2 \\ -Ex_3 \end{bmatrix}$$

Layout models



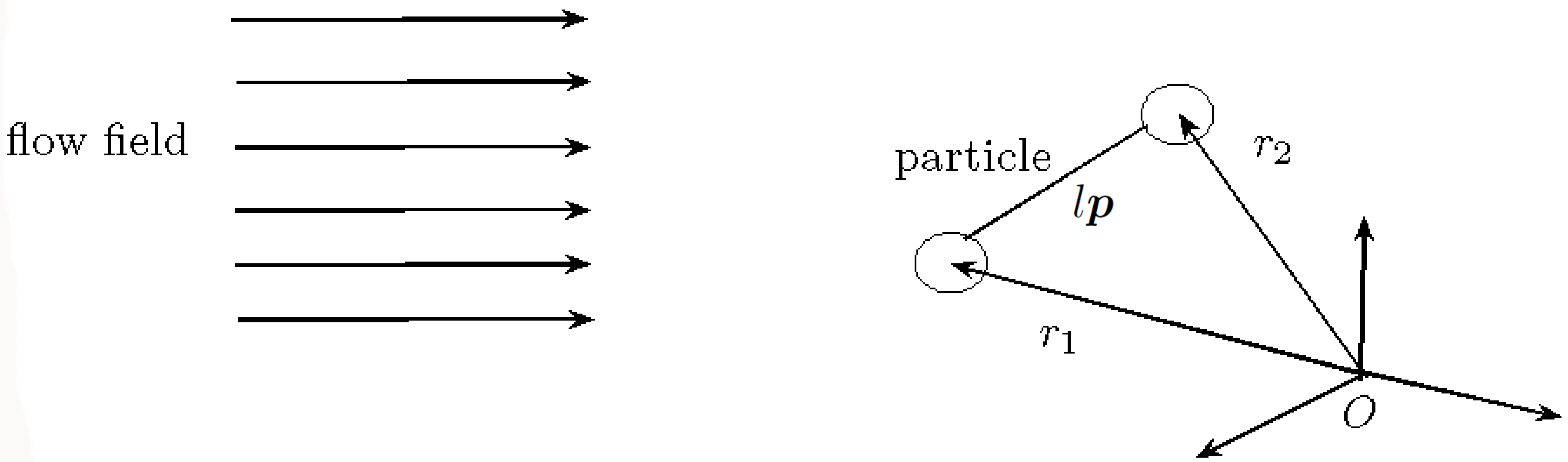
Jeffery's equation

Ellipsoidal particle immersed in a viscosity dominated fluid

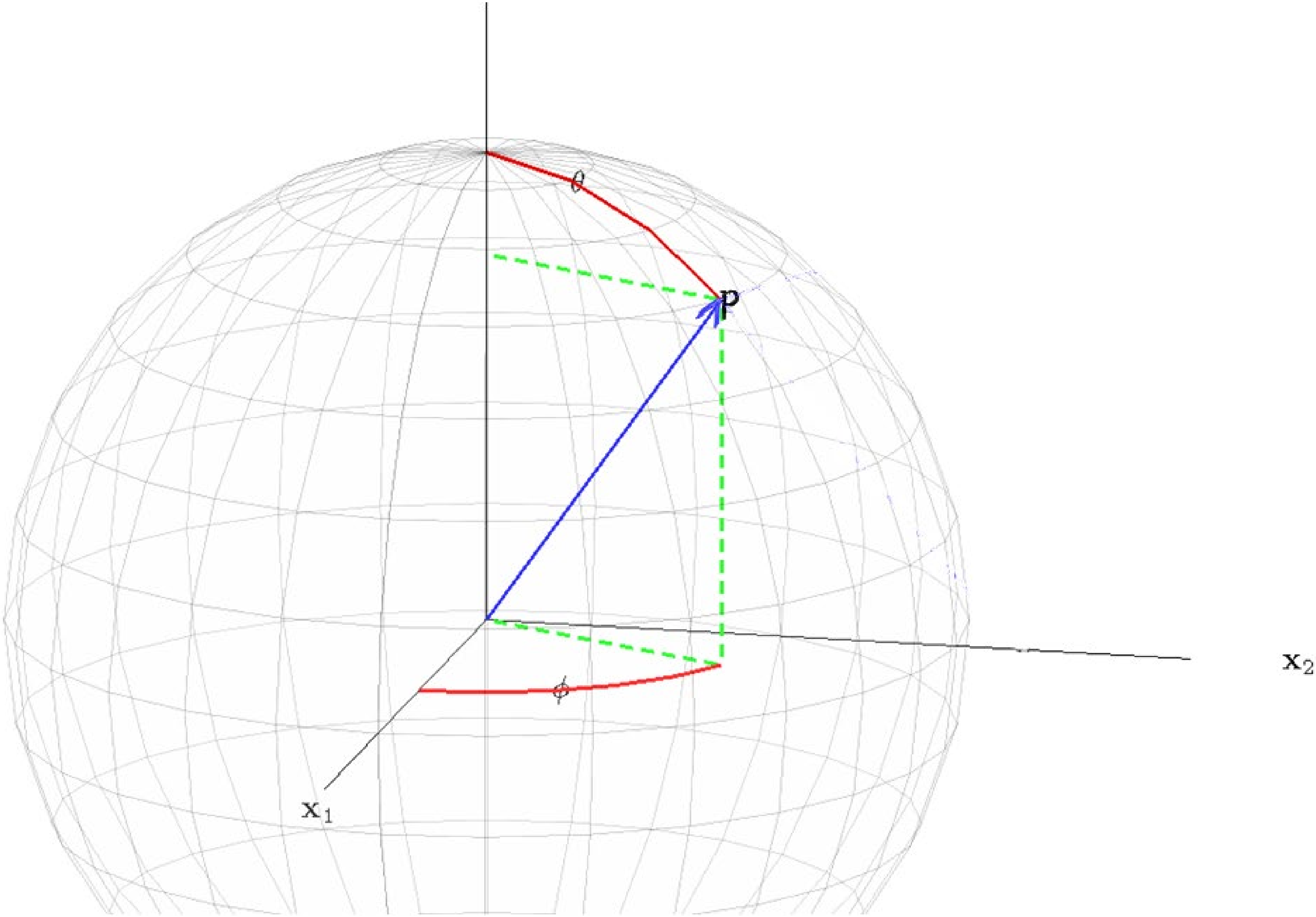


Jeffery's equation

viscous dominated / Stokes flow



Jeffery's equation



Jeffery's equation

Balance between *viscous stresses from the flow field* and *internal stresses of the fiber* leads to

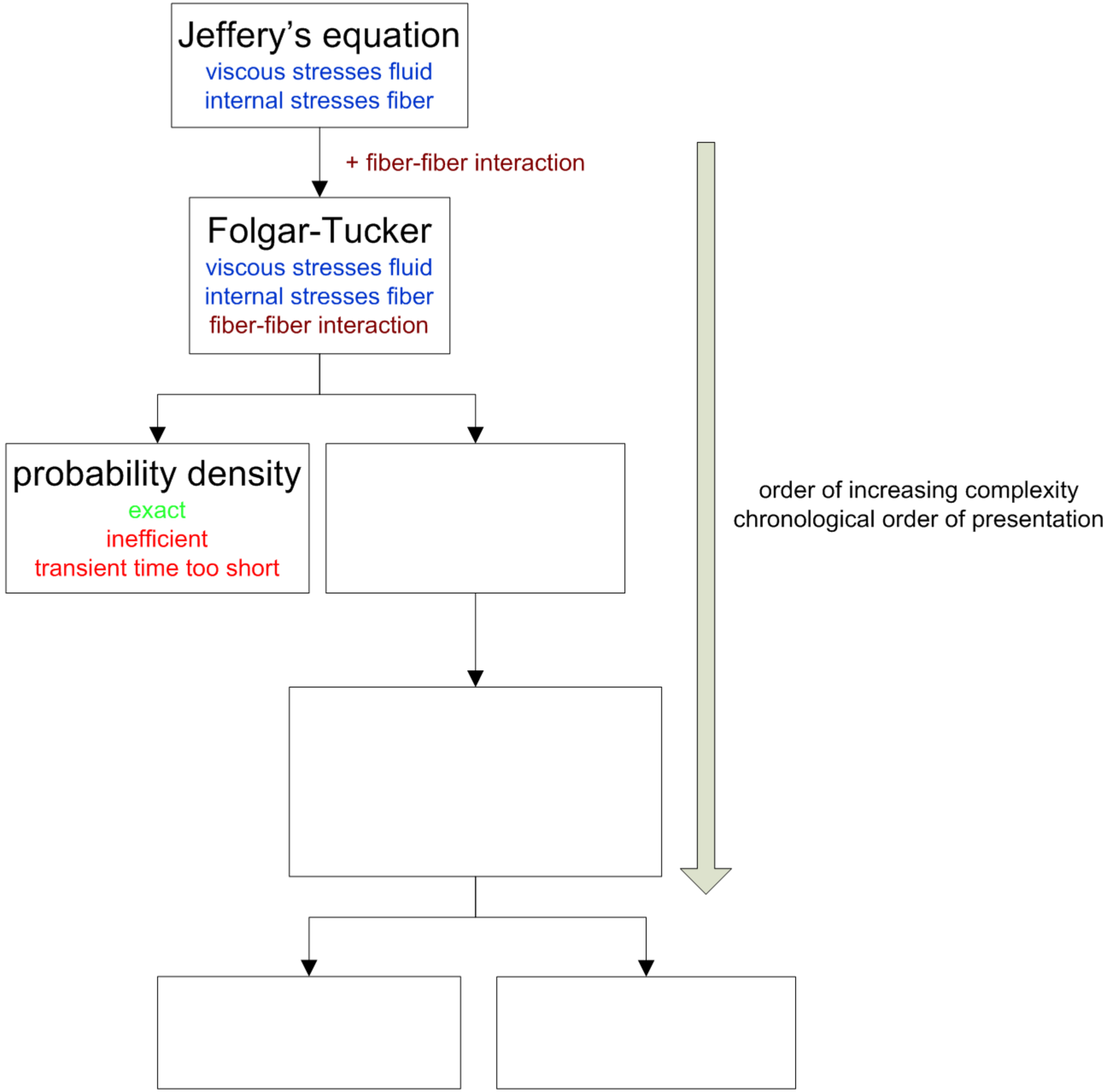
$$\underbrace{\dot{p} - \boldsymbol{W} \cdot p - \xi \boldsymbol{D} \cdot p}_{\text{difference between velocity flow and velocity fiber}} = \underbrace{-\xi \boldsymbol{D} : ppp}_{\text{stress within fiber}}$$

$$\boldsymbol{D} = \frac{1}{2}(\boldsymbol{K} + \boldsymbol{K}^T), \quad \boldsymbol{W} = \frac{1}{2}(\boldsymbol{K} - \boldsymbol{K}^T) \quad \boldsymbol{K} = (\nabla \boldsymbol{v})^T$$

$$\xi = \frac{r_e^2 - 1}{r_e^2 + 1}, \quad r_e = \sqrt{-\frac{\xi + 1}{\xi - 1}}, \quad r_e = \frac{l}{d}$$

The r_e is the *aspect ratio* of the ellipsoidal particle. The ξ is a function of this aspect ratio.

Layout models



Folgar-Tucker model

Model *fiber-fiber interaction* deterministically or stochastically?

Folgar-Tucker model

Outcome of a throw of a dice.

•Hard to say in a deterministic sense.

•Easy to say in a stochastic (probabilistic) sense.

Same holds for fiber-fiber interaction.

Folgar-Tucker model

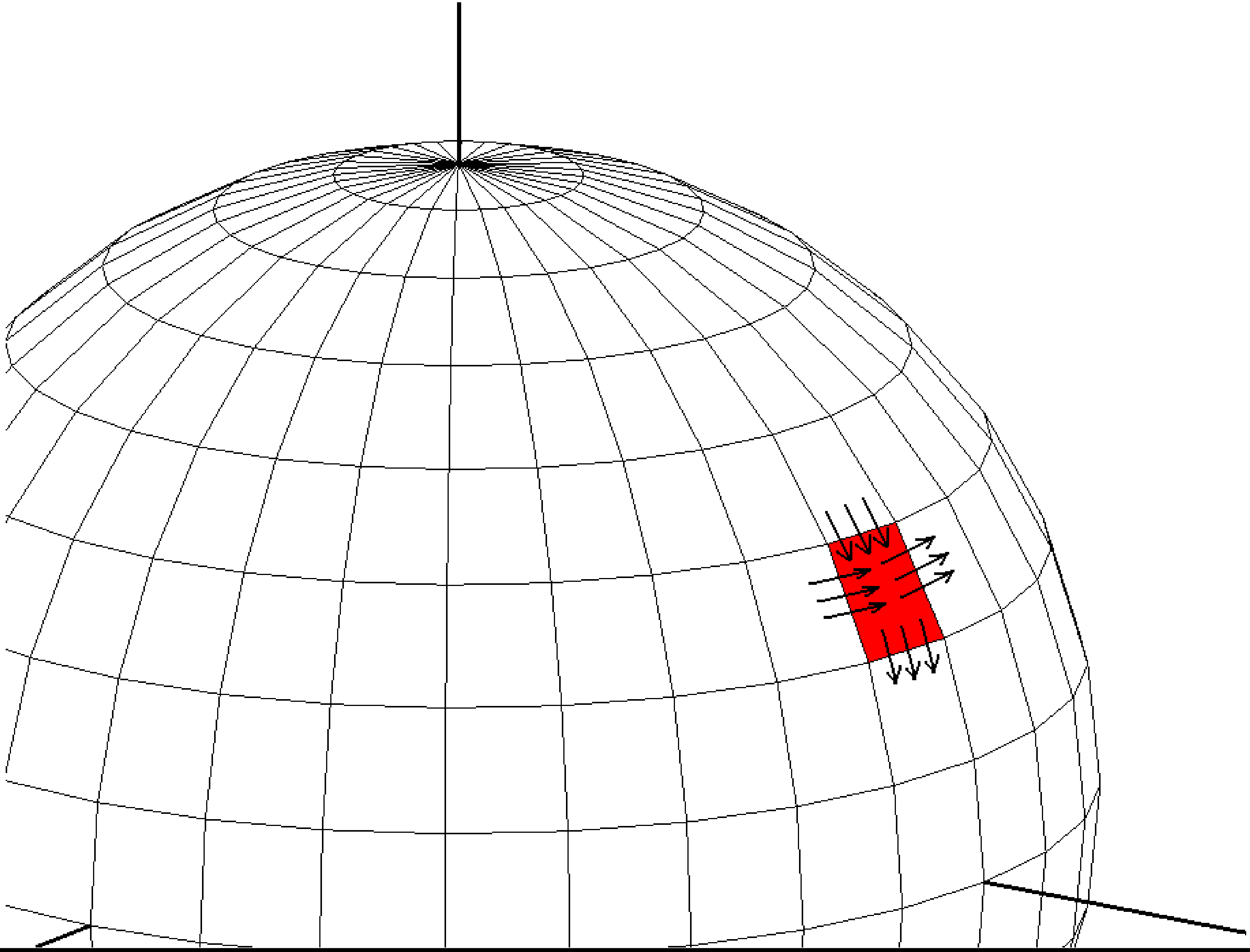
$$\underbrace{\dot{p} = \boldsymbol{W} \cdot p + \xi(\boldsymbol{D} \cdot p}_{\text{viscous stresses}} \quad \underbrace{-\boldsymbol{D} : ppp}_{\text{internal stresses}} \quad)$$

↓

$$\underbrace{\dot{p} = \boldsymbol{W} \cdot p + \xi(\boldsymbol{D} \cdot p}_{\text{viscous stresses}} \quad \underbrace{-\boldsymbol{D} : ppp}_{\text{internal stresses}} \quad) \quad \underbrace{-C_I \dot{\gamma} \tilde{\boldsymbol{\nabla}} \ln \psi}_{\text{fiber-fiber interaction}}$$

Three equations, four unknowns, not solvable.

Folgar-Tucker model



Folgar-Tucker model

$$\dot{\psi} = -\tilde{\boldsymbol{\nabla}} \cdot (\psi \dot{\boldsymbol{p}})$$

$$\dot{\boldsymbol{p}} = \boldsymbol{W} \cdot \boldsymbol{p} + \xi(\boldsymbol{D} \cdot \boldsymbol{p} - \boldsymbol{D} : \boldsymbol{ppp}) - C_I \dot{\gamma} \tilde{\boldsymbol{\nabla}} \ln \psi$$

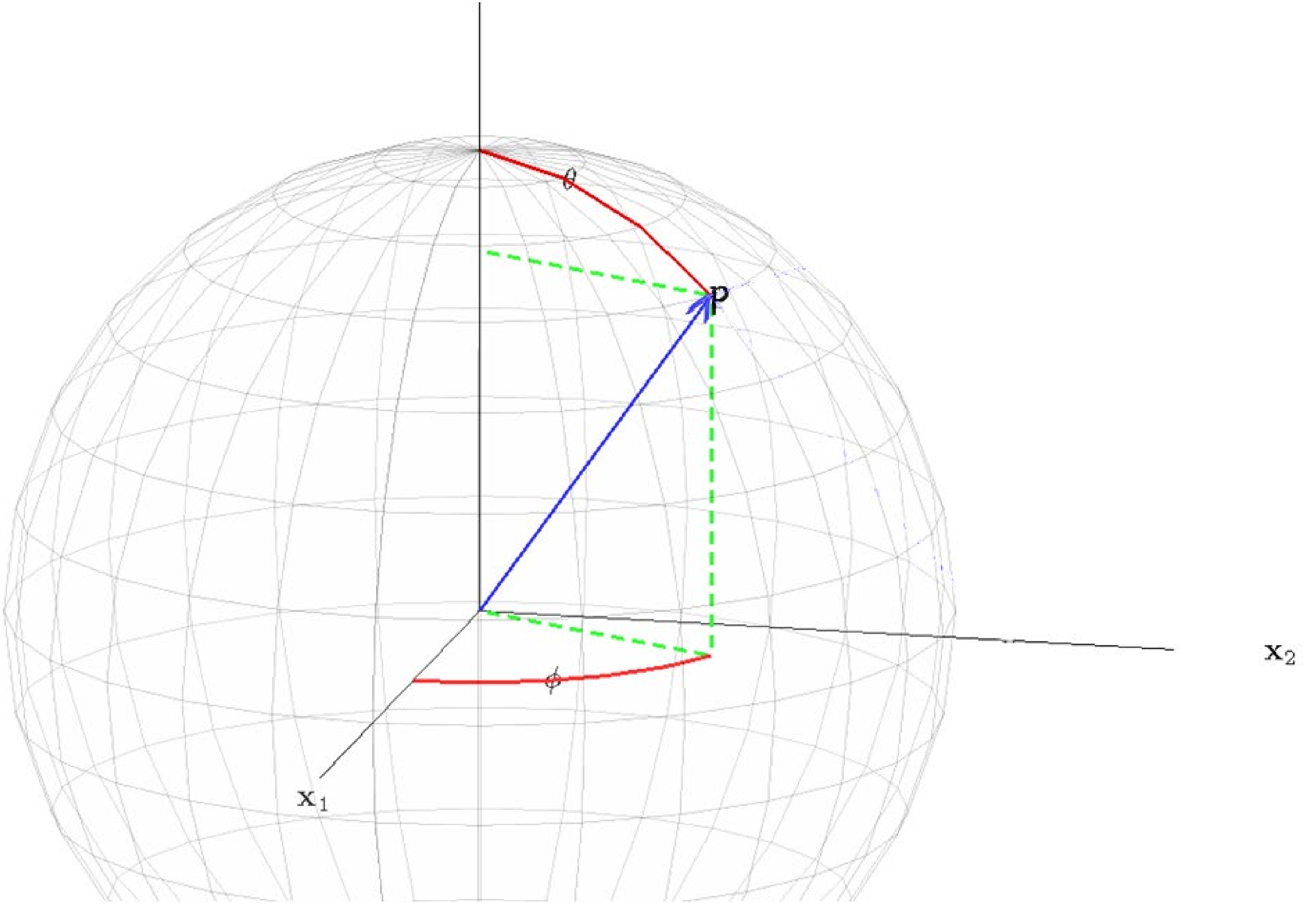
Four equations, four unknowns, so solvable.

Folgar-Tucker model

$$\underbrace{\dot{\psi}}_{\text{time rate of change}} = \underbrace{-\tilde{\boldsymbol{\nabla}} \cdot (\dot{\boldsymbol{p}}_J \psi)}_{\text{convection}} + \underbrace{C_I \dot{\gamma} \tilde{\boldsymbol{\nabla}} \cdot \tilde{\boldsymbol{\nabla}} \psi}_{\text{diffusion}}$$

- Viscous and internal stresses of a *convective* nature.
- Fiber-fiber interaction of a *diffusive* nature.

Jeffery's equation

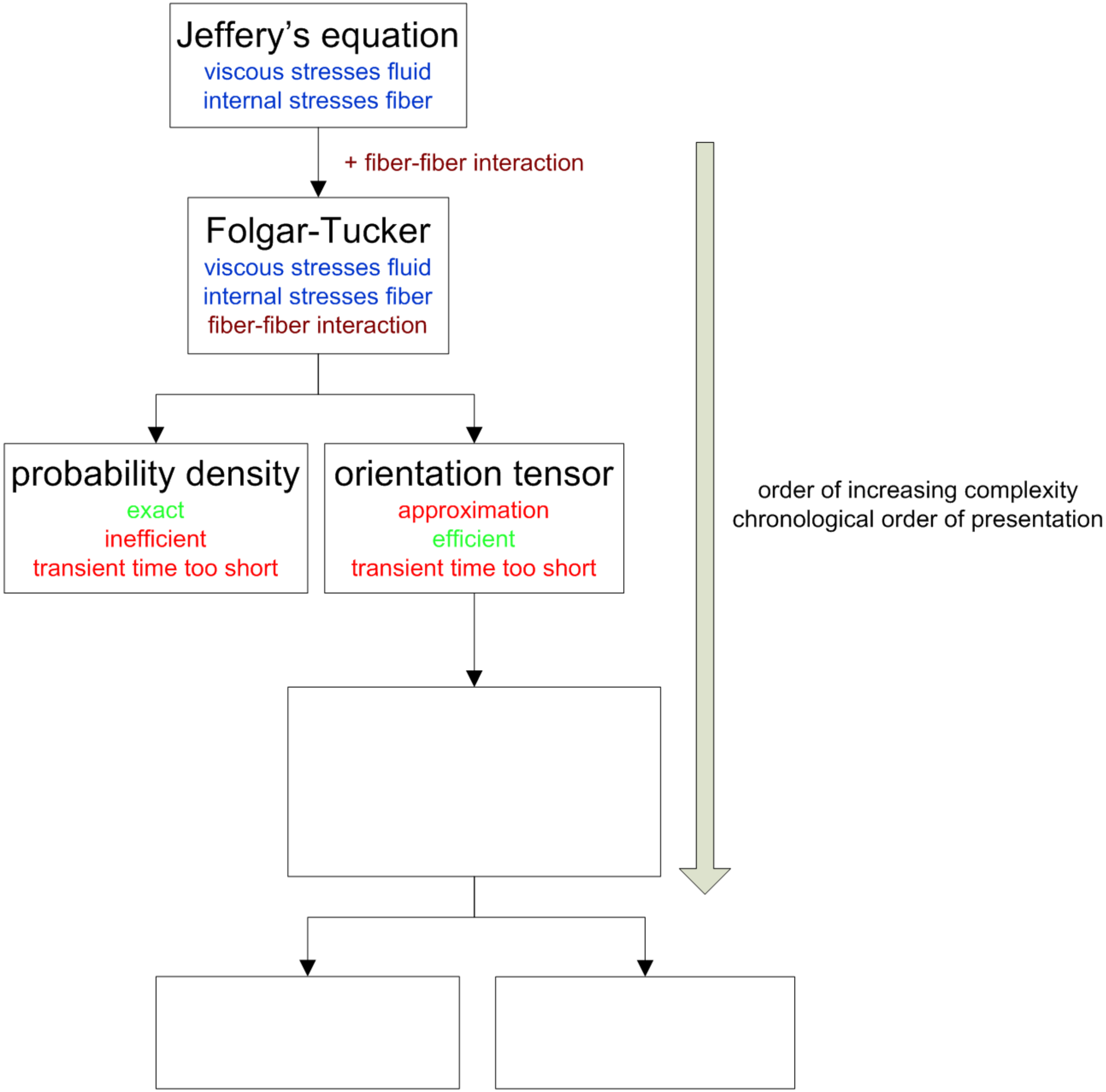


Partial information

Solving the probability density is very demanding in the computational sense.

Is there a computationally less expensive approach?

Layout models



Partial information

$$\psi(\boldsymbol{p},t) = f_0 V_0 + \sum_{i,j}[f_{ij}(\boldsymbol{p})V_{ij}(t)] + \sum_{i,j,k,l}[f_{ijkl}(\boldsymbol{p})V_{ijkl}(t)] + \dots$$

$$= \frac{1}{4\pi} + O(\boldsymbol{p}\otimes\boldsymbol{p}) + O(\boldsymbol{p}\otimes\boldsymbol{p}\otimes\boldsymbol{p}\otimes\boldsymbol{p}) + \dots$$

--> less information

The only unknowns are the *orientation tensors*

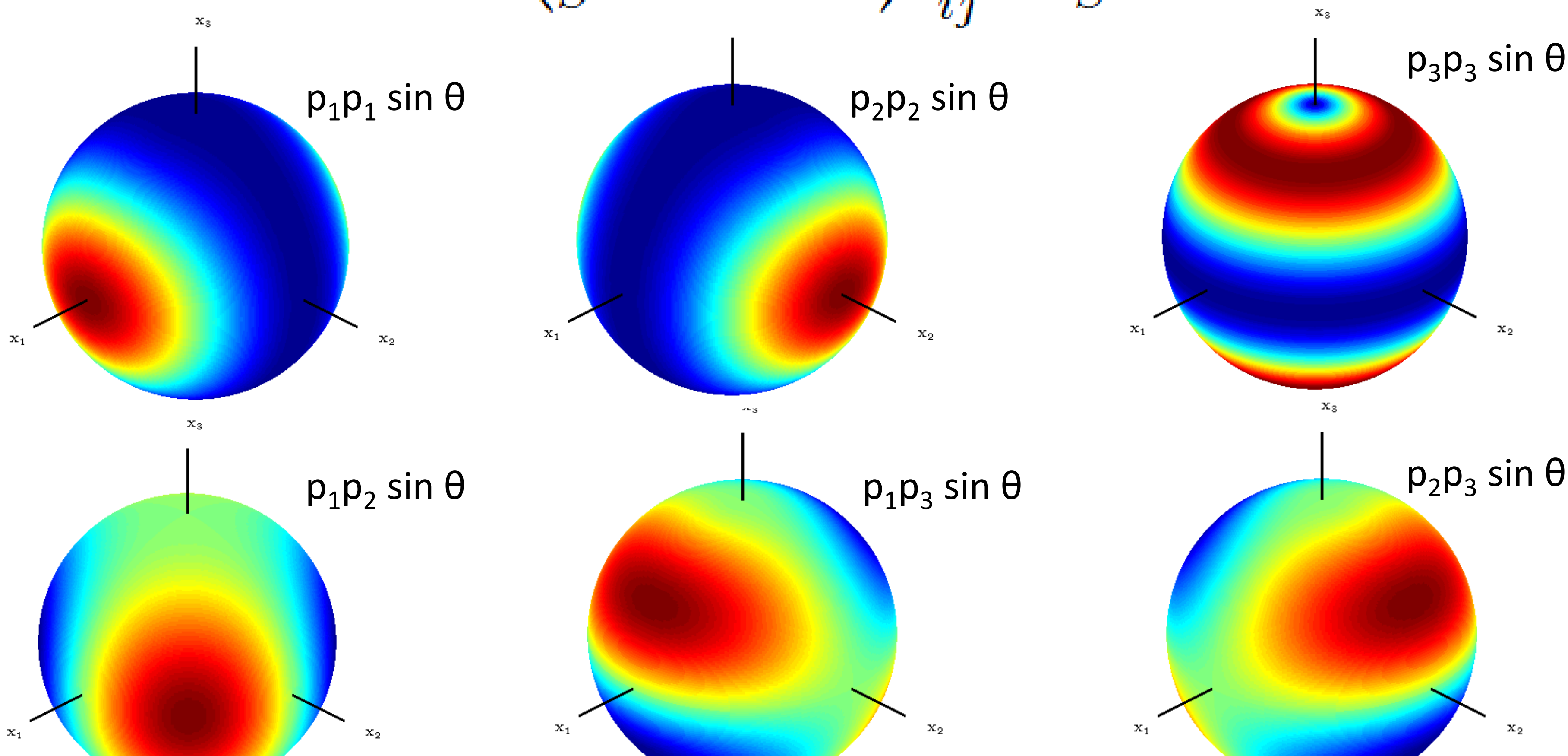
$$\mathbf{A}(t) = \oint_S \psi(\boldsymbol{p},t)\boldsymbol{p}\boldsymbol{p}\, d^2\boldsymbol{p}, \quad \mathbb{A}(t) = \oint_S \psi(\boldsymbol{p},t)\boldsymbol{p}\boldsymbol{p}\boldsymbol{p}\boldsymbol{p}\, d^2\boldsymbol{p}, \quad \dots.$$

Sum is infinite! **Maybe a set of lower order terms already give enough information on the fiber orientation.**

Partial information

Let us first consider the *symmetric* second order tensor.

$$A_{ij} := (\boldsymbol{A})_{ij} = \left(\oint\limits_S \psi \boldsymbol{p}\boldsymbol{p} \, d^2\boldsymbol{p} \right)_{ij} = \oint\limits_S \psi p_i p_j \, d^2\boldsymbol{p}.$$



Partial information

The orientation tensor already gives sufficient information on the fiber orientation.

But can it be solved more efficiently?

Folgar-Tucker tensor form

The rate equation for A.

$$\dot{\boldsymbol{A}} = \boldsymbol{W} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot \boldsymbol{W} + \xi(\boldsymbol{D} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{D} - 2\mathbb{A} : \boldsymbol{D}) + 2C_I\dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{A})$$

Not a function of orientation p. Only of time t.

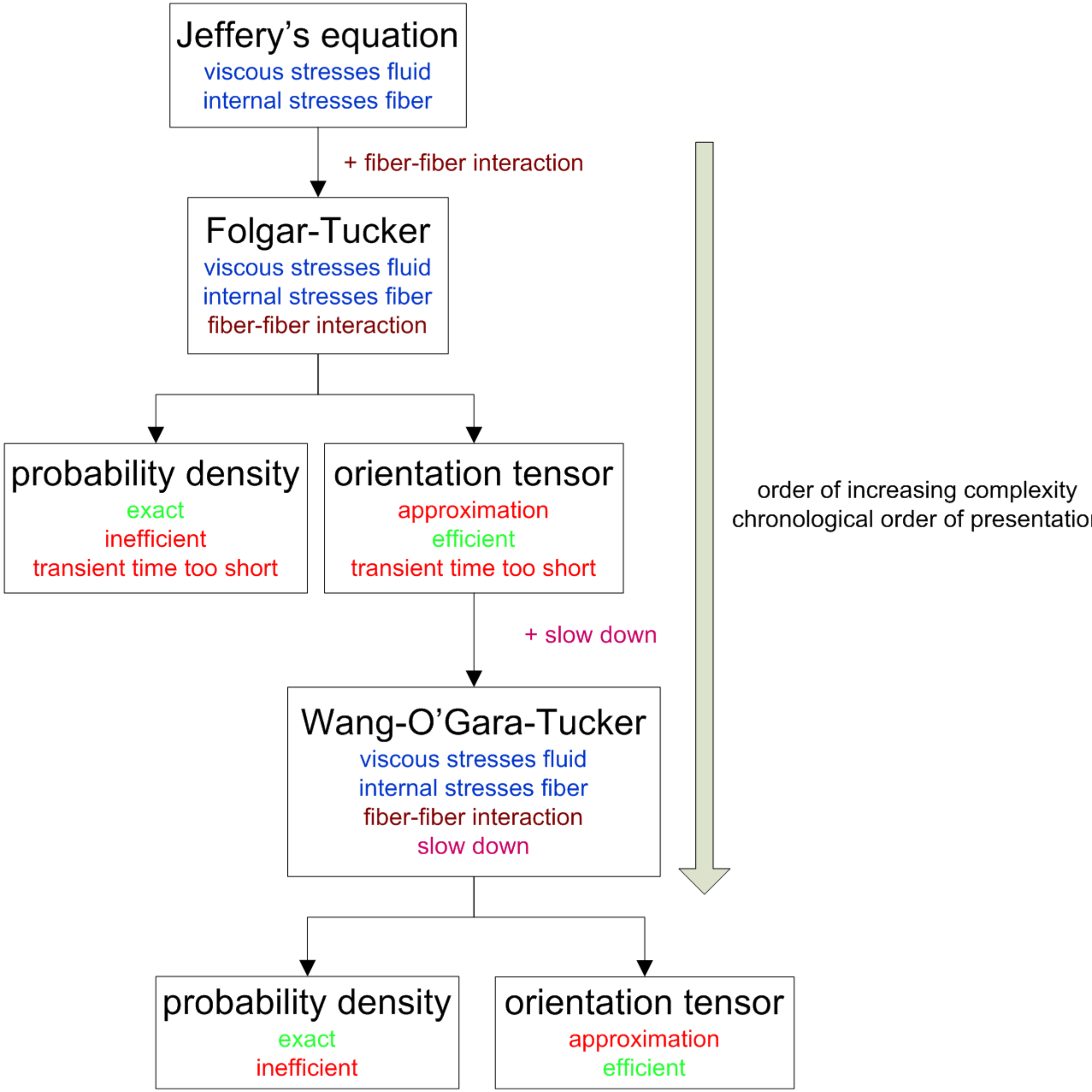
We have realized a reduction of the #DOF from three to one. **The tensor form can be solved more efficiently**.

The rate equation for A.

$$\dot{\boldsymbol{A}} = \boldsymbol{W} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot \boldsymbol{W} + \xi(\boldsymbol{D} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{D} - 2\mathbb{A} : \boldsymbol{D}) + 2C_I \dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{A})$$

Comparison with experimental results show that the transient time is too short.

Layout models



Correction

We need to ‘correct’ the rate equation.

How should we do this?

Correction

A straightforward way would be

$$\dot{\boldsymbol{A}} = \boldsymbol{W} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot \boldsymbol{W} + \xi(\boldsymbol{D} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{D} - 2\mathbb{A} : \boldsymbol{D}) + 2C_I\dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{A})$$

↓

$$\dot{\boldsymbol{A}} = \kappa\left(\boldsymbol{W} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot \boldsymbol{W} + \xi(\boldsymbol{D} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{D} - 2\mathbb{A} : \boldsymbol{D}) + 2C_I\dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{A})\right), \quad 0 < \kappa < 1$$

Model is not objective.

Wang-O'Gara-Tucker

In 2008, Wang, O'Gara and Tucker found a way to prolong the transient time in an objective way.

Because the orientation tensor is symmetric, it has a *spectral decomposition*.

$$\boldsymbol{A} = \sum_i \lambda_i \boldsymbol{e}_i \boldsymbol{e}_i$$

$$\begin{aligned} \dot{\lambda}_i &= f(\lambda_i, \boldsymbol{e}_i) \\ \dot{\boldsymbol{e}}_i &= \boldsymbol{g}(\lambda_i, \boldsymbol{e}_i) \end{aligned} \longrightarrow \begin{aligned} \dot{\lambda}_i &= \kappa f(\lambda_i, \boldsymbol{e}_i) \\ \dot{\boldsymbol{e}}_i &= \boldsymbol{g}(\lambda_i, \boldsymbol{e}_i) \end{aligned}$$

$$0 < \kappa \leq 1$$

Wang-O'Gara-Tucker

$$\dot{\boldsymbol{A}} = \boldsymbol{W} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot \boldsymbol{W} + \xi(\boldsymbol{D} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{D} - 2\mathbb{A} : \boldsymbol{D}) + 2C_I\dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{A})$$

$$\downarrow$$

$$\dot{\boldsymbol{A}} = \boldsymbol{W} \cdot \boldsymbol{A} - \boldsymbol{A} \cdot \boldsymbol{W} + \xi\{\boldsymbol{D} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \boldsymbol{D} - 2[\mathbb{A} + (1-\kappa)(\mathbb{L} - \mathbb{M} : \mathbb{A})] : \boldsymbol{D}\} + 2\kappa C_I\dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{A})$$

$$\mathbb{L} = \sum_i \lambda_i \boldsymbol{e}_i\boldsymbol{e}_i\boldsymbol{e}_i\boldsymbol{e}_i \quad \wedge \quad \mathbb{M} = \sum_i \boldsymbol{e}_i\boldsymbol{e}_i\boldsymbol{e}_i\boldsymbol{e}_i$$

Is objective!

But the equation is not solvable.

Closure approximation

Fourth order tensor is unknown.

$$\mathbb{A}(t) = \oint_S \psi(\boldsymbol{p},t)\boldsymbol{pppp}d^2\boldsymbol{p}$$

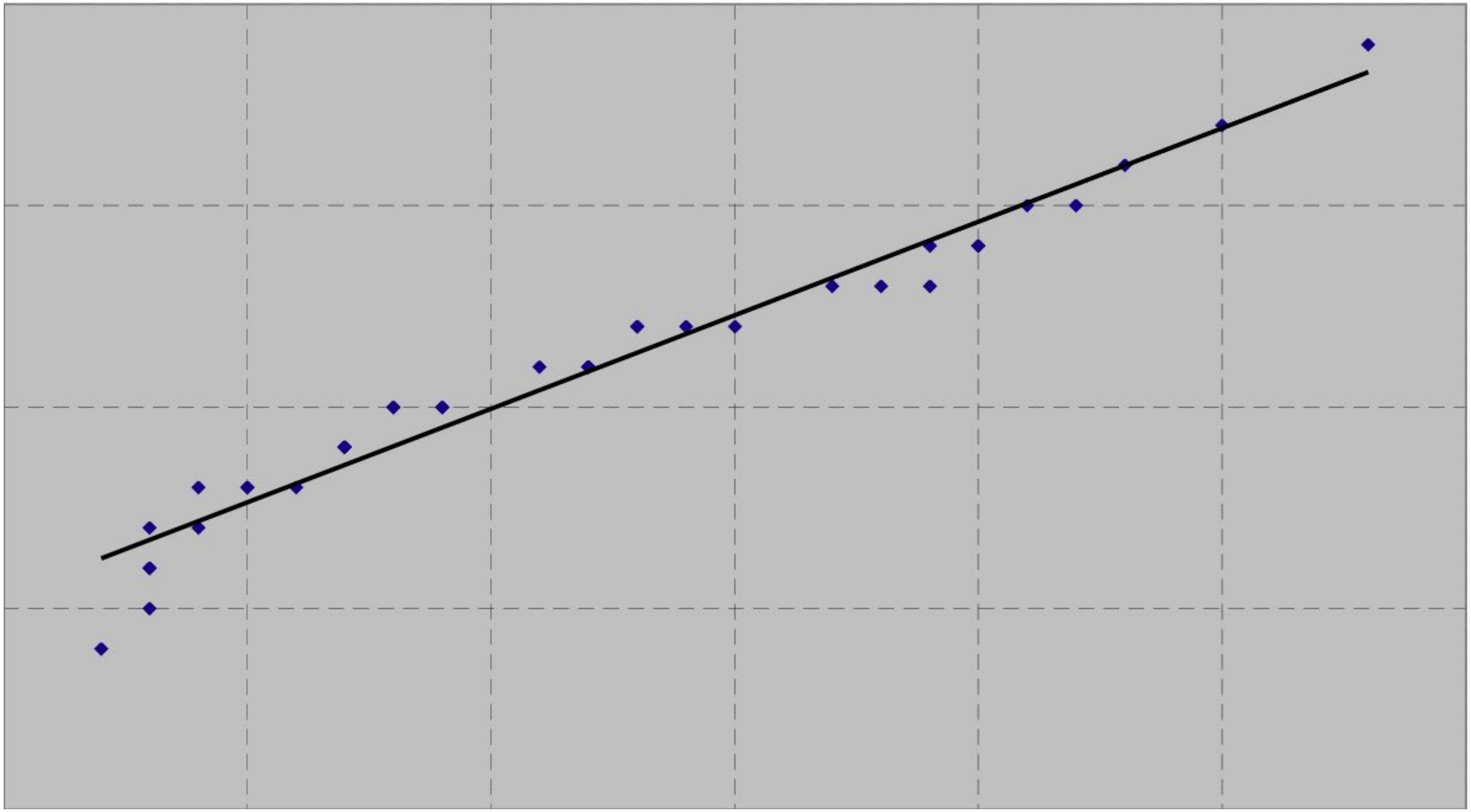
With relations with the second order orientation tensor and solving ψ for some easy cases, we can construct

$$\mathbb{A} = \mathbb{F}(\boldsymbol{A})$$

and solve the rate equation.

F is called a *closure approximation* as it close the problem in an approximate way.

The idea is *fitting*.

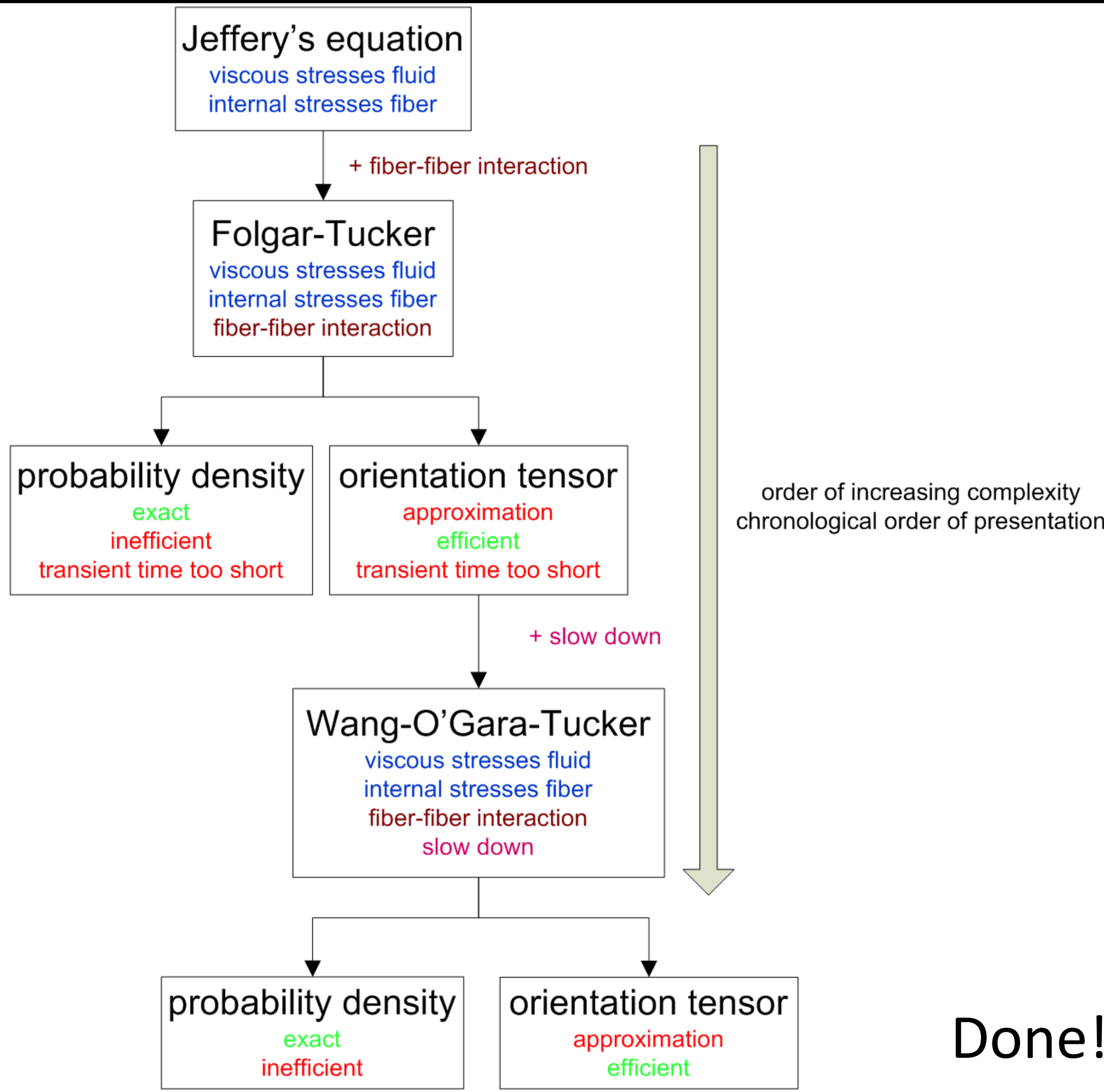


The F can be constructed in many ways!

Closure approximation

We have to investigate the quality of the approximation.

Layout models



Done!

Solution strategy

We solve the equations with

- finite volume method in space and
- Euler forward in time

for the probability density function, and

- Euler forward in time
- several closure approximations

for the orientation tensor.

We have to compare the *quality of the approximations*.

Test case

Simple shear

Simple shear flow field is described by

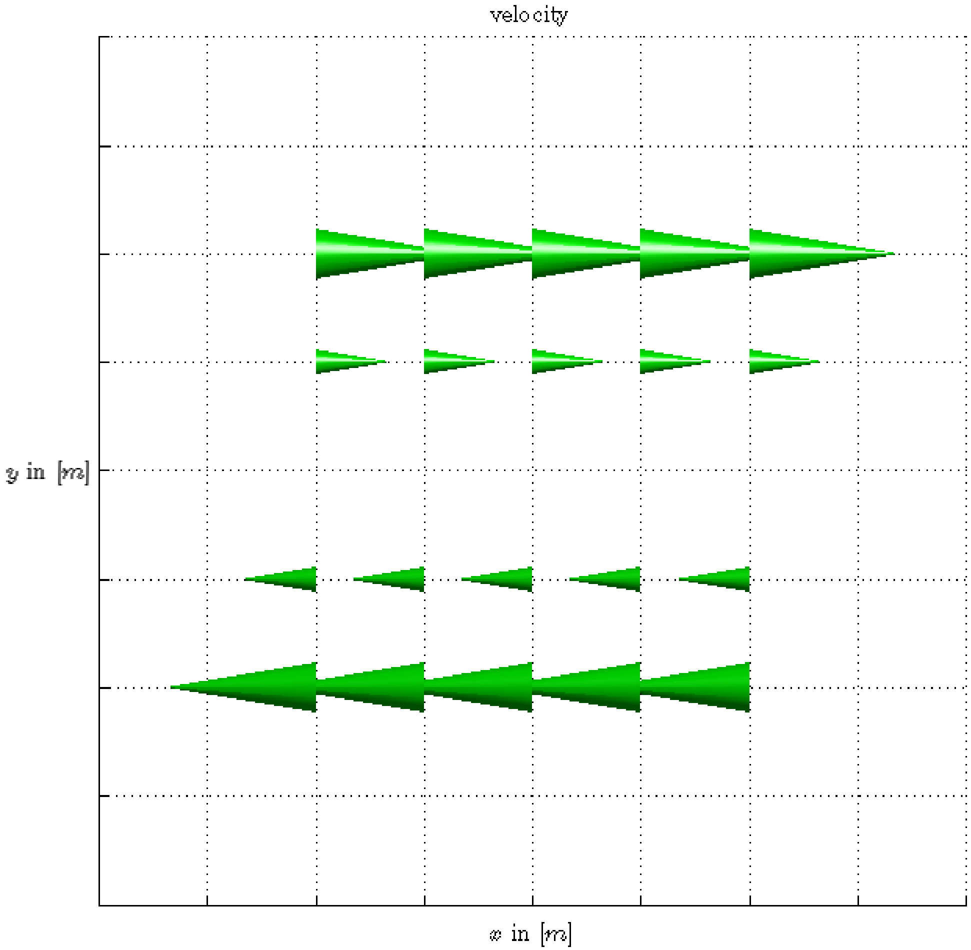
$$\boldsymbol{v} = \begin{bmatrix} 0 & G & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \cdot \boldsymbol{x} = \begin{bmatrix} Gx_2 \\ 0 \\ 0 \end{bmatrix}$$

v = velocity in [m/s]

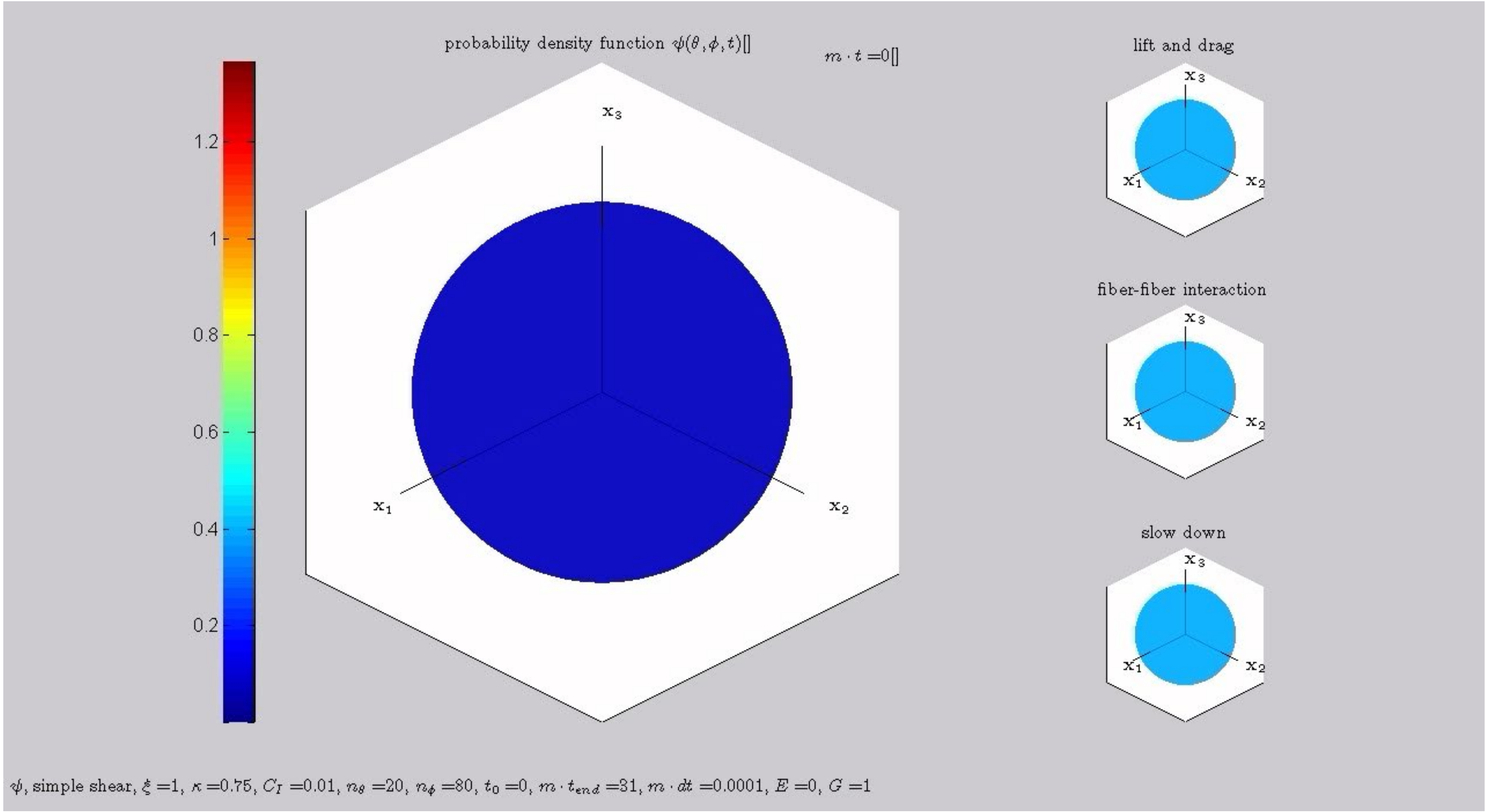
x = space in [m]

G = shear rate in [1/s]

Simple shear flow field



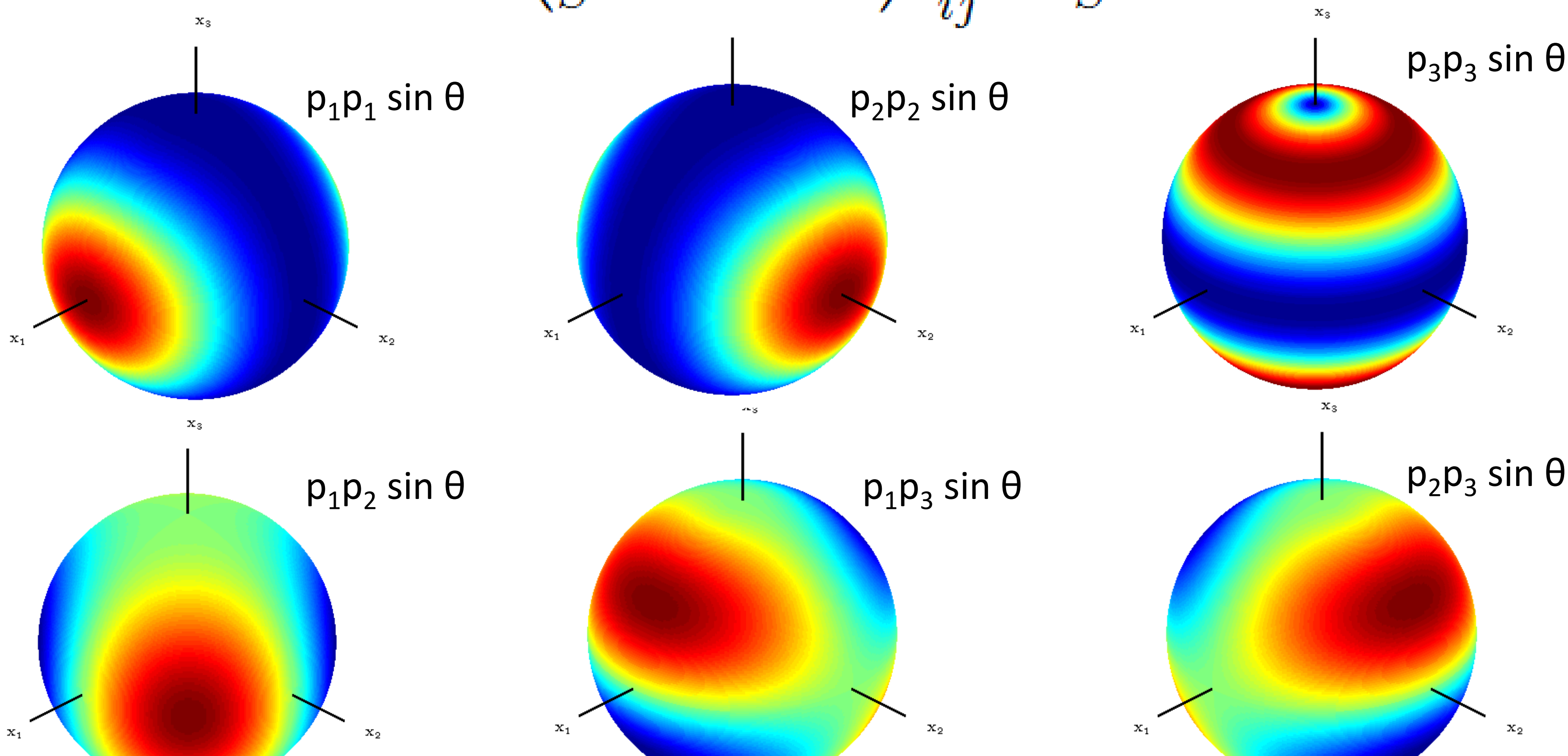
Simple shear



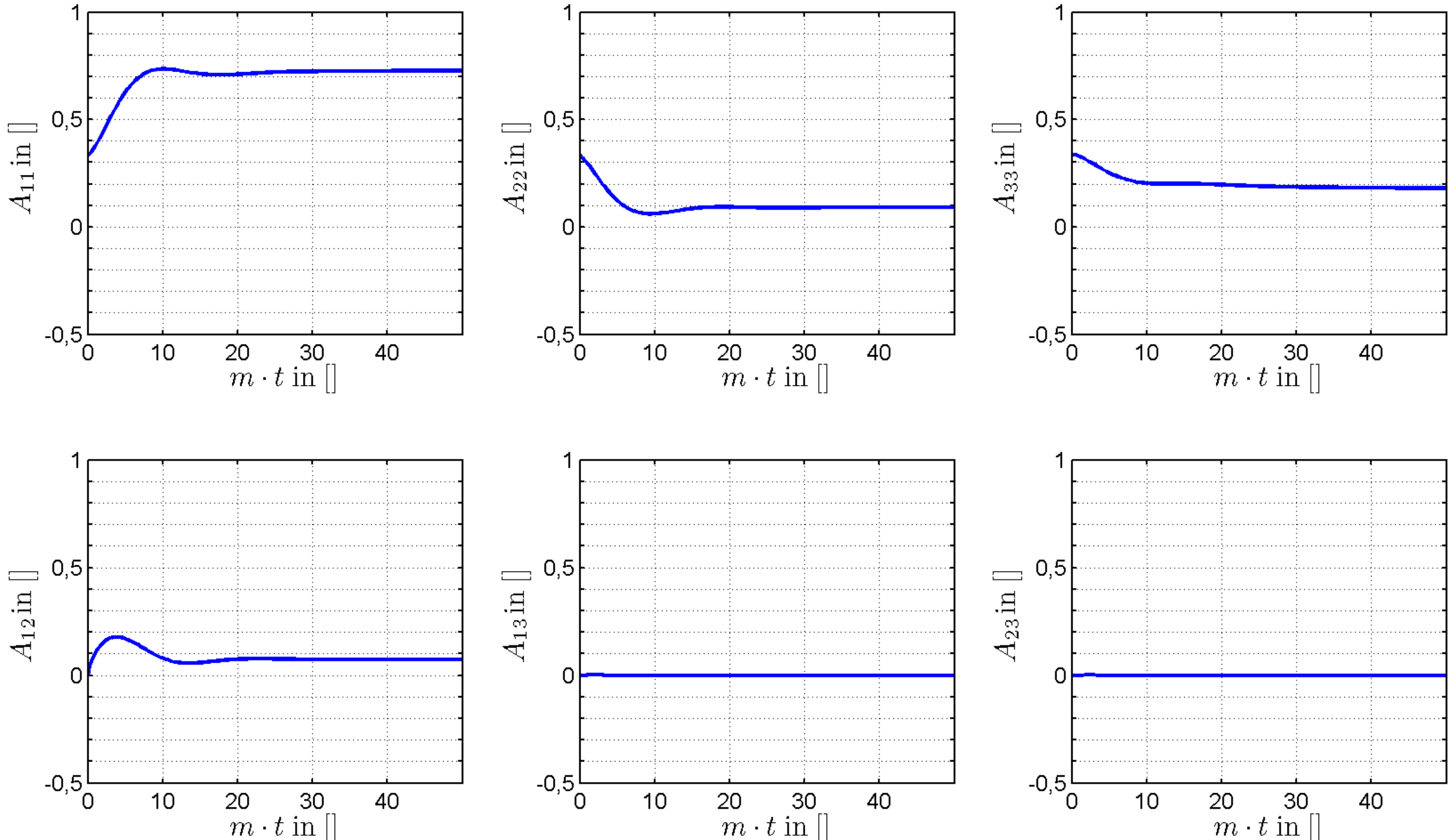
Partial information

Let us consider the *symmetric* second order tensor.

$$A_{ij} := (\boldsymbol{A})_{ij} = \left(\oint_S \psi \boldsymbol{p}\boldsymbol{p}\, d^2\boldsymbol{p} \right)_{ij} = \oint_S \psi p_i p_j \, d^2\boldsymbol{p}.$$

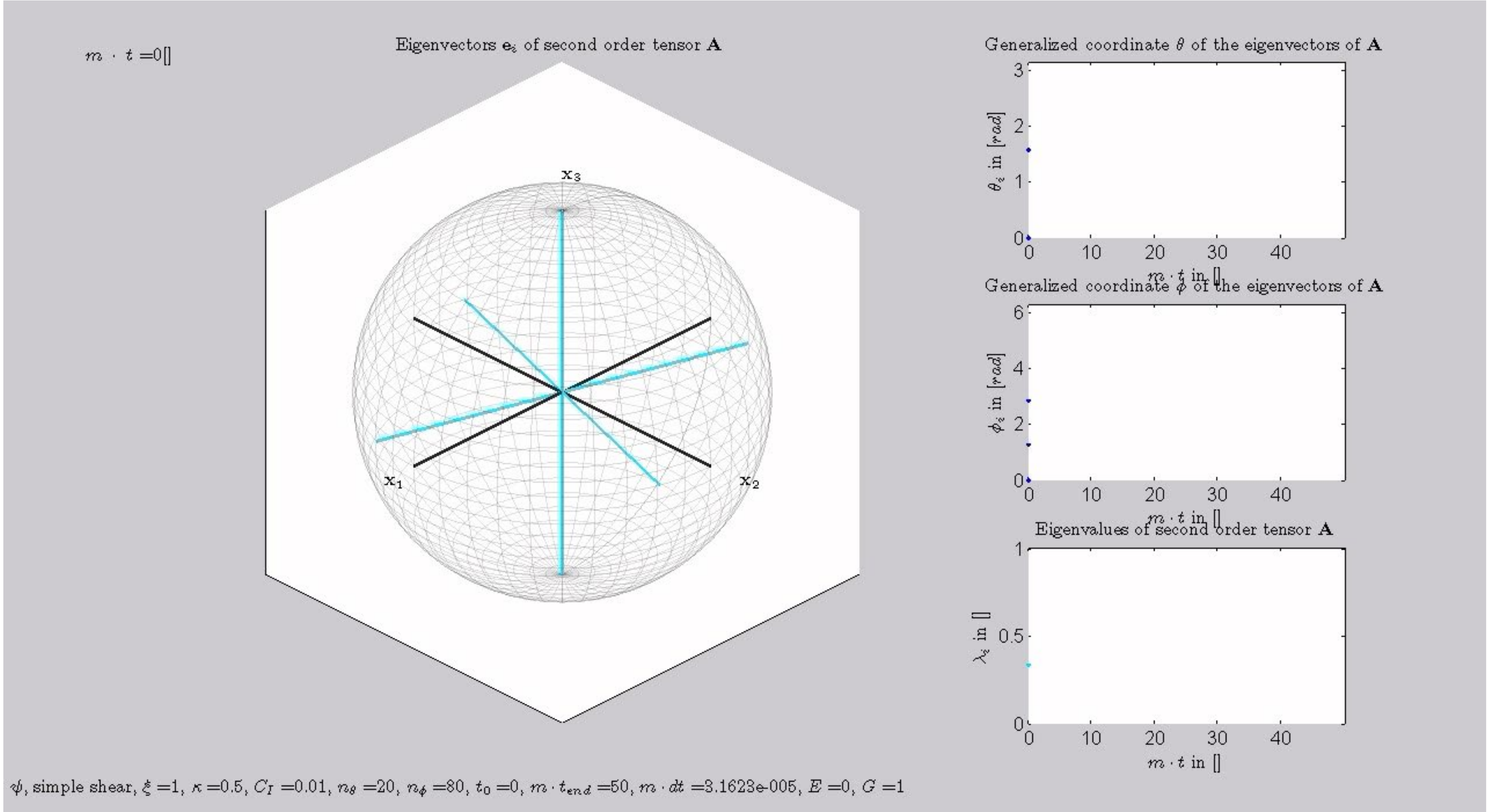


Simple shear



ψ, simple shear, $\xi = 1$, $\kappa = 0.5$, $C_I = 0.01$, $n_\theta = 20$, $n_\phi = 80$, $t_0 = 0$, $m \cdot t_{end} = 50$, $m \cdot dt = 3.1623\text{e-}005$, $E = 0$, $G = 1$

Simple shear



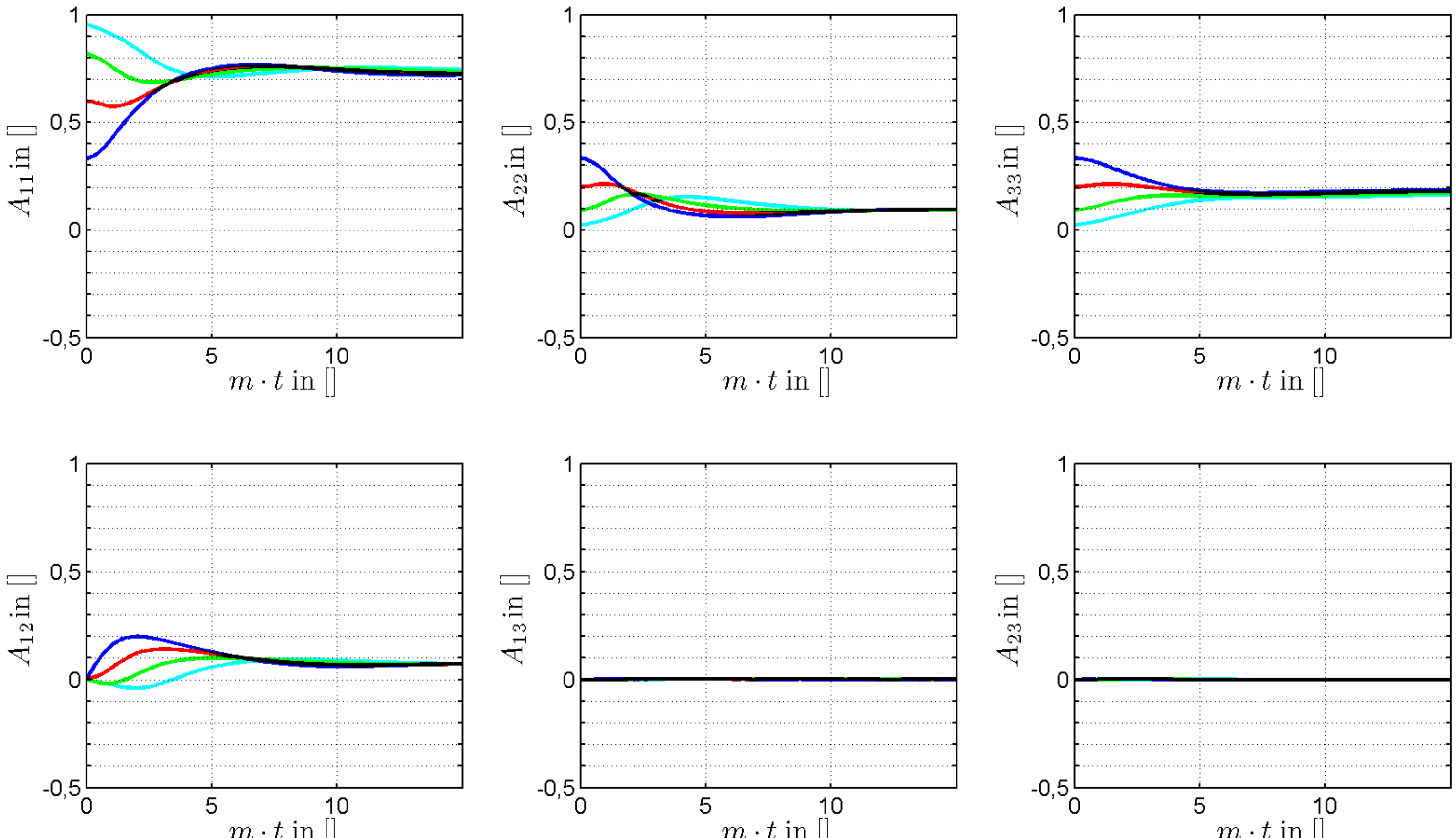
Simple shear

Balance between contributions can be varied by changing

- the *initial condition* and
- the *time dependence of the strain and shear rates*.

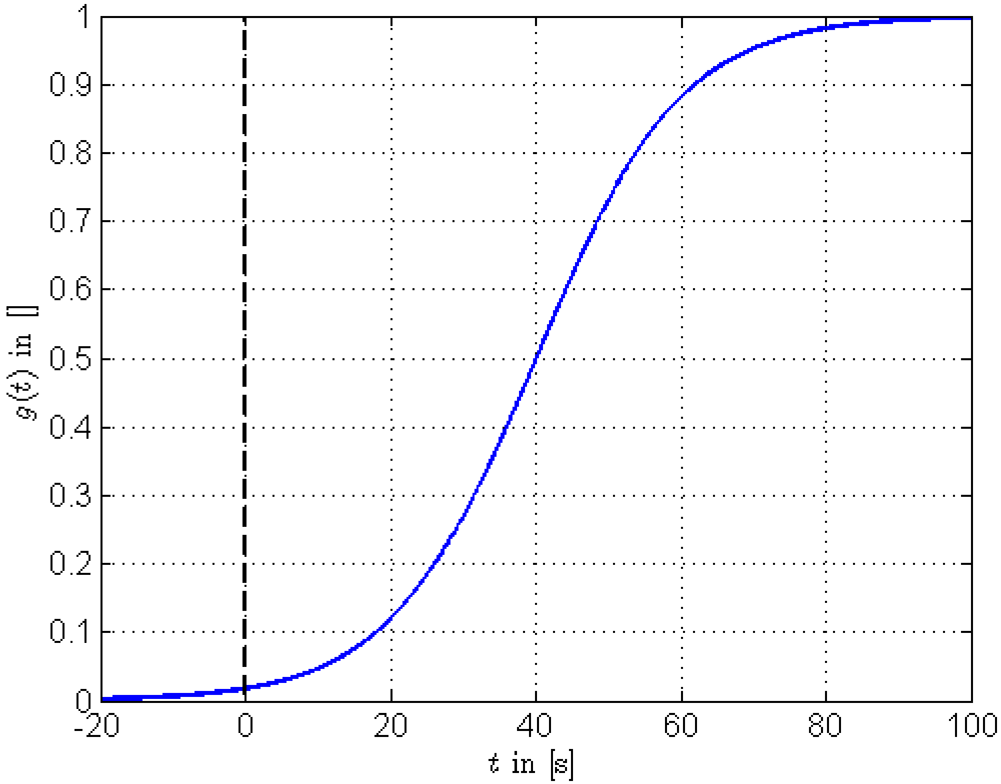
Gives an indication of *dependence on history*.

ICs taken with orientation already towards the x_1 direction

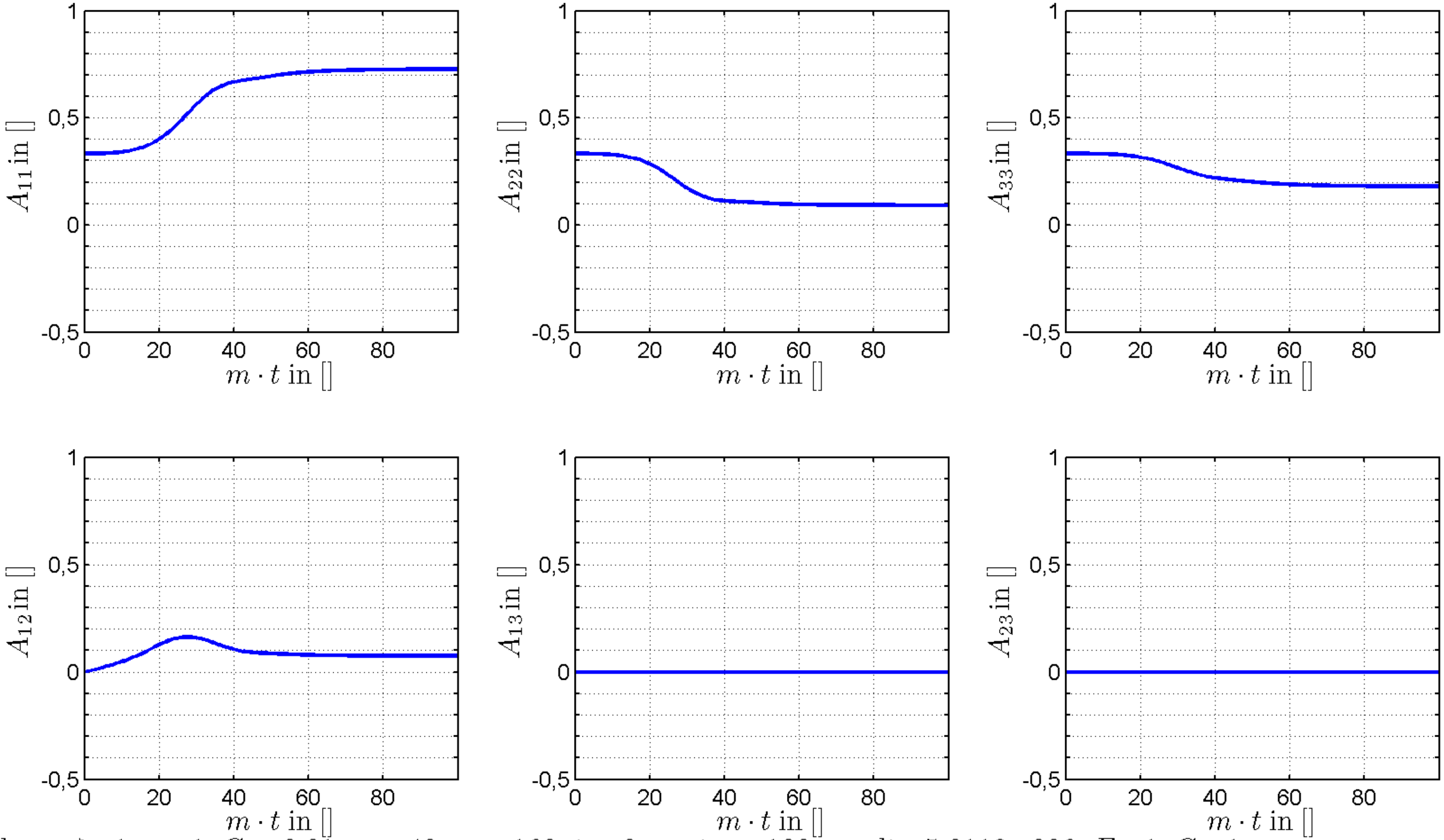


ψ, simple shear, $\xi = 1$, $\kappa = 1$, $C_I = 0.01$, $n_\theta = 40$, $n_\phi = 160$, $t_0 = 0$, $m \cdot t_{end} = 15$, $m \cdot dt = 5.0119\text{e-}006$, $E = 1$, $G = 1$

Simple shear

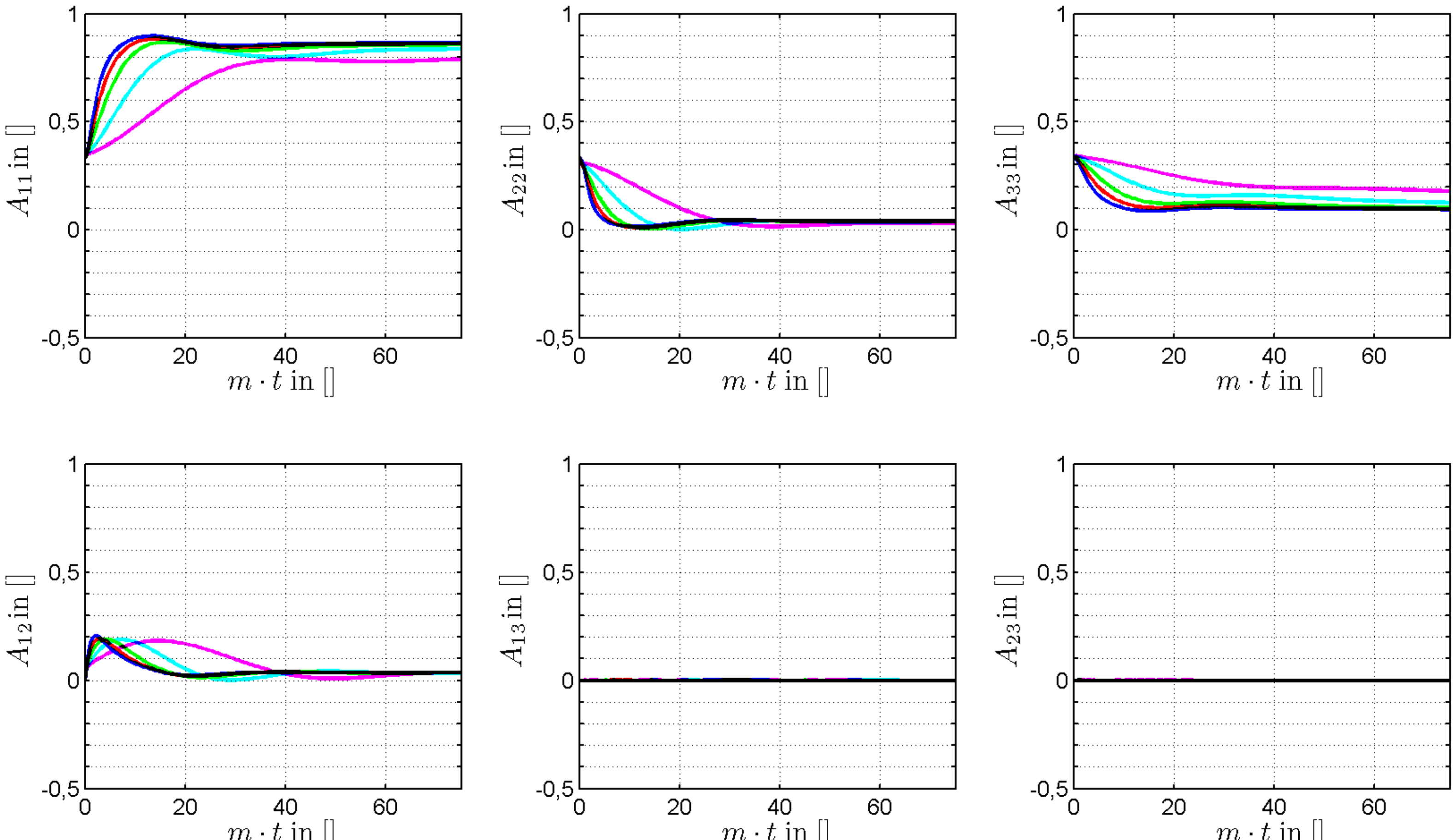


Simple shear



ψ, simple shear, $\xi = 1$, $\kappa = 1$, $C_I = 0.01$, $n_\theta = 40$, $n_\phi = 160$, $t_0 = 0$, $m \cdot t_{end} = 100$, $m \cdot dt = 5.0119\text{e-}006$, $E = 1$, $G = 1$

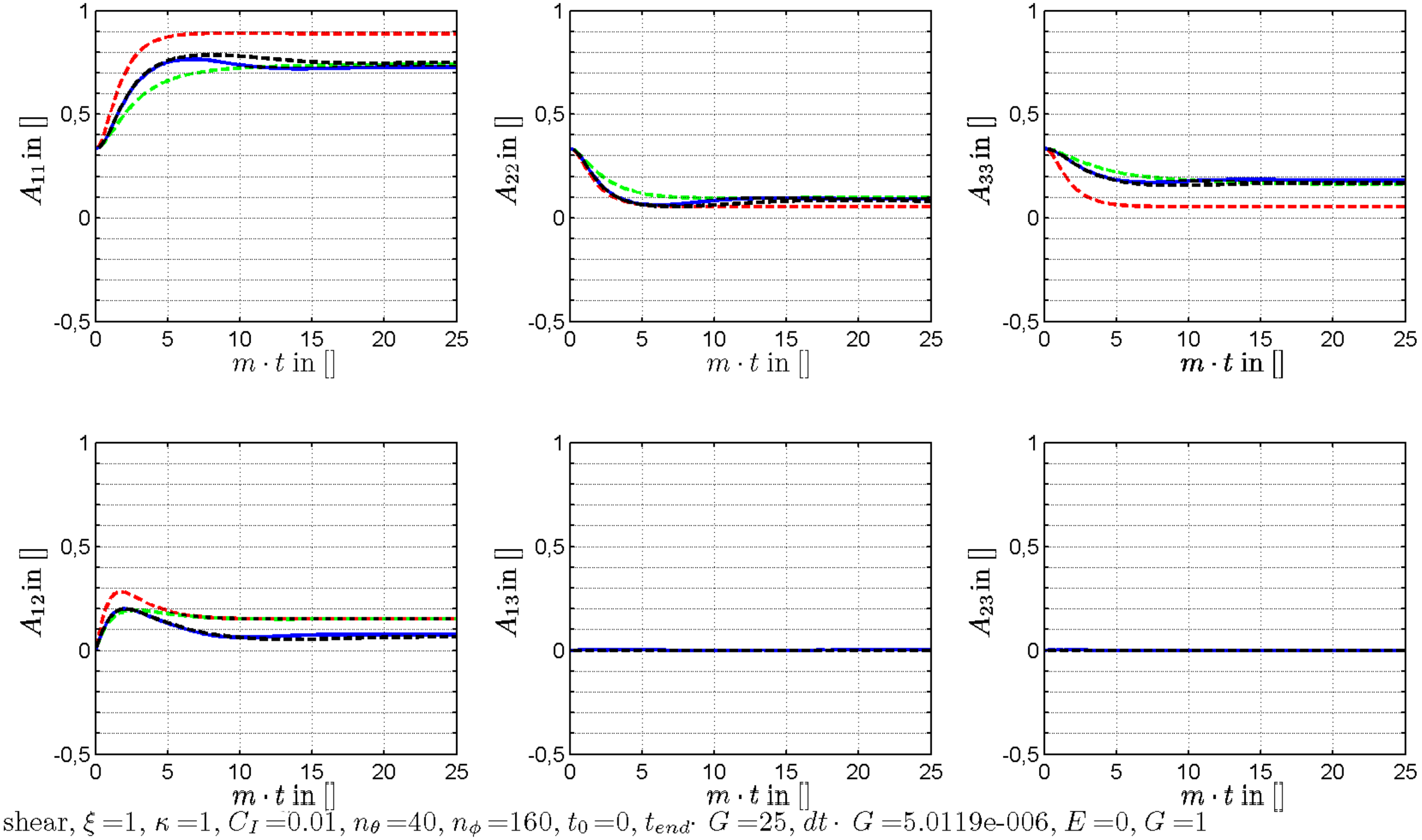
Phenomenological parameter kappa to prolong the transient time.



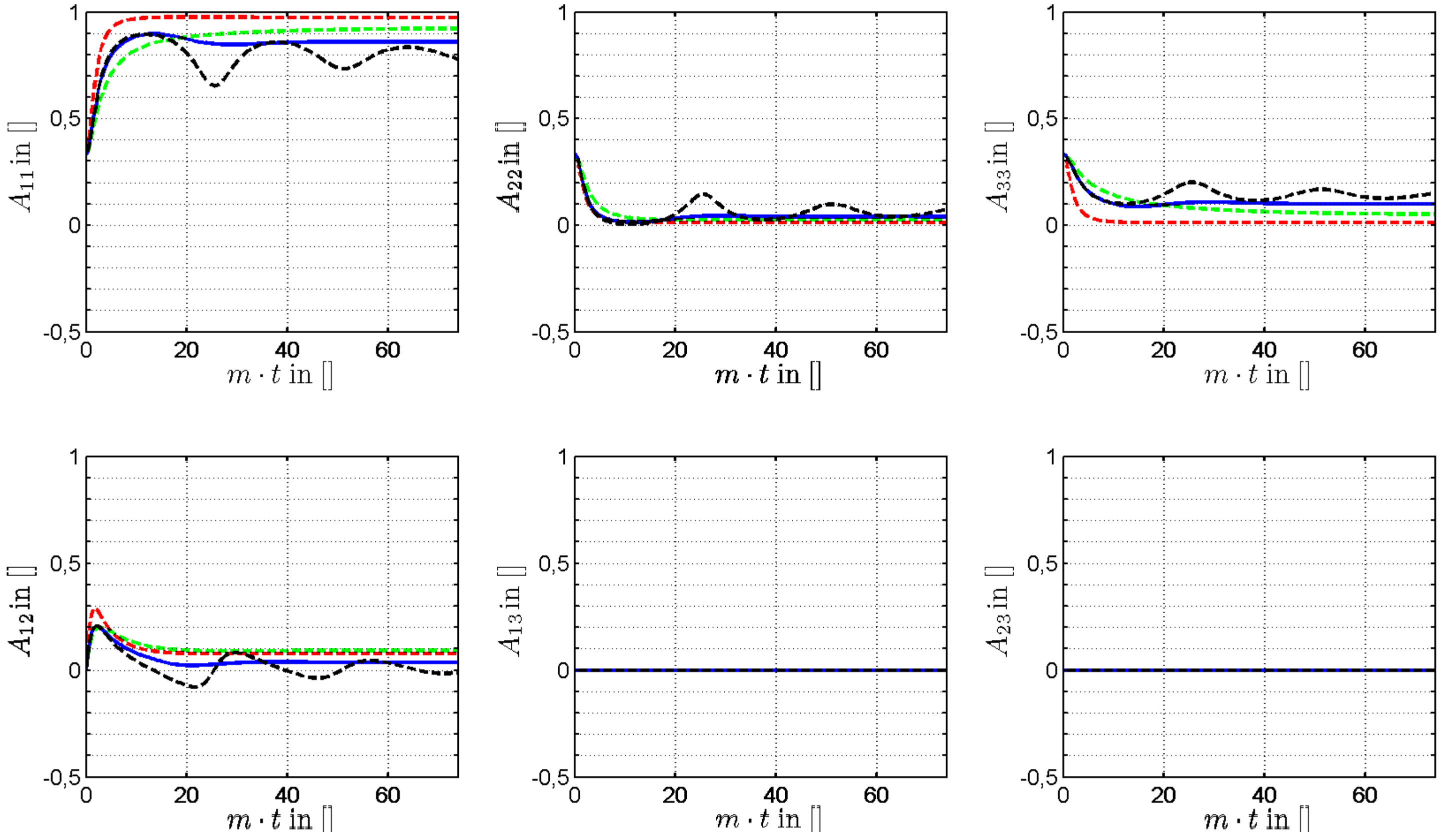
ψ, simple shear, $\xi = 1$, $\kappa = 1$, $C_I = 0.001$, $n_\theta = 20$, $n_\phi = 80$, $t_0 = 0$, $m \cdot t_{end} = 75$, $m \cdot dt = 3.1623\text{e-}005$, $E = 0$, $G = 1$

Simple shear

Comparison of the solutions of the kinetic theory and the tensor approximations.



Taking another parameter set results in a *decay of the quality* of the approximations.



simple shear, $\xi = 1$, $\kappa = 1$, $C_I = 0.001$, $n_\theta = 50$, $n_\phi = 200$, $t_0 = 0$, $t_{end} \cdot G = 74$, $dt \cdot G = 1e\text{-}005$, $E = 0$, $G = 1$

Conclusions and recommendations

Conclusions and recommendations

Conclusions

- The numerical approach for the probability density and orientation tensor are sufficiently fast.
- The convection and diffusion of the probability density strongly depend on the initial condition and the time dependence of the strain and shear rates.
- The slow down will help fitting to experimental results.
- The quality of the closure approximations varies with the parameters and the flow fields.

Recommendations

- Further study of the literature.
- Closure approximations should be investigated.

Questions?