Multiphase Flow Laboratory
University of Udine

COST Training Schoool (Action FP1005)

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Project supported by COST - European Cooperation in Science and Technology

Lecture 2:
The Art of Modelling
Elongated Particles as Points

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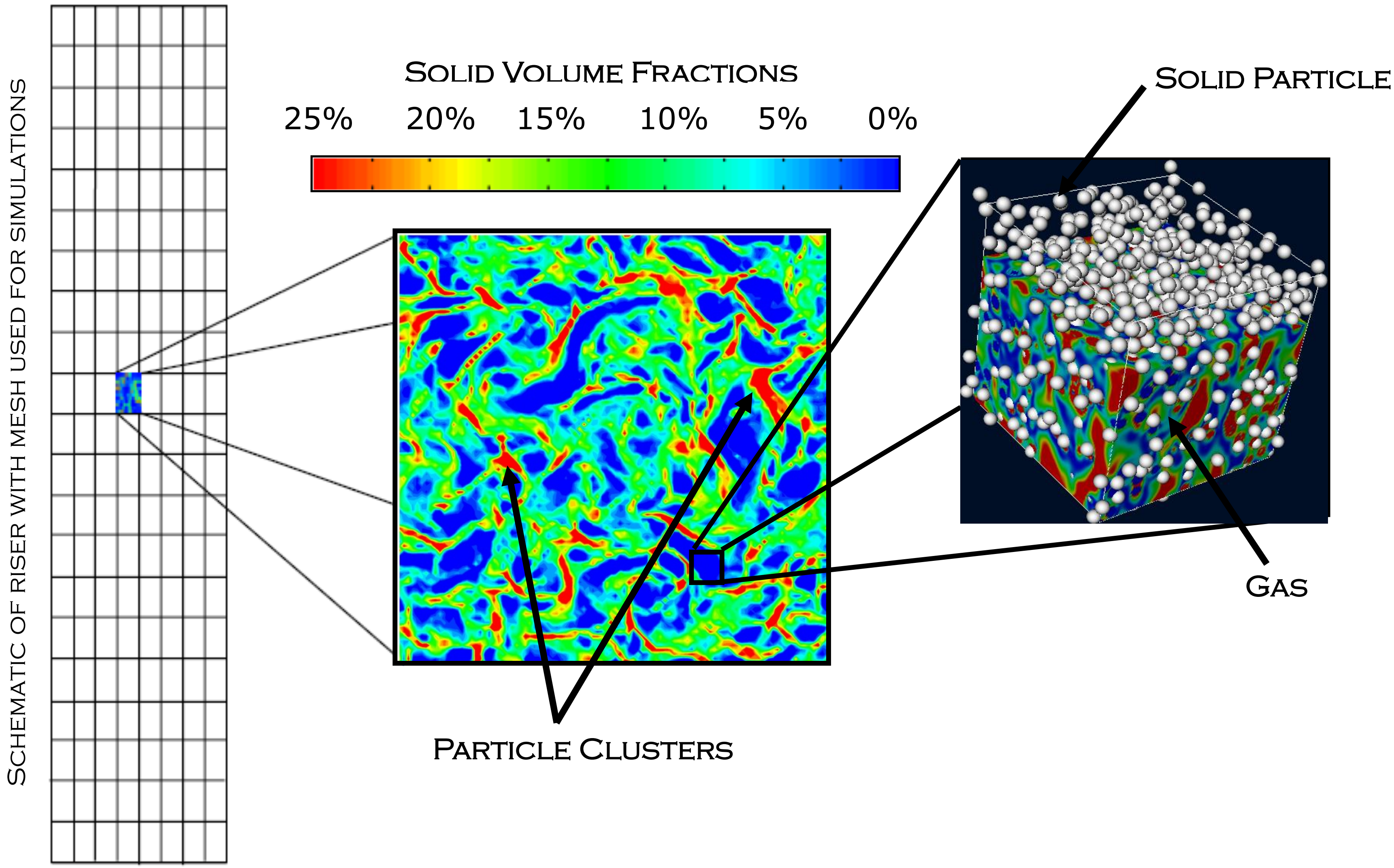
PREMISE: MULTIPHASE FLOWS ARE MULTISCALE -> HIERARCHIC APPROACH

GLOBAL APPROACH | SIMULATION OF FLOW DYNAMICS | DNS/LES: LOCAL



Macro-scale (cm-m) Meso-scale (mm – cm) Micro-scale (μm)

Outline of Lecture 2

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1.1 Multi-Parameter Description of Non-Spherical Particle Dynamics
- 1.1.1 Lagrangian Equations of Motion

1.2 Translational Dynamics
- 1.2.1 Force Models (Drag, Lift)

1.3 Kinematics
- 1.3.1 frames of reference
- 1.3.2 transformation matrix
- 1.3.3 quaternions

1.4 Rotational Dynamics
- 1.4.1 rotational torque

1.5 Example: rigid fibers in (dilute) turbulent channel flow

1.6 Homework

The Pointwise Approximation

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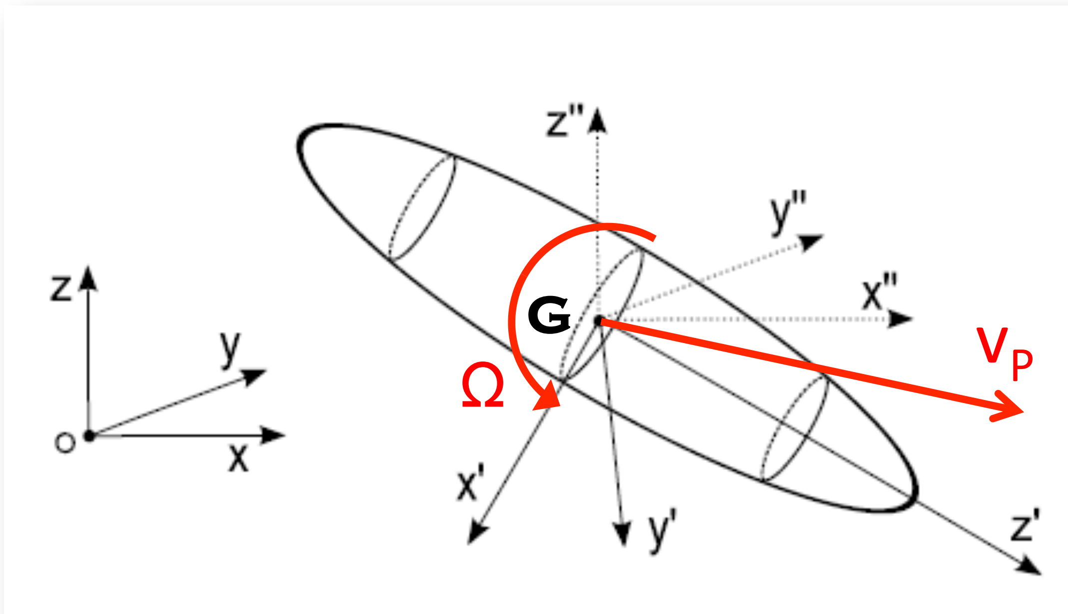
The simplest approach to deal with non-spherical particles is to describe their translation and rotation with a "lumped-variable" model



Basically, our particle is a Lagrangian point moving in a 3D space.

Finite-size effects are neglected.

Recall: Lagrangian Equation of Particle Motion

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- Translational dynamics (enough for a spherical particle)

$$m_p \frac{d\mathbf{v}_p}{dt} = \sum_i \mathbf{F}_i = \mathbf{F}_D + \mathbf{F}_g + \mathbf{F}_L + \mathbf{F}_{PG} + \mathbf{F}_{AM} + \mathbf{F}_B + \ldots$$

- Rotational dynamics (needed for a non-spherical particle)

$$\begin{cases} I_x \dfrac{d\omega_x}{dt} = \sum_i T_{x,i} + \omega_y \omega_z \left(I_y - I_z\right) \\ I_y \dfrac{d\omega_y}{dt} = \sum_i T_{y,i} + \omega_z \omega_x \left(I_z - I_x\right) \\ I_z \dfrac{d\omega_z}{dt} = \sum_i T_{z,i} + \omega_x \omega_y \left(I_x - I_y\right) \end{cases}$$

Modelling Forces for Non-Spherical Particles

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Consider translational dynamics first.

We need force models that account for shape and orientation .

One option is to assume **creeping flow** conditions.

For drag:

$$\boxed{f_\lambda = \frac{F_D\left(\lambda, Re_p \to 0\right)}{3\pi d_p \mu_f u_{rel}}}$$

$$\boxed{f_{\lambda||} = \frac{(4/3)\lambda^{-1/3}(1-\lambda^2)}{\lambda - \frac{(2\lambda^2-1)\ln\left(\lambda+\sqrt{\lambda^2-1}\right)}{\sqrt{\lambda^2-1}}}}$$

$$\boxed{f_{\lambda\perp} = \frac{(8/3)\lambda^{-1/3}(\lambda^2-1)}{\lambda + \frac{(2\lambda^2-3)\ln\left(\lambda+\sqrt{\lambda^2-1}\right)}{\sqrt{\lambda^2-1}}}}$$

$$\boxed{\mathbf{F}_D\left(\lambda, Re_p \to 0\right) = 3\pi d_p \mu_f \left(\mathbf{u}_{rel||}\cdot f_{\lambda||} + \mathbf{u}_{rel\perp}\cdot f_{\lambda\perp}\right)}$$

Modelling Forces for Non-Spherical Particles

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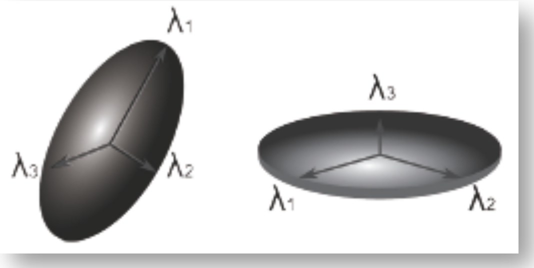
For an ellipsoid:

$$\boxed{\mathbf{F}_D\left(\lambda, \mathrm{Re}_p \to 0\right) = 3\pi d_p \mu_f \left(\mathbf{u}_{rel,1} \cdot f_{\lambda 1} + \mathbf{u}_{rel,2} \cdot f_{\lambda 2} + \mathbf{u}_{rel,3} \cdot f_{\lambda 3}\right)}$$

For a spheroid: $f_{\lambda 1} = f_{\lambda \|}$ and $f_{\lambda 2} = f_{\lambda 3} = f_{\lambda \perp}$



Note 1 - minimum drag shape is obtained:

- for a sphere averaging over all orientations
- for a prolate spheroid with λ= 1.955 for a stationary orientation (parallel to the axis of symmetry)

Note 2 – creeping flow conditions hold if:

$$\boxed{\mathbf{u}_{rel,1} = \mathbf{u}_{f@p} - \mathbf{v}_p \cong 0}$$ and/or if: $$\boxed{d_p << \eta_f}$$

(small slip velocity)

(small particles, yet not Brownian ...)

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Modelling Forces for Non-Spherical Particles

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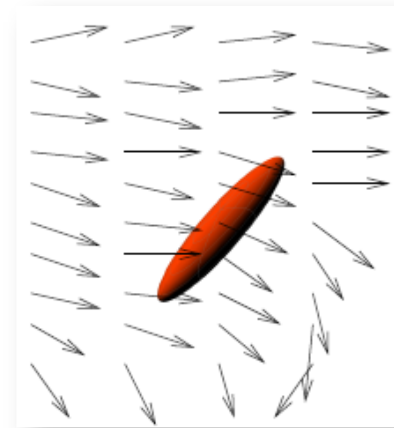
Following Bretherton (1962), Brenner (1964, 1965, 1972), and Gallily & Cohen (1979):



$$\mathbf{F}_D\left(\lambda, \mathrm{Re}_p \to 0\right) = 6\pi a \mu_f \overline{\overline{\mathbf{K}}} \cdot \left(\mathbf{u}_{f@p} - \mathbf{v}_p\right)$$

where $\overline{\overline{\mathbf{K}}}$ = translational resistance tensor for arbitrary-shape particle in arbitrary flow field

By analogy, the shear-induced lift force model is:

$$C_L = \frac{\mathbf{F}_L(\mathrm{Re}_p \to 0, \lambda)}{\frac{1}{2}\rho \mathbf{u}_{rel}^2 \frac{\pi}{4} d_p^2}$$

$$\mathbf{F}_L\left(\lambda, \mathrm{Re}_p \to 0\right) = \frac{\pi^2 \mu_f a^2}{\sqrt{\nu}} \Gamma \cdot \overline{\overline{\mathbf{L}}} \cdot \left(\mathbf{u}_{f@p} - \mathbf{v}_p\right)$$

with:

$$\Gamma = \left(\partial u_{f@p,i} \big/ \partial x_j \right) \cdot \left(\left| \partial u_{f@p,i} \big/ \partial x_j \right| \right)^{-1/2}$$

Modelling Forces for Non-Spherical Particles

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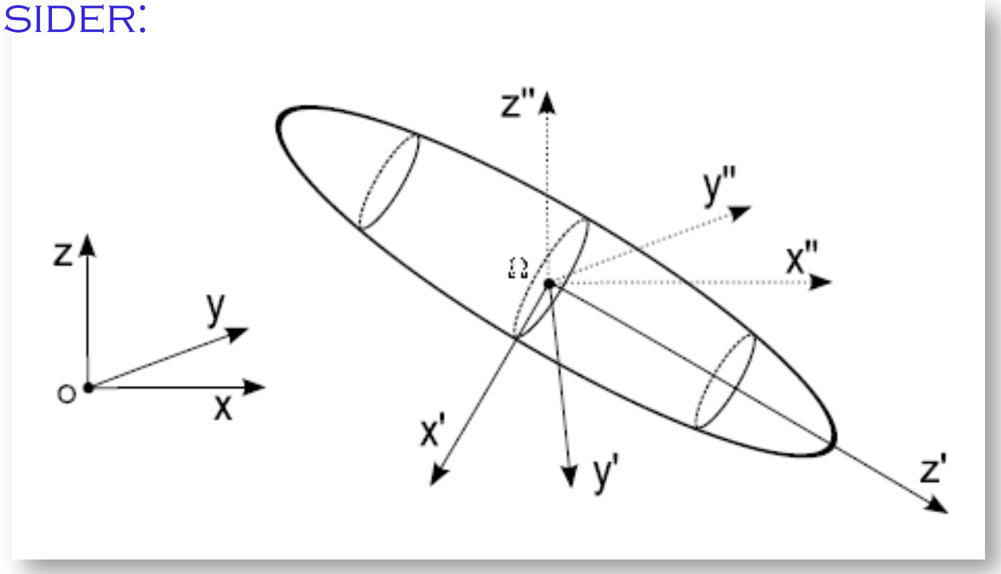
Tensors $\bar{\bar{\mathbf{K}}}$ and $\bar{\bar{\mathbf{L}}}$ can be conveniently expressed with respect to a frame of reference with:

- origin at the particle center of mass
- axes being the principal axes of the particle

The "usual" approach is to consider:

1. Inertial Frame **X**=[x,y,z]
2. Particle Frame **X'**=[x',y',z']
3. Co-moving frame **X''**=[x'',y'',z'']



Modelling Forces for Non-Spherical Particles

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In the particle frame:

$$\overline{\overline{\mathbf{K}}}' = \begin{bmatrix} k_{x'x'} & 0 & 0 \\ 0 & k_{y'y'} & 0 \\ 0 & 0 & k_{z'z'} \end{bmatrix}$$

$$k_{x'x'} = k_{y'y'} = \frac{(1-\lambda^2)}{\lambda - \dfrac{(2\lambda^2-1)\ln\left(\lambda+\sqrt{\lambda^2-1}\right)}{\sqrt{\lambda^2-1}}}$$

$$k_{z'z'} = \frac{(\lambda^2-1)}{\lambda + \dfrac{(2\lambda^2-3)\ln\left(\lambda+\sqrt{\lambda^2-1}\right)}{\sqrt{\lambda^2-1}}}$$

$$\overline{\overline{\mathbf{L}}}' = \begin{bmatrix} 0.0501 & 0.0329 & 0.00 \\ 0.0182 & 0.0173 & 0.00 \\ 0.00 & 0.00 & 0.0373 \end{bmatrix}$$

Note: for a sphere the original Saffman model is recovered

Rigid Body Kinematics

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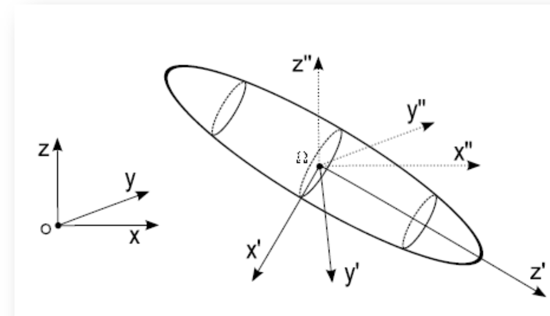
How to go from $\bar{\bar{\mathbf{K}}}'$ to $\bar{\bar{\mathbf{K}}}$?

$$\boxed{\bar{\bar{\mathbf{K}}}_{(\varphi,\theta,\psi)} = R_{eul}^T \bar{\bar{\mathbf{K}}}' R_{eul}}$$



where R_{EUL} = rotation matrix,

obtained from the Euler angles:

- Nutation:

  $\theta \in [0 : \pi]$

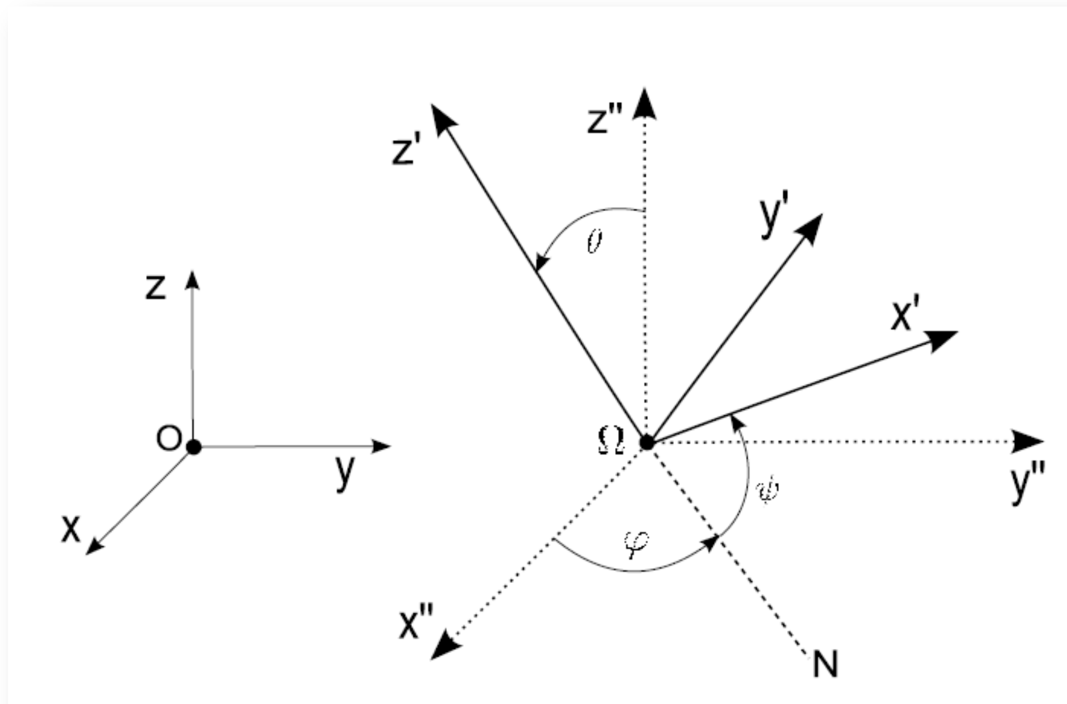
- Precession:

  $\varphi \in [0 : 2\pi]$

- Proper Rotation:

  $\psi \in [0 : 2\pi]$

$$\mathbf{x}' = R_{Eul}\mathbf{x}''$$



Rigid Body Kinematics

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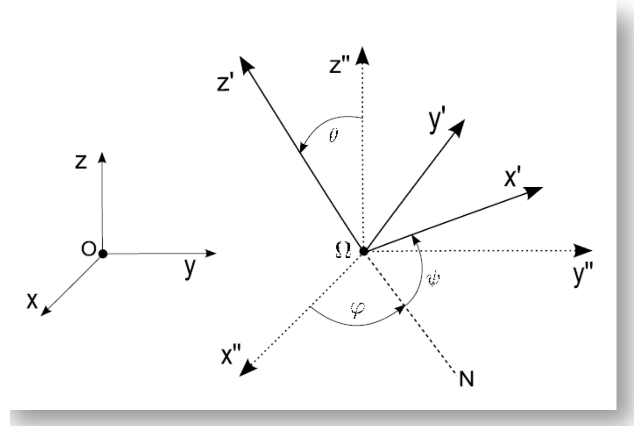
$$R_1 = \begin{bmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$R_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}$$

$$R_3 = \begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



Physical interpretation: columns are the "world" space directions that the "body" space axes transform to.

Issues: loss of orthonormality (matrix multiplication), gimbal lock (matrix singularity)

$$R_{Eul} = \begin{bmatrix} \cos\psi\cos\varphi - \cos\theta\sin\varphi\sin\psi & \cos\psi\sin\varphi + \cos\theta\cos\varphi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\varphi - \cos\theta\sin\varphi\cos\psi & -\sin\psi\sin\varphi + \cos\theta\cos\varphi\cos\psi & \cos\psi\cos\theta \\ \sin\theta\sin\varphi & -\sin\theta\cos\varphi & \cos\theta \end{bmatrix}$$

$$R_{eul}^{-1} = R_{eul}^{T} \longrightarrow R_{eul}R_{eul}^{-1} = R_{eul}R_{eul}^{T} = I$$

Rigid Body Kinematics

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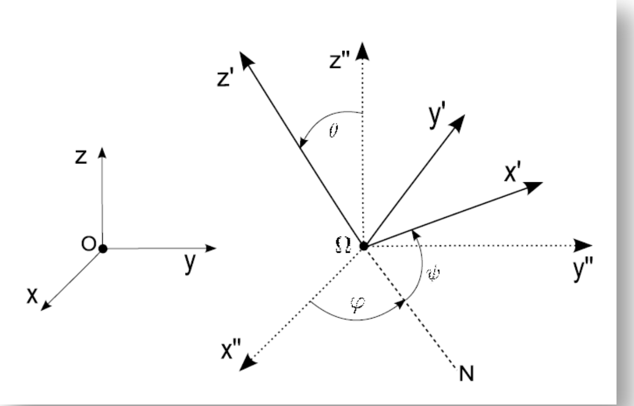
The rotation matrix can also be written in terms of the Euler parameters (aka quanternions):

- $e_0 = \cos\left[\frac{1}{2}(\psi + \varphi)\right]\cos\left(\frac{\theta}{2}\right)$
- $e_1 = \cos\left[\frac{1}{2}(\psi - \varphi)\right]\sin\left(\frac{\theta}{2}\right)$
- $e_2 = \sin\left[\frac{1}{2}(\psi - \varphi)\right]\sin\left(\frac{\theta}{2}\right)$
- $e_3 = \sin\left[\frac{1}{2}(\psi + \varphi)\right]\cos\left(\frac{\theta}{2}\right)$
- $e_0^2 + e_1^2 + e_2^2 + e_3^2 = 1$



Note: quanternions do not suffer from gimbal lock problems (but require normalization...)

$$R_{eul} = \begin{bmatrix} e_0^2 + e_1^2 - e_2^2 - e_3^2 & 2(e_1e_2 + e_0e_3) & 2(e_1e_3 - e_0e_2) \\ 2(e_1e_2 - e_0e_3) & e_0^2 - e_1^2 + e_2^2 - e_3^2 & 2(e_2e_3 + e_0e_1) \\ 2(e_1e_3 + e_0e_2) & 2(e_2e_3 - e_0e_1) & e_0^2 - e_1^2 - e_2^2 + e_3^2 \end{bmatrix}$$

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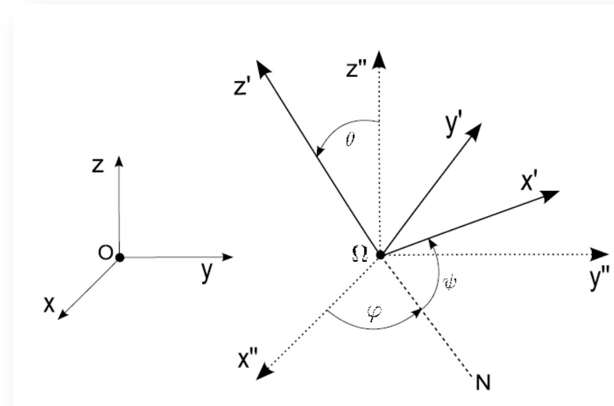
Rigid Body Kinematics

The rotation matrix can be evolved in time using the following set of ODEs for the 4 quaternions:

$$\begin{pmatrix} \dot{e_0} \\ \dot{e_1} \\ \dot{e_2} \\ \dot{e_3} \end{pmatrix} = \frac{1}{2} \begin{bmatrix} e_0 & -e_1 & -e_2 & e_3 \\ e_1 & e_0 & -e_3 & e_2 \\ e_2 & e_3 & e_0 & -e_1 \\ e_3 & -e_2 & e_1 & e_0 \end{bmatrix} \cdot \begin{pmatrix} 0 \\ \omega_{x'} \\ \omega_{y'} \\ \omega_{z'} \end{pmatrix}$$



that replace the Euler kinematic equations:

$$\begin{pmatrix} \dot{\varphi} \\ \dot{\theta} \\ \dot{\psi} \end{pmatrix} = \begin{bmatrix} \frac{\sin\psi}{\sin\theta} & \frac{\cos\psi}{\sin\theta} & 0 \\ \cos\psi & -\sin\psi & 0 \\ -\frac{\sin\psi\cos\theta}{\sin\theta} & -\frac{\cos\psi\cos\theta}{\sin\theta} & 1 \end{bmatrix} \cdot \begin{pmatrix} \omega_{x'} \\ \omega_{y'} \\ \omega_{z'} \end{pmatrix}$$

Singularities may arise!!!

Rigid Body Kinematics

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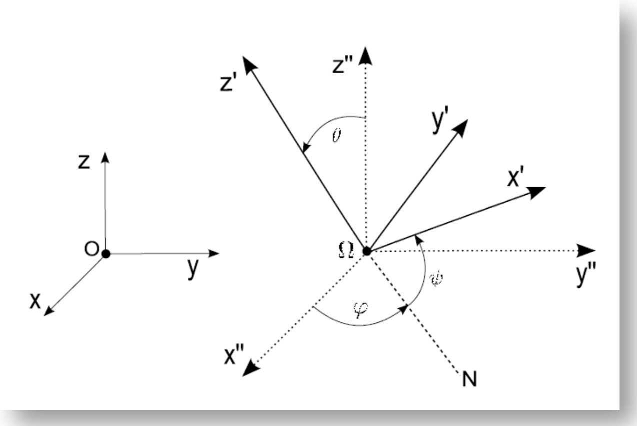
In summary, compute the resistance tensor in the particle frame as:



$$\mathbf{F}'_{drag} = \mu \pi a \bar{\bar{\mathbf{K}}}'(\mathbf{u}' - \mathbf{v}')$$

Then apply the transformation from the particle frame to the inertial frame:

$$\mathbf{F}_{drag} = R_{eul}^{-1}\mathbf{F}'_{drag} = R_{eul}^{T}\mathbf{F}'_{drag} = \mu\pi a R_{eul}^{T}\bar{\bar{\mathbf{K}}}'(\mathbf{u}' - \mathbf{v}') =$$

$$= \mu\pi a R_{eul}^{T}\bar{\bar{\mathbf{K}}}'(R_{eul}\mathbf{u} - R_{eul}\mathbf{v}) = \mu\pi a R_{eul}^{T}\bar{\bar{\mathbf{K}}}' R_{eul}(\mathbf{u} - \mathbf{v})$$

to get:

$$\mathbf{F}_{drag} = \mu\pi a \bar{\bar{\mathbf{K}}}_{(\varphi,\theta,\psi)}(\mathbf{u} - \mathbf{v})$$

Rigid Body Kinematics

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For the lift force (Harper & Chang, JFM,1968; Hogg , JFM, 1994):

$$\boxed{\mathbf{F}_L = \frac{\pi^2 \mu_f a^2}{\sqrt{\nu}} \Gamma \cdot \left(\overline{\overline{\mathbf{K}}} \cdot \overline{\overline{\mathbf{L}}}' \cdot \overline{\overline{\mathbf{K}}} \right) \cdot \left(\mathbf{u}_{f@p} - \mathbf{v}_p \right)}$$

Note that:

- Lift force is non-zero at any non-zero shear rate
- $\mathbf{F}_L \propto a^2$ i.e. the semi-minor axis of an ellipsoid squared therefore lift counts for large particles
- Derived for unidirectional shear
- no wall effects included (only available for spheres)
- In general, very little effort done to lift force models for non-spherical particles

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"Final" Equation of Translational Motion

$$\overbrace{m_p \frac{d\mathbf{v}_p}{dt}}^{\text{Inertia}} = \overbrace{\mu_f \pi a \overline{\overline{\mathbf{K}}}_{(\varphi,\theta,\psi)} \cdot \left(\mathbf{u}_{f@p} - \mathbf{v}_p\right)}^{\text{drag}} +$$

$$\underbrace{+ \frac{\pi^2 \mu_f a^2}{\sqrt{\nu}} \Gamma \cdot \left(\overline{\overline{\mathbf{K}}} \cdot \overline{\overline{\mathbf{L}}}' \cdot \overline{\overline{\mathbf{K}}}\right) \cdot \left(\mathbf{u}_{f@p} - \mathbf{v}_p\right)}_{\text{lift}} + \underbrace{\left(m_p - m_f\right)\mathbf{g}}_{\text{Buoyancy}}$$

plus $\dfrac{d\mathbf{x}_p}{dt} = \mathbf{v}_p$ to compute particle trajectory

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Rotational Dynamics

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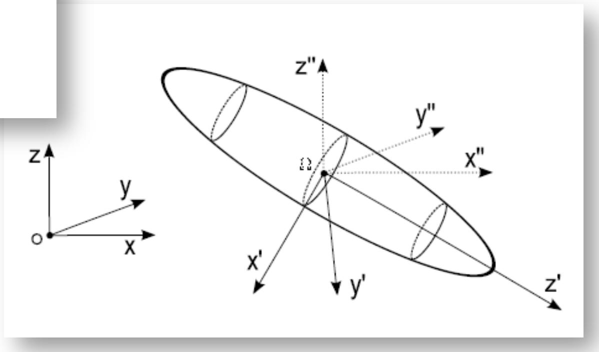
Start from the 2nd cardinal eq. of dynamics in the particle frame:

$$\begin{cases} I_{x'x'}\dot{\omega}_{x'} + \omega_{y'}\omega_{z'}(I_{z'z'} - I_{y'y'}) = M_{x'}^{est} \\ I_{y'y'}\dot{\omega}_{y'} + \omega_{x'}\omega_{z'}(I_{z'z'} - I_{x'x'}) = M_{y'}^{est} \\ I_{z'z'}\dot{\omega}_{z'} + \omega_{x'}\omega_{y'}(I_{y'y'} - I_{x'x'}) = M_{z'}^{est} \end{cases}$$

Note - in the particle frame the inertia tensor is constant:

$$I_{x'x'} = I_{y'y'} = \frac{(1+\lambda^2)a^2}{5} m_P$$

$$I_{z'z'} = \frac{2a^2}{5} m_P$$



with: $$m_P = \left(\frac{4}{3}\pi a^3\right) \lambda S \rho_P$$

Rotational Dynamics

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The hydrodynamic torque acting on the particle wrt the principal axes of the particle is computed using Jeffery's formulation:

$$M_{x'}^{Jeff} = \frac{16\pi\mu a^3\lambda}{3(\beta_0+\lambda^2\gamma_0)}\left[(1-\lambda^2)f' + (1+\lambda^2)(\xi' - \omega_{x'})\right]$$

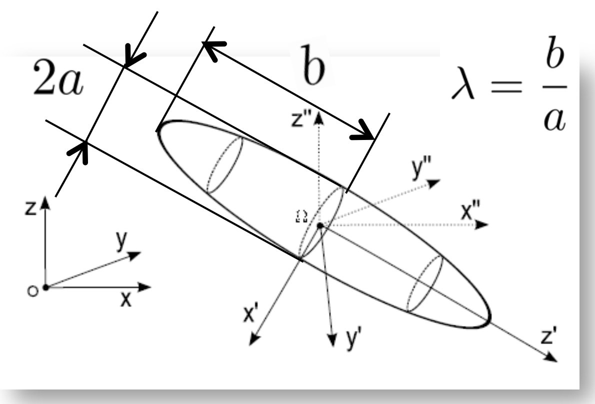
$$M_{y'}^{Jeff} = \frac{16\pi\mu a^3\lambda}{3(\alpha_0+\lambda^2\gamma_0)}\left[(\lambda^2-1)g' + (1+\lambda^2)(\eta' - \omega_{y'})\right]$$

$$M_{z'}^{Jeff} = \frac{32\pi\mu a^3\lambda}{3(\beta_0+\alpha_0)}(\chi' - \omega_{z'})$$

with parameters (Gallily & Cohen, 1979):

$$\alpha_0 = \beta_0 = \frac{2\lambda^2\sqrt{\lambda^2-1} + \lambda\cdot ln\left(\frac{\lambda-\sqrt{\lambda^2-1}}{\lambda+\sqrt{\lambda^2-1}}\right)}{2(\lambda^2-1)^{3/2}}$$

$$\gamma_0 = \frac{2\sqrt{\lambda^2-1} + \lambda\cdot ln\left(\frac{\lambda-\sqrt{\lambda^2-1}}{\lambda+\sqrt{\lambda^2-1}}\right)}{(\lambda^2-1)^{3/2}}$$



Rotational Dynamics

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The hydrodynamic torques depend on the elements of:

- rate of strain tensor:

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \quad \left\{ \begin{aligned} f' &= \frac{1}{2}\left(\frac{\partial u_{z'}}{\partial y'} + \frac{\partial u_{y'}}{\partial z'}\right) \\ g' &= \frac{1}{2}\left(\frac{\partial u_{x'}}{\partial z'} + \frac{\partial u_{z'}}{\partial x'}\right) \end{aligned} \right.$$

- rate of rotation tensor:

$$\Omega_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right) \quad \left\{ \begin{aligned} \xi' &= \frac{1}{2}\left(\frac{\partial u_{z'}}{\partial y'} - \frac{\partial u_{y'}}{\partial z'}\right) \\ \eta' &= \frac{1}{2}\left(\frac{\partial u_{x'}}{\partial z'} - \frac{\partial u_{z'}}{\partial x'}\right) \\ \chi' &= \frac{1}{2}\left(\frac{\partial u_{x'}}{\partial y'} - \frac{\partial u_{y'}}{\partial x'}\right) \end{aligned} \right.$$

computed in the particle frame: $\bar{\bar{\mathbf{G}}}' = R_{eul}\bar{\bar{\mathbf{G}}}R_{eul}^T$

Rotational Dynamics

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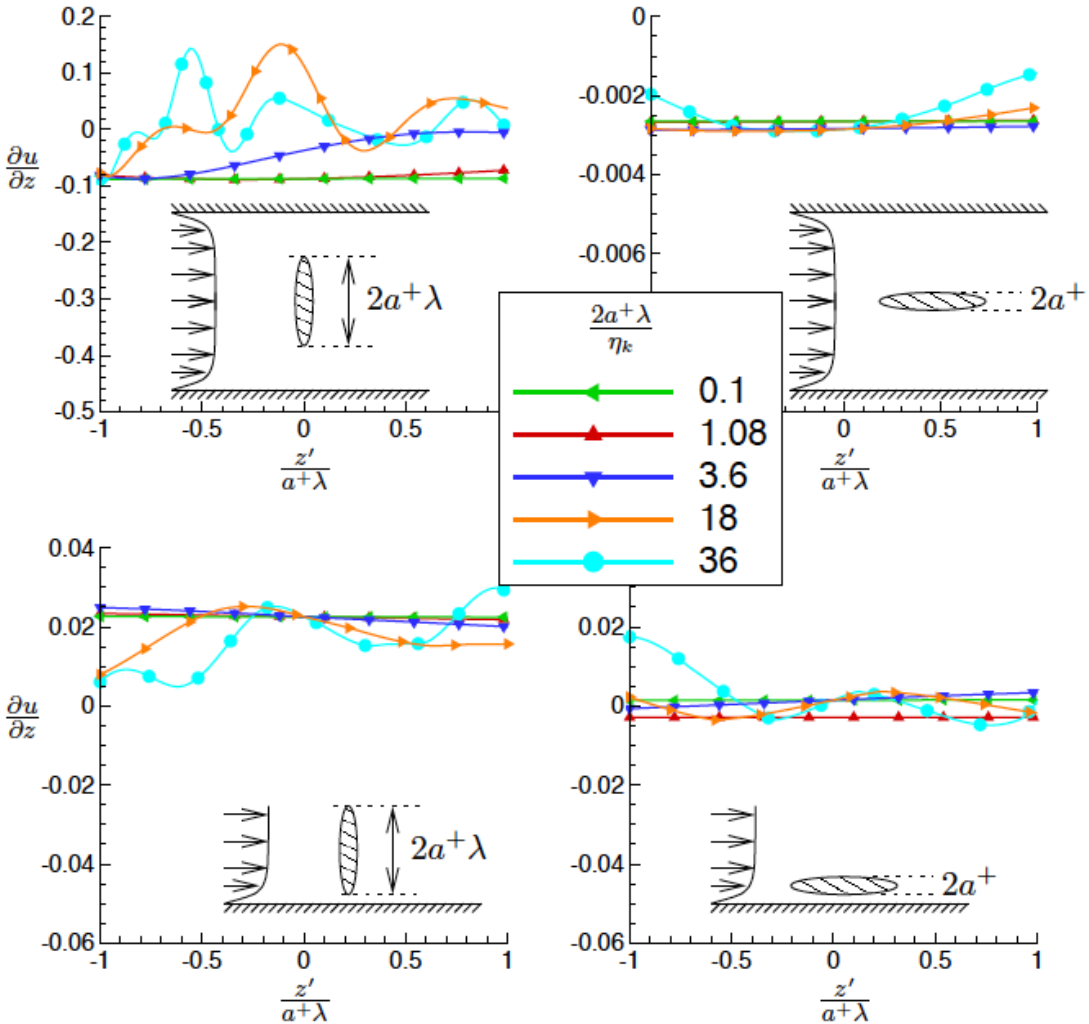
Caveat: How accurate is Jeffery's formulation?

Channel center...

Near the wall...



Instantaneous velocity gradient along the fiber at varying aspect ratio

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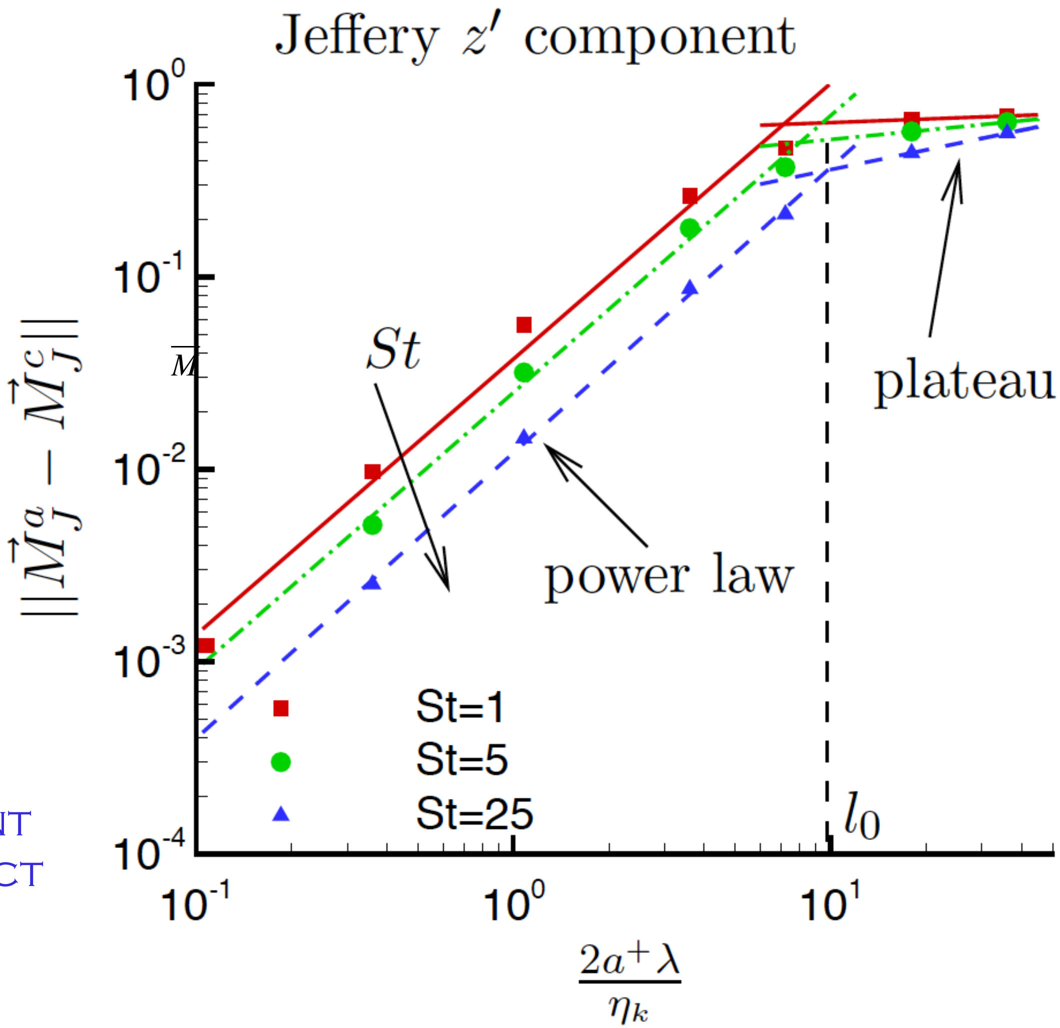
Rotational Dynamics

Caveat: How accurate is Jeffery's formulation?

Relative RMS norm:

$$\left\| \vec{M}_J^a - \vec{M}_J^c \right\| = \sqrt{\frac{\sum_i \left(\vec{M}_{J,i}^a - \vec{M}_{J,i}^c \right)^2}{\sum_i \left(\vec{M}_{J,i}^c \right)^2}}$$



Instantaneous velocity gradient along the fiber at varying aspect ratio and inertia.

Complete System of Dimensional Equations

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$$
\begin{cases}
\underline{Kinematics:} \\
\dfrac{d\mathbf{x}_{(G)}}{dt} = \mathbf{v} \\
\dot{e_0} = \dfrac{1}{2}(-e_1\omega_{x'} - e_2\omega_{y'} - e_3\omega_{z'}) \\
\dot{e_1} = \dfrac{1}{2}(e_0\omega_{x'} - e_3\omega_{y'} + e_2\omega_{z'}) \\
\dot{e_2} = \dfrac{1}{2}(e_3\omega_{x'} + e_0\omega_{y'} - e_1\omega_{z'}) \\
\dot{e_3} = \dfrac{1}{2}(-e_2\omega_{x'} + e_1\omega_{y'} + e_0\omega_{z'}) \\
\underline{Dynamics:} \\
m_P\dfrac{d\mathbf{v}}{dt} = (m_P - m_F)\mathbf{g} + \mu\bar{\bar{\mathbf{K}}}_{(e_0,e_1,e_2,e_3)} \cdot (\mathbf{u} - \mathbf{v}) \\
I_{x'x'}\dot{\omega}_{x'} + \omega_{y'}\omega_{z'}(I_{z'z'} - I_{y'y'}) = M_{x'}^{Jeff} \\
I_{y'y'}\dot{\omega}_{y'} + \omega_{x'}\omega_{z'}(I_{z'z'} - I_{x'x'}) = M_{y'}^{Jeff} \\
I_{z'z'}\dot{\omega}_{z'} + \omega_{x'}\omega_{y'}(I_{y'y'} - I_{x'x'}) = M_{z'}^{Jeff}
\end{cases}
$$

Example: Dilute Suspension
Rigid fibers in wall turbulence

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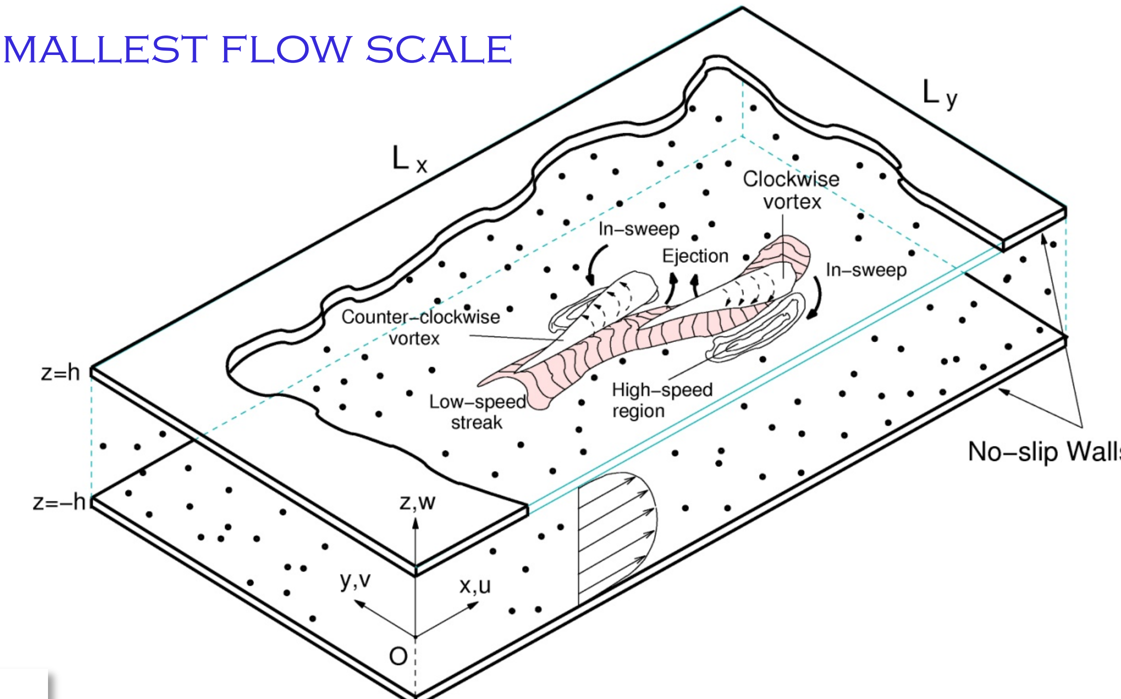
Fibers are modelled as non-deformable prolate ellipsoids evolving in 3D time-dependent fully-turbulent flow (e.g. Marchioli et al, 2010)

Assume:

- Fibers smaller than the smallest flow scale
  - > pointwise
  - > Stokes regime
- Dilute flow
  - > no turbulence modulation
  - > no collisions



First: work with non-dimensional equations!

$$a^+ = \frac{a}{\delta_\nu} = \frac{a u_\tau}{\nu} \quad , \quad \mathbf{x}^+ = \frac{\mathbf{x}}{\delta_\nu} = \frac{\mathbf{x} u_\tau}{\nu}$$

$$t^+ = \frac{t u_\tau^2}{\nu} \quad v_i^+ = \frac{v_i}{u_\tau} \quad , \quad \omega_{i'}^+ = \frac{\omega_{i'} \nu}{u_\tau^2}$$

with $u_\tau = \sqrt{\dfrac{\tau_w}{\rho}}$ the shear velocity

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Complete System of Non-Dimensional Equations

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$$a^+ = \frac{a}{\delta_\nu} = \frac{a u_\tau}{\nu} \quad , \quad \mathbf{x}^+ = \frac{\mathbf{x}}{\delta_\nu} = \frac{\mathbf{x} u_\tau}{\nu}$$

$$t^+ = \frac{t u_\tau^2}{\nu} \qquad v_i^+ = \frac{v_i}{u_\tau} \quad , \quad \omega_{i'}^+ = \frac{\omega_{i'}\nu}{u_\tau^2}$$

$$\begin{cases}
\underline{Kinematics:} \\
\dfrac{d\mathbf{x}^+_{(G)}}{dt} = \mathbf{v}^+ \\
\dfrac{de_0}{dt^+} = \dfrac{1}{2}(-e_1\omega^+_{x'} - e_2\omega^+_{y'} - e_3\omega^+_{z'}) \\
\dfrac{de_1}{dt^+} = \dfrac{1}{2}(e_0\omega^+_{x'} - e_3\omega^+_{y'} + e_2\omega^+_{z'}) \\
\dfrac{de_2}{dt^+} = \dfrac{1}{2}(e_3\omega^+_{x'} + e_0\omega^+_{y'} - e_1\omega^+_{z'}) \\
\dfrac{de_3}{dt^+} = \dfrac{1}{2}(-e_2\omega^+_{x'} + e_1\omega^+_{y'} + e_0\omega^+_{z'}) \\
\underline{Dynamics:} \\
\dfrac{d\mathbf{v}^+}{dt^+} = (\dfrac{S-1}{S})\mathbf{g}^+ + \dfrac{3}{4\lambda S {a^+}^2}\bar{\bar{\mathbf{K}}}_{(e_0,e_1,e_2,e_3)} \cdot (\mathbf{u}^+ - \mathbf{v}^+) \\
\dfrac{d\omega^+_{x'}}{dt^+} = \omega^+_{y'}\omega^+_{z'}\left(1 - \dfrac{2}{1+\lambda^2}\right) + \dfrac{20\left[(1-\lambda^2)f' + (1+\lambda^2)(\xi' - \omega^+_{x'})\right]}{(\alpha_0 + \lambda^2\gamma_0)(1+\lambda^2)S{a^+}^2} \\
\dfrac{d\omega^+_{y'}}{dt^+} = \omega^+_{x'}\omega^+_{z'}\left(\dfrac{2}{1+\lambda^2} - 1\right) + \dfrac{20\left[(\lambda^2-1)g' + (\lambda^2+1)(\eta' - \omega^+_{y'})\right]}{(\alpha_0 + \lambda^2\gamma_0)(1+\lambda^2)S{a^+}^2} \\
\dfrac{d\omega^+_{z'}}{dt^+} = \dfrac{20}{(2\alpha_0)S{a^+}^2}(\chi' - \omega^+_{z'})
\end{cases}$$

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Example: Dilute Suspension of Rigid fibers in wall turbulence

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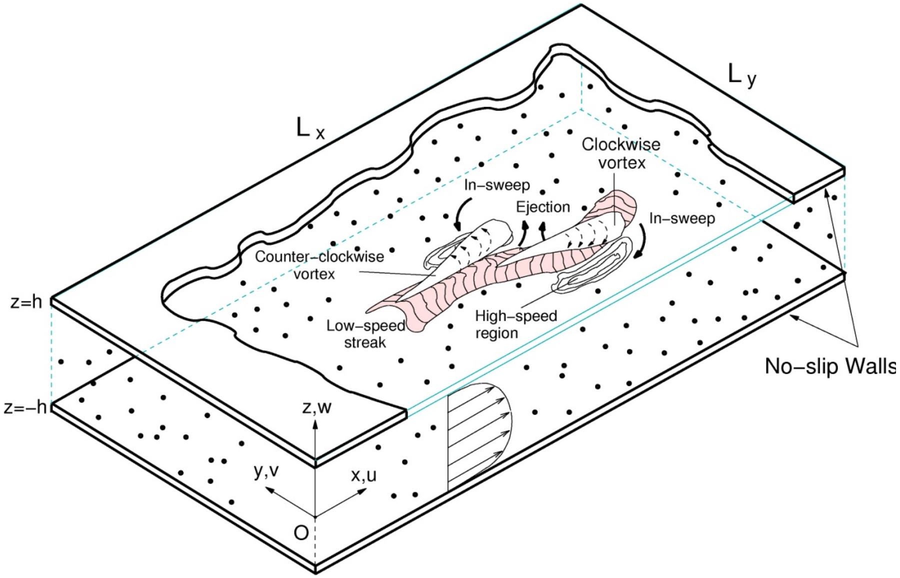
The physics of the problem is controlled by a small set of parameters:

- Turbulence

  flow Reynolds number $$Re_\tau = \frac{u_\tau h}{\nu}$$

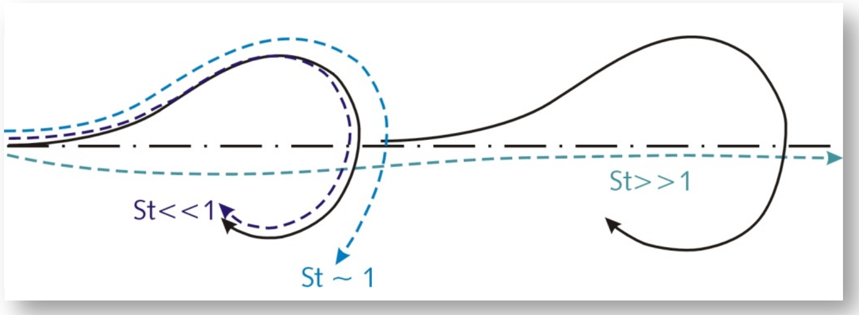


- Fibers

  aspect ratio (shape) $$\lambda = \frac{b}{a}$$

  specific density $$S = \frac{\rho_P}{\rho_F}$$

  response time (inertia) $$St = \frac{\tau_P}{\tau_F} = \frac{\tau_P u_\tau^2}{\nu}$$



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Example: Dilute Suspension of Rigid Fibers in Wall Turbulence

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Response time for non-spherical particles:

- Shapiro & Goldenberg (1993) assumed isotropic particle orientation and used the averaged mobility dyadic (inverse of the translation dyadic)

$$\boxed{\tau_p = \frac{4\lambda \mathrm{Sa}^2}{9\nu}\left(\frac{1}{k_{x'x'}} + \frac{1}{k_{y'y'}} + \frac{1}{k_{z'z'}}\right) = \frac{2\lambda \mathrm{Sa}^2}{9\nu}\,\frac{\ln\left(\lambda + \sqrt{\lambda^2 - 1}\right)}{\sqrt{\lambda^2 - 1}}}$$

- Fan & Ahmadi (1995) used the orientation-averaged translation dyadic

$$\boxed{\tau_p = \frac{4\lambda \mathrm{Sa}^2}{\nu\left(k_{x'x'} + k_{y'y'} + k_{z'z'}\right)}}$$

In the $\lambda = 1$ limit (sphere), both reduce to $\tau_p = \dfrac{2\mathrm{Sa}^2}{\nu}$

Ellipsoids also have a rotational response time (equal to $\tau_r = \dfrac{\mathrm{Sa}^2}{15\nu}$ for sphere) but no expression has been proposed so far.

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Example: Dilute Suspension of Rigid fibers in wall turbulence

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Rotational response time for ellipsoidal particles:

- rotation around *z'* in the fiber frame:

$$\frac{d\omega_{z'}^{+}}{dt^{+}} = \frac{20}{(\alpha_0+\beta_0)Sa^{+2}}\Delta\omega_{z'}^{+} = \frac{1}{\tau_{r,z'}^{+}}\Delta\omega_{z'}^{+} \quad \rightarrow \quad \boxed{\tau_{r,z'}^{+} = \frac{\alpha_0 Sa^{+2}}{10}}$$

- rotation around *x'* or *y'* in the fiber frame:

$$\frac{d\omega_{y'}^{+}}{dt^{+}} = \underbrace{\omega_{x'}^{+}\omega_{z'}^{+}\left(\frac{2}{1+\lambda^2}-1\right)}_{A} + \underbrace{\frac{20(\lambda^2-1)}{(\alpha_0+\lambda^2\gamma_0)(1+\lambda^2)Sa^{+2}}g'}_{B} + \underbrace{\frac{20(\lambda^2+1)}{(\alpha_0+\lambda^2\gamma_0)(1+\lambda^2)Sa^{+2}}}_{1/\tau_{r,y'}}\Delta\omega_{y'}^{+}$$

$$\rightarrow \quad \boxed{\tau_{r,y'} = \frac{(\alpha_0+\lambda^2\gamma_0)}{20}Sa^{+2} \equiv \tau_{r,x'}}$$

- assuming isotropic orientation would yield:

$$\boxed{\tau_r^{+} = \frac{1}{3}(\tau_{r,x'}+\tau_{r,y'}+\tau_{r,z'}) = \frac{2\alpha_0+\lambda^2\gamma_0}{30}Sa^{+2} = \frac{3}{10}\tau_p^{+} \quad \forall\lambda}$$

Example: Dilute Suspension of Rigid fibers in wall turbulence

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Possible simulation parameters for a test case calculation:

- Fluid

Re_τ	Fluid	$\rho_F\ [kg/m^3]$	$\nu\ [m^2/s]$	$h\ [cm]$	$u_\tau\ [m/s]$	$\overline{u_x}\ [m/s]$
150	Air	1.3	$1.57 \cdot 10^{-5}$	2.0	0.11775	1.77
150	Water	1000	$1.00 \cdot 10^{-6}$	0.5	0.03000	0.45

- Particles

Set	τ_p^+	λ	S	$2b^+$	(μm)	(kg/m^3)
F1-1	1	1.001	34.72	0.72	96.07	45.14
F1-3	1	3	18.57	2.16	287.93	24.14
F1-10	1	10	11.54	7.20	960.09	15.01
F1-50	1	50	7.54	36.00	4800.01	9.80
F5-1	5	1.001	173.60	0.72	96.07	225.68
F5-3	5	3	92.90	2.16	287.93	120.77
F5-10	5	10	57.70	7.20	960.09	75.01
F5-50	5	50	37.69	36.00	4800.01	49.00
F30-1	30	1.001	1041.70	0.72	96.07	1354.21
F30-3	30	3	557.10	2.16	287.93	724.23
F30-10	30	10	346.30	7.20	960.09	450.19
F30-50	30	50	226.15	36.00	4800.01	294.00
F100-1	100	1.001	3472.33	0.72	96.07	4514.03
F100-3	100	3	1857.00	2.16	287.93	2414.10
F100-10	100	10	1154.33	7.20	960.09	1500.63
F100-50	100	50	753.83	36.00	4800.01	979.98

Example: Dilute Suspension of Rigid fibers in wall turbulence

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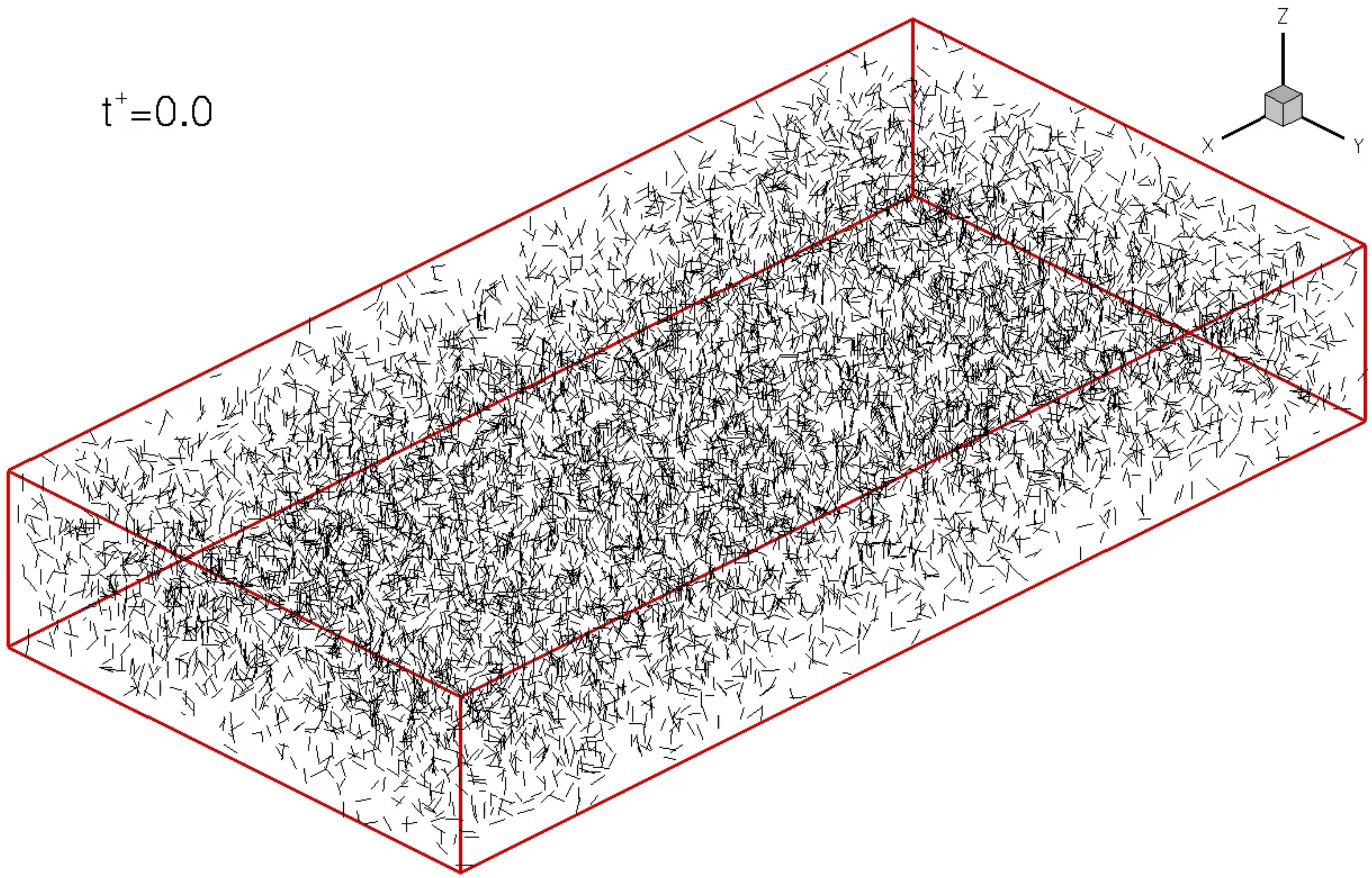
Qualitative results: animation of collective fiber motion at Re= 150



Fiber parameters: St = 30, λ = 10, a^+ = 0.36

Example: Dilute Suspension of Rigid fibers in wall turbulence

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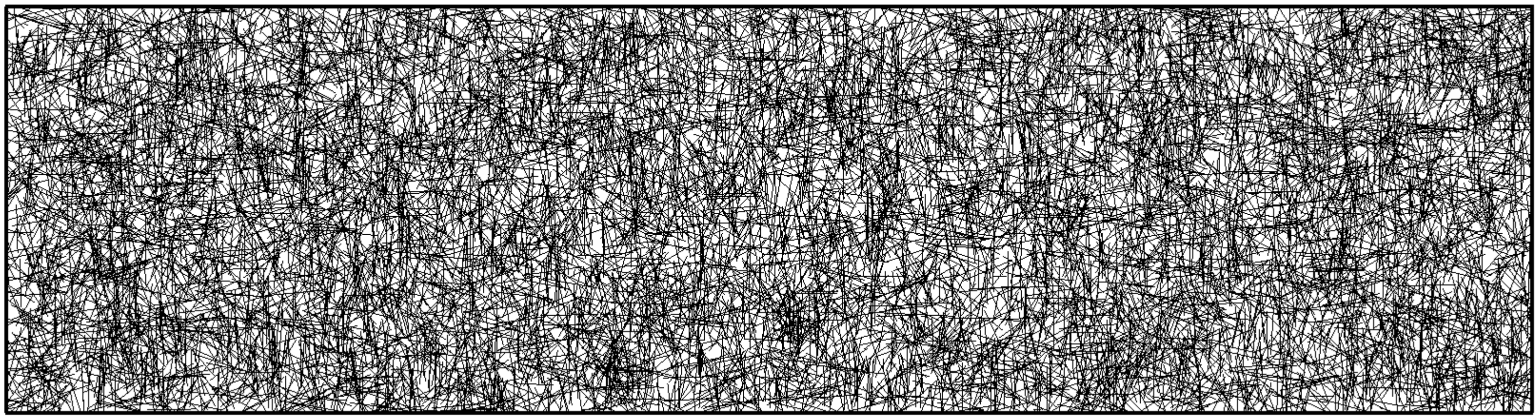
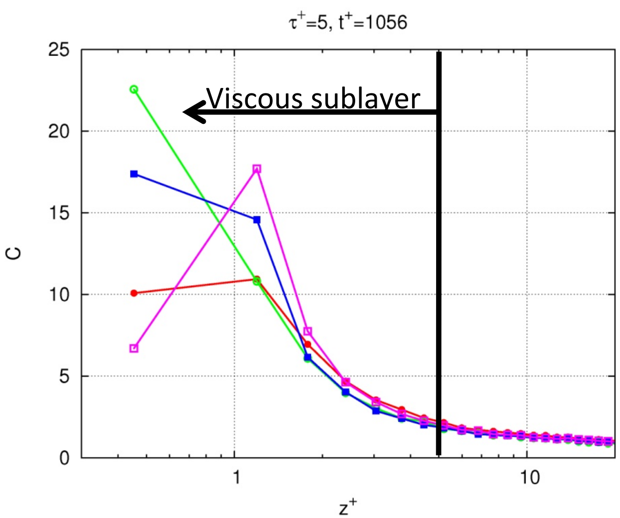
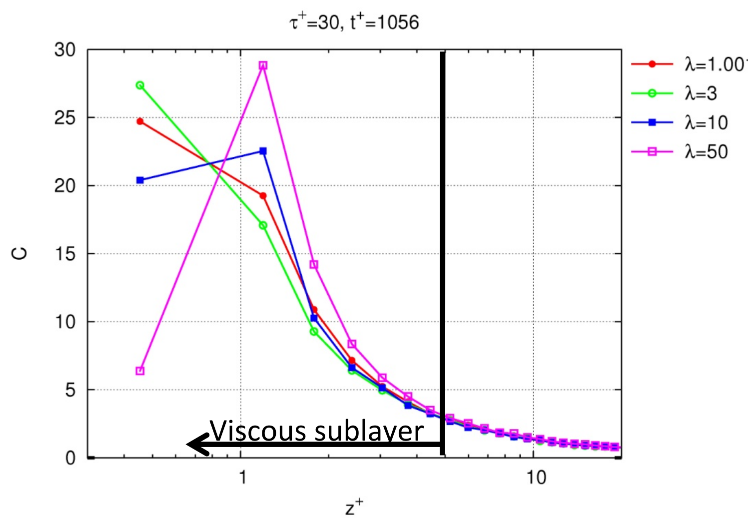
Qualitative results: front view



Fiber parameters: St = 30, λ = 50, $a^+ = 0.36$





Example: Dilute Suspension of Rigid fibers in wall turbulence

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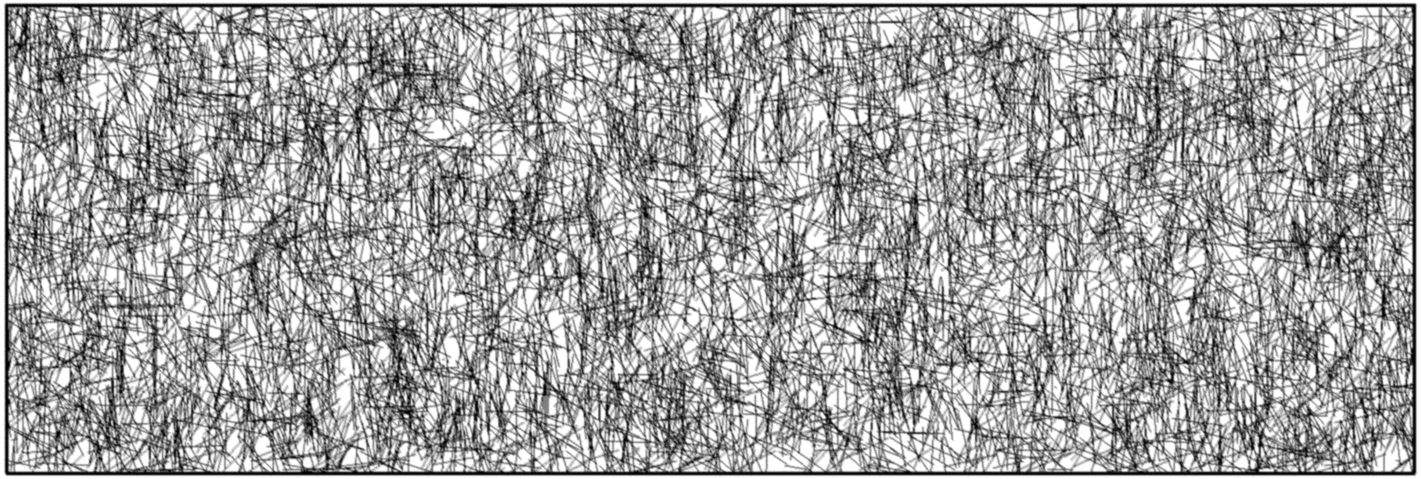
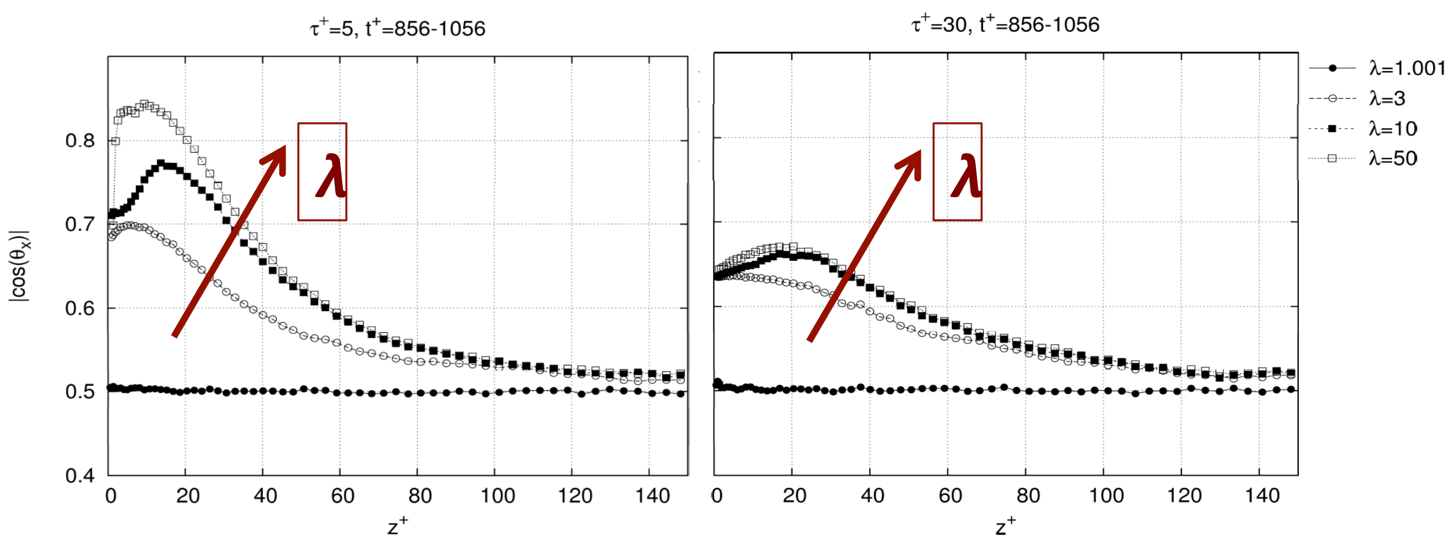
Qualitative results: side view



Fiber parameters: St = 30, λ = 50, $a^+ = 0.36$



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Example: Dilute Suspension of Rigid fibers in wall turbulence

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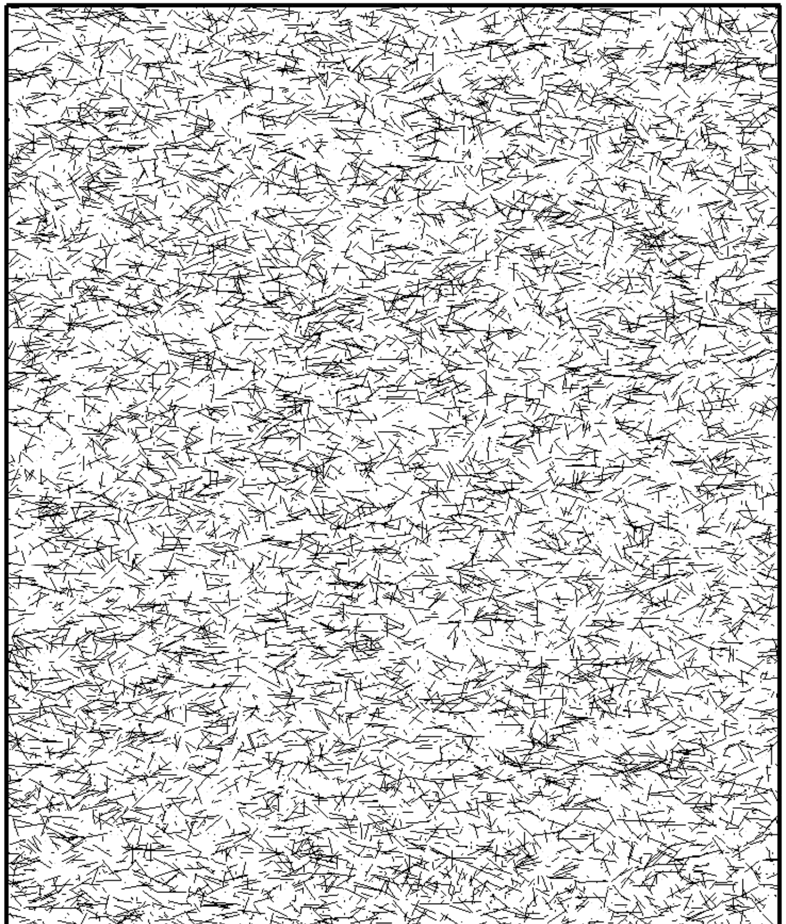
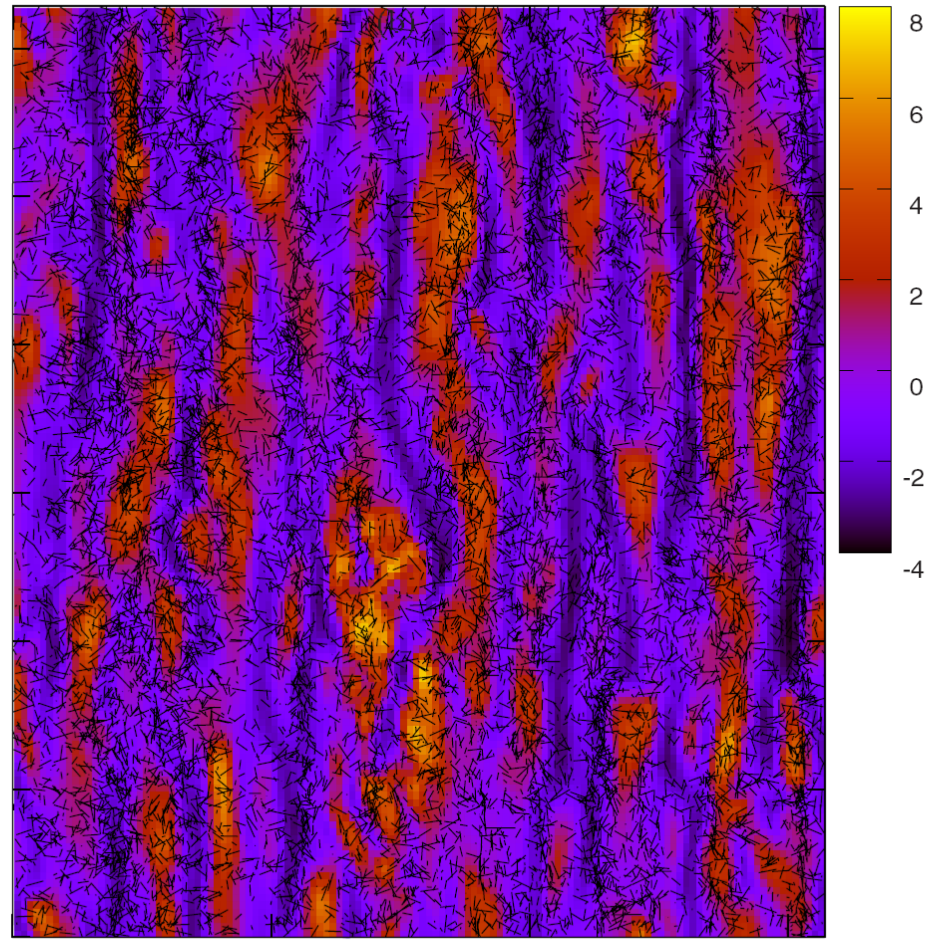
Qualitative results: top view





Fiber parameters: St = 30, λ = 50, a^+ = 0.36

Example: Dilute Suspension of Rigid fibers in wall turbulence

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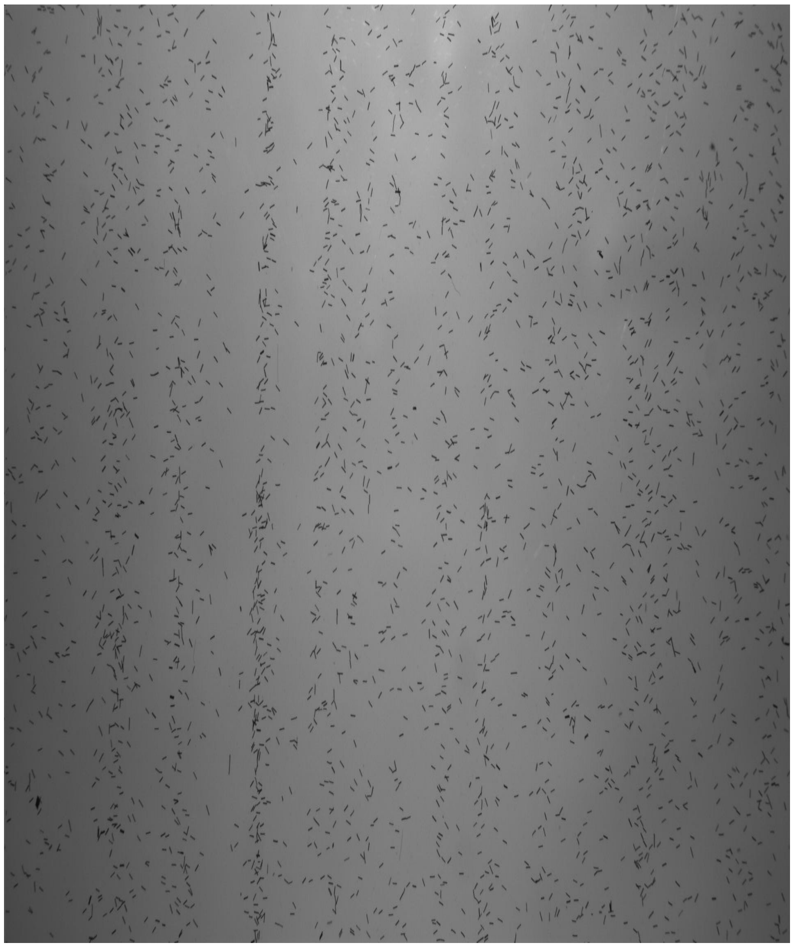
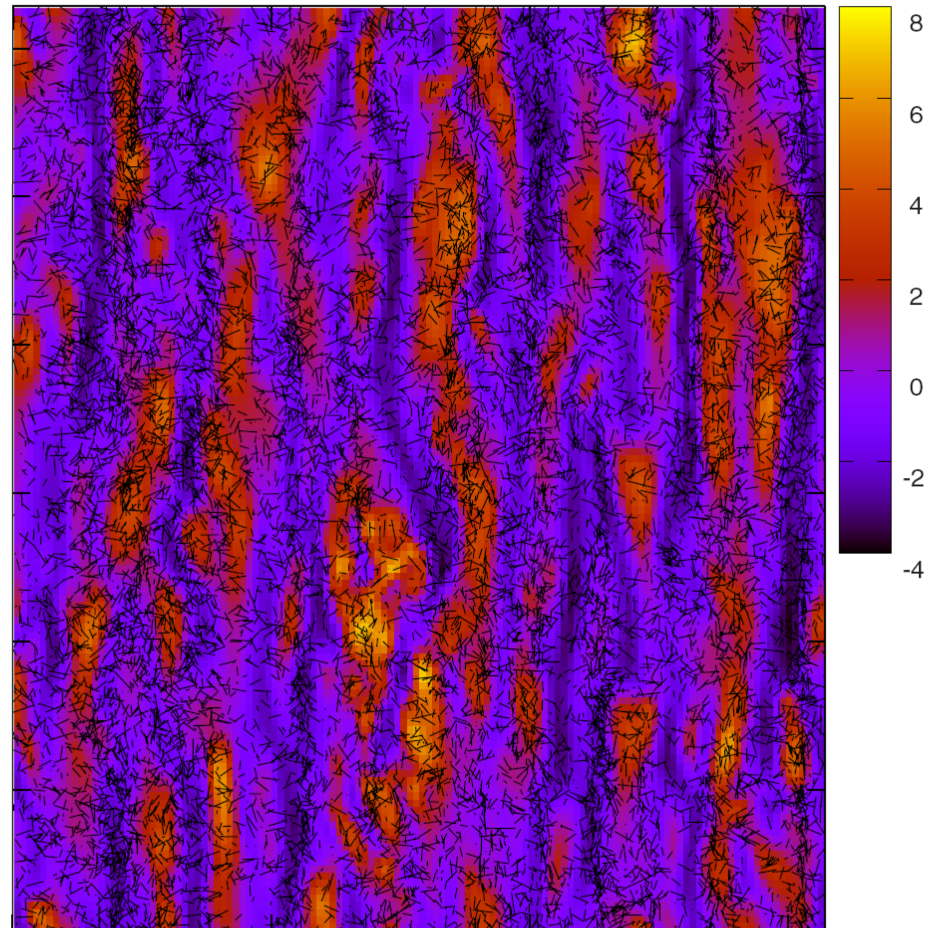
Compare with experimental results





Fiber parameters: St = 30, λ = 50, a^{+} = 0.36

Example: Dilute Suspension of Rigid fibers in wall turbulence

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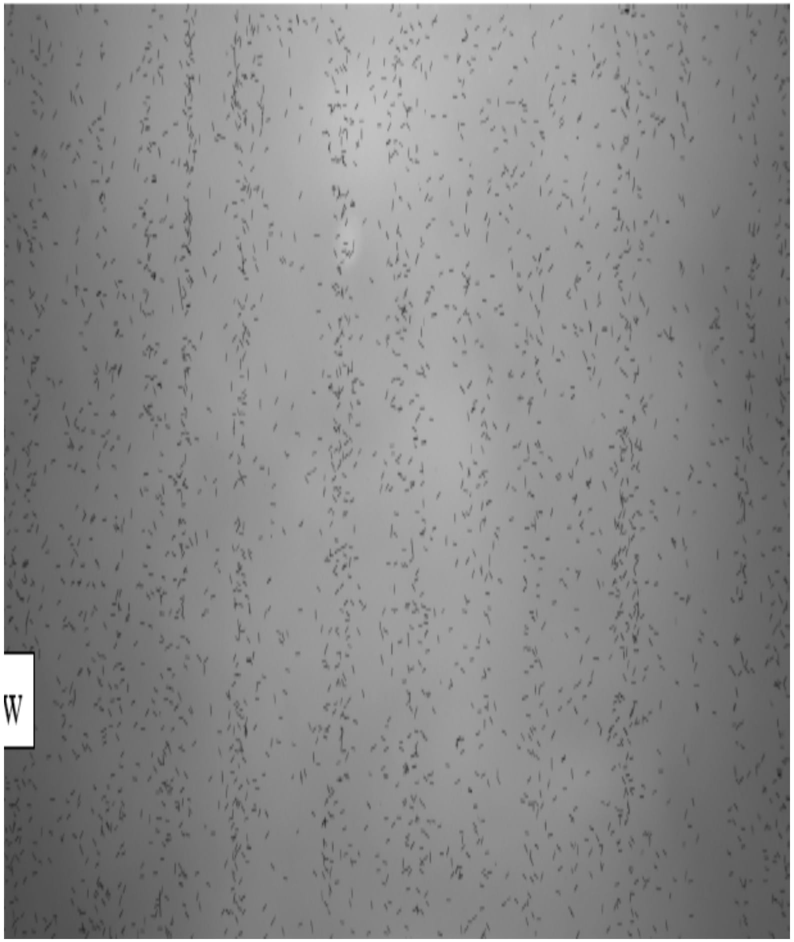
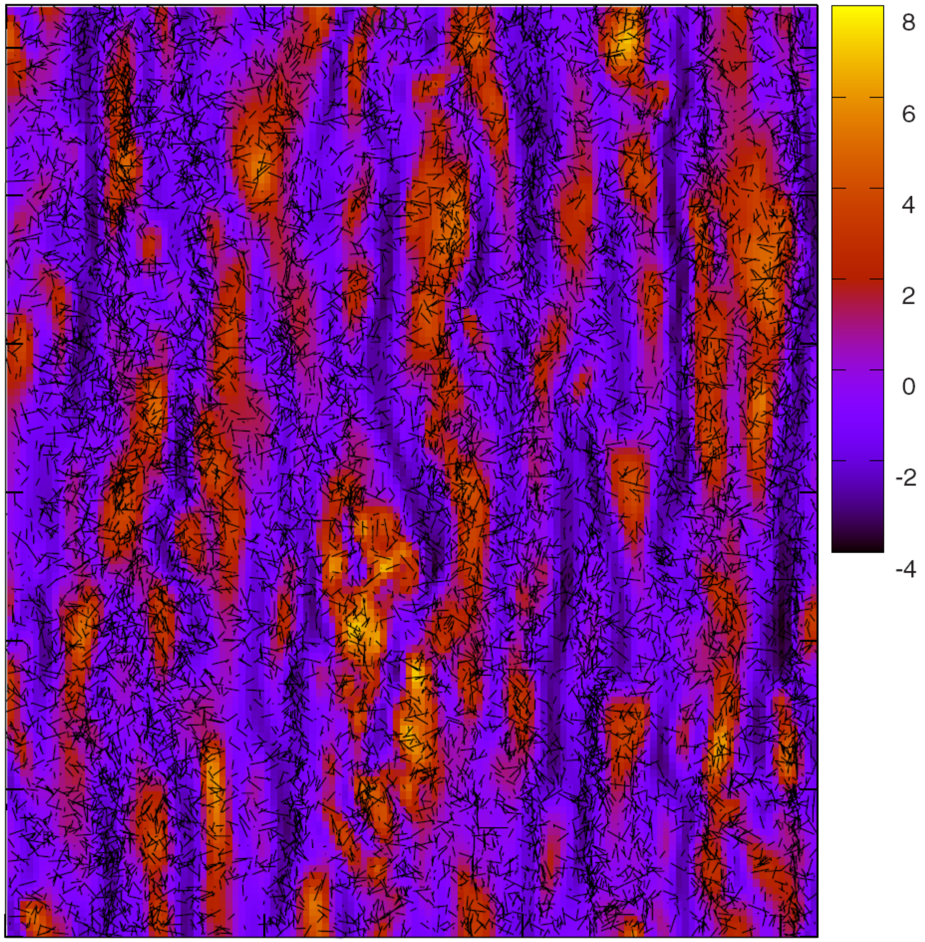
Compare with experimental results





Fiber parameters: St = 30, λ = 50, a^{+} = 0.36

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Homework: Settling of fibers in cellular flow field

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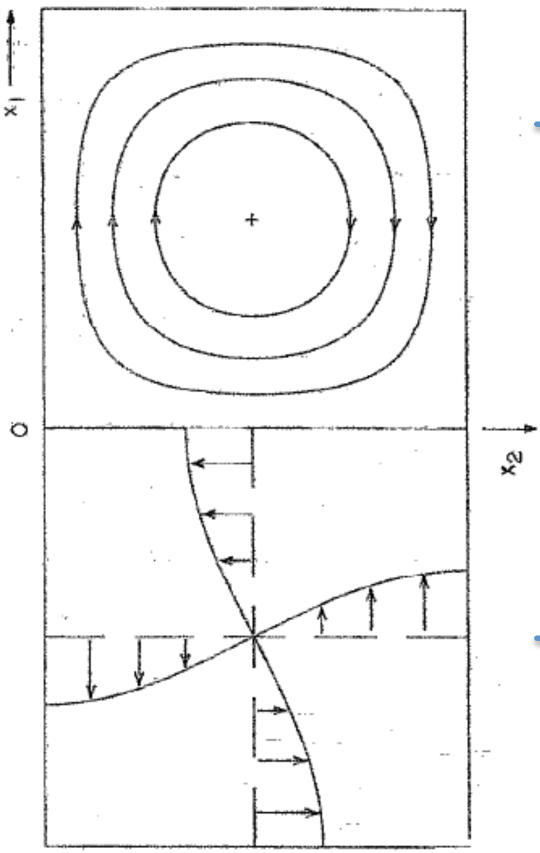
The settling of nonspherical particles in a cellular flow field

R. Mallier and M. Maxey

Division of Applied Mathematics, Brown University, Providence, Rhode Island 02912

Phys. Fluids A 3 (6), June 1991



$$\mathbf{V}(t)=\frac{d\mathbf{X}}{dt}=\mathbf{u}(\mathbf{X}(t),t)+W_1(\hat{\mathbf{g}}\cdot\mathbf{m})\mathbf{m}+W_2[\hat{\mathbf{g}}-(\hat{\mathbf{g}}\cdot\mathbf{m})\mathbf{m}].$$

$$\boldsymbol{\Omega}(t)=\tfrac{1}{2}\boldsymbol{\omega}(\mathbf{X}(t),t)+D\mathbf{m}\times(\mathbf{E}\cdot\mathbf{m})$$

$$\boxed{\psi=U_0L\sin(x_1/L)\sin(x_2/L)}$$

$$V_1=\sin\pi X_1\cos\pi X_2+(W_1-W_2)\sin\theta\cos\theta,$$

$$V_2=-\cos\pi X_1\sin\pi X_2+W_2+(W_1-W_2)\sin^2\theta,$$

$$\frac{d\theta}{dt}=\pi\sin\pi X_1\sin\pi X_2-2D\pi\cos\pi X_1\cos\pi X_2\sin\theta\cos\theta.$$

Homework: Settling of fibers in cellular flow field

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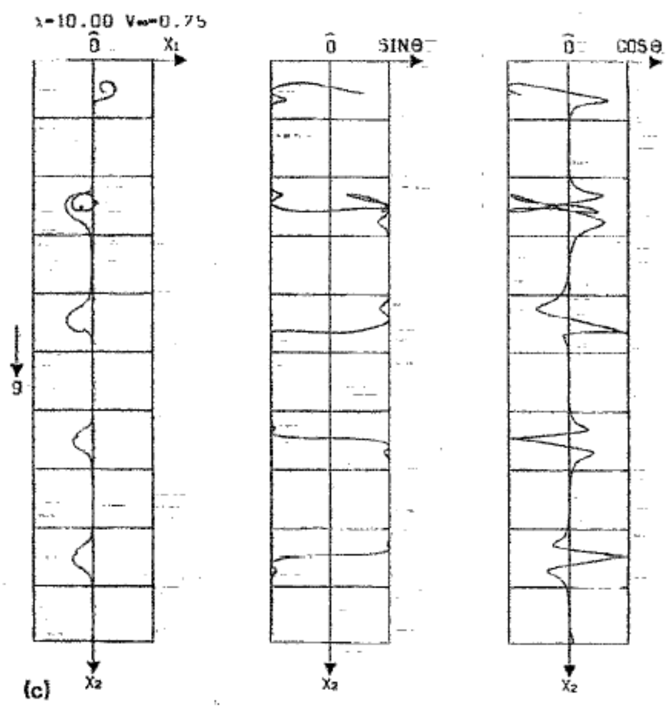
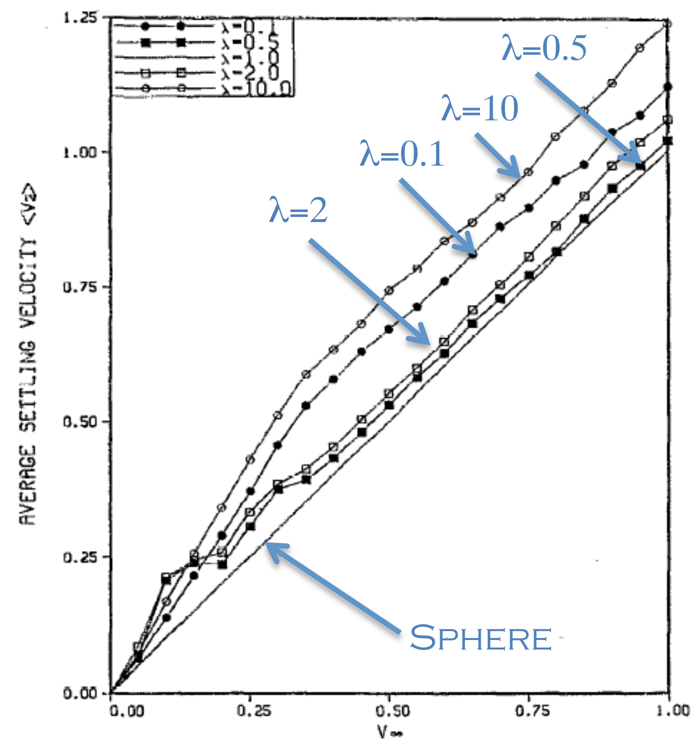


Sample trajectories and orientation of settling spheroidal particles with $\lambda = 10$



Average settling velocity of spheroidal particles at varying λ vs fall speed V_∞

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LESSONS LEARNED

L1. A Lagrangian framework for numerical simulation of non-spherical particles dynamics (in dilute flow conditions) has been presented

L2. Equations for particle translation and rotation were derived for particles with arbitrary shape in the Stokes regime (creeping flow)

L3. The resulting lumped-parameter model provides strong mathematical coupling between Translation and rotation (drag and lift depend on particle orientation)

L4. Particle rotation can be conveniently described using the quaternion formalism

L5. Equations yield accurate results if particles are small (limit on aspect ratio) and/or have small slip velocity

L6. Many modelling issues remain open (force models, force coupling schemes, torque coupling schemes, collisions, ...)

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Thank You
For Your Kind Attention!

Any questions?