Dynamics of diatoms in a turbulent flow

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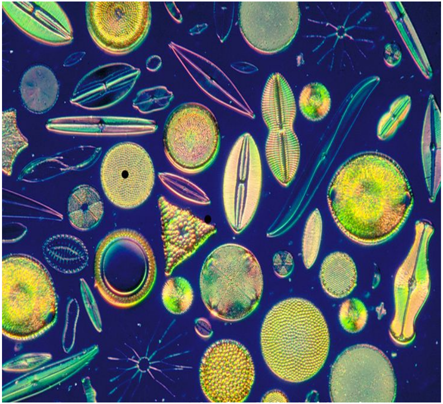
Diatoms

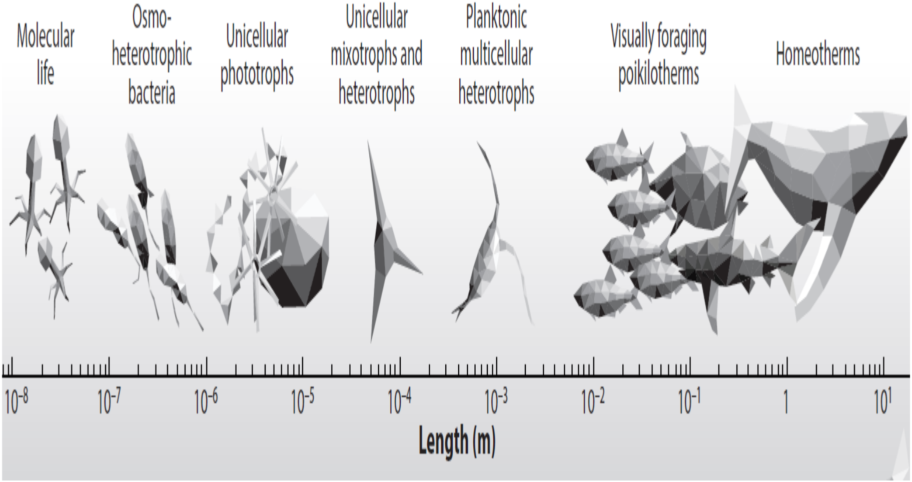


A family of plankton called Phytoplankton.

Why Phytoplankons ?
As they are unicellular, free floating and non swimming microrganism.

How big are diatoms ?

- Roughly 2 μm to 500 μm

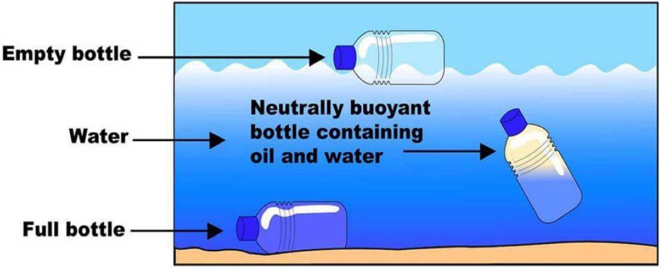


Non motile and neutrally buoyant

- Move passively by water turbulence.
- Neither sinks nor floats.

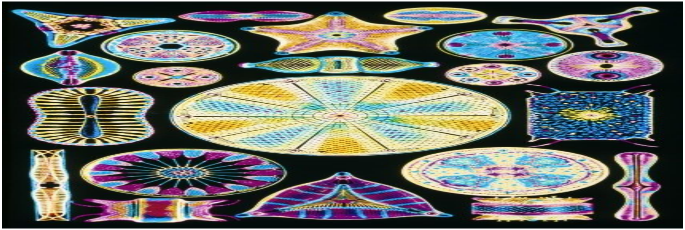
Neutrally buoyant

weight of object = Upward buoyant force exerted by water



Shape and classes of diatoms ?

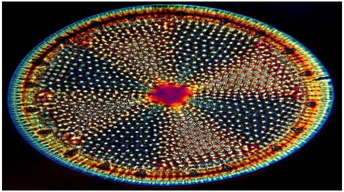
- Usually axisymmetric shape.



Two general category of diatoms.

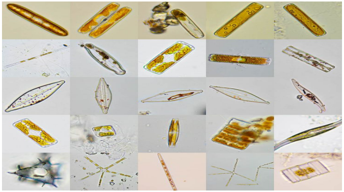
Centrales

Radial symmetry

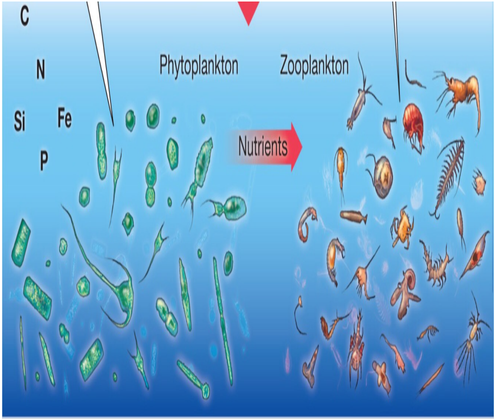


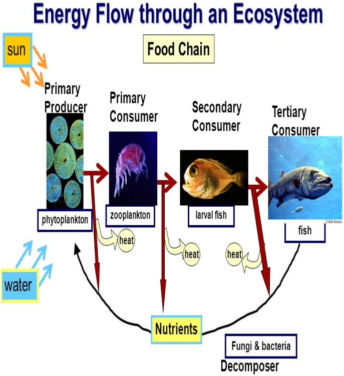
Pennales

Bilateral symmetry



- Phytoplanktons eats nutrients,nutrients are more smaller then phytoplanktons.
- Can be modelled as passive tracers or scalar field which are subjected to diffusion.

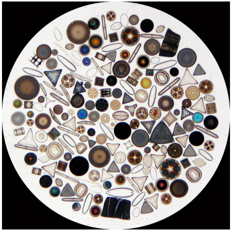




- Homogeneous turbulent flow
- $Re_\lambda \approx 100$ and $\eta \approx 200\mu m$
- Size of the nutrients
- Passive scalar

Why this shape ?

- For collection nutrients
- Adaptation to turbulent environment.
- Evolution

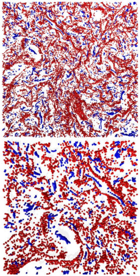


Shapes of planktons

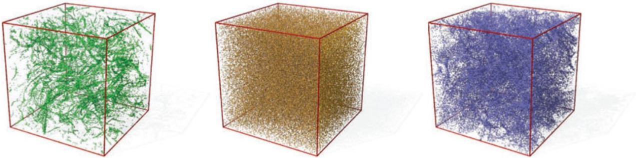
Turbulent environment

Dispersion of inertial particles in turbulent flow

- Preferential concentration based on inertia
- Alignment of the diatoms



Distribution of the particles w.r.t density



Lower to higher density of particles

- Navier stokes for fluid simulation + forcing

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} + F \tag{1}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2}$$

- Advection diffusion equation

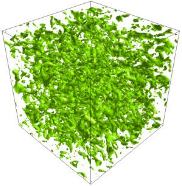
$$\frac{\partial}{\partial t} C + u_j \cdot \frac{\partial}{\partial x_j} C = \alpha \frac{\partial^2}{\partial x_j^2} C + S \tag{3}$$

where F is the forcing term and S is the source term for the scalar

- Refinement due to variation of force and source in the terms with depth

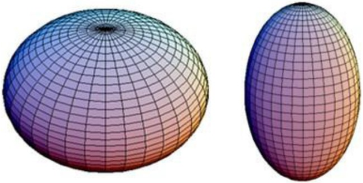
Assumptions and Consideration for simulation

- Fluid assumption
  - Incompressible
  - Homogeneous
  - Isotropic
- Particle assumption
  - Shape of particle (Oblate and Prolate)
  - Symmetry is shape
  - One way coupling



Simulation of turbulence

(Visualization of vorticity)



oblate spheroid *prolate spheroid*

- Newton equation

$$m \cdot \frac{dv_p}{dt} = F \tag{4}$$

- Drag force [3]

$$F = \mu \pi a \cdot R K^b R^T (u_f - v_p) \tag{5}$$

where K is the resistance tensor.

$$K^b_{xx} = K^b_{yy} = \frac{16(\beta^2 - 1)}{(2\beta^2 - 3) ln \frac{\beta + \sqrt{\beta^2 - 1}}{\sqrt{\beta^2 - 1)}} + \beta}$$

$$K^b_{zz} = \frac{8(\beta^2 - 1)}{(2\beta^2 - 1) ln \frac{\beta + \sqrt{\beta^2 - 1}}{\sqrt{\beta^2 - 1)}} - \beta}$$

β = aspect ratio

3. Gallily, I. and Cohen, A. (1979). On the orderly nature of the motion of nonspherical aerosol particles. II. Inertial collision between a spherical large droplet and an axially symmetrical elongated particle. Journal of Colloid and Interface Science, 68(2), 338(356).

Modeling of diatoms w.r.t orientation

- Euler equation

$$\frac{d}{dt}(I \cdot \omega) + \omega \times (I \cdot \omega) = T \tag{6}$$

- Torque [4]

$$T_i = \frac{16 \times \pi \times \mu \times a^3 \times \beta}{3 \times (\beta_0 + \beta^2 \cdot \gamma_0)} \times ((1-\beta^2) \times S_{kj} + (1+\beta^2) \times (\omega_{jk} - \omega_i) \tag{7}$$

where,
β = aspect ratio
ω_{jk} = strain rate tensor $(\frac{1}{2}(\frac{du_k}{dx_j} + \frac{du_j}{dx_k}))$
S_{kj} = rotation tensor $(\frac{1}{2}(\frac{du_k}{dx_j} - \frac{du_j}{dx_k}))$

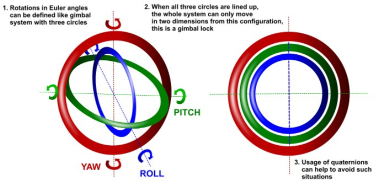
- Homogeneous in density

4. Jeffery, G. B. (1922). The motion of ellipsoidal particles immersed in a viscous fluid. Royal Society of London. Series A,, 102(715), 161(179).

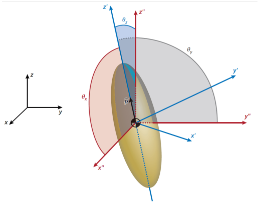
Difficulty in the numerical simulation

- 12 unknown variables ($x_i, v_i, \omega_i, \theta, \psi, \phi$)
- Lab frame to body frame
- Singularity problem (Rotation Matrix)
- Gimbal lock (Euler angles)

Lab frame(x, y, z) and body frame(x'', y'', z'')



Gimbal lock configuration



Coordinate frames

Solution and optimization

- Quaternions

$$q = [q_0, q_1, q_2, q_3] \tag{8}$$

Property of quaternions

$$q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1 \tag{9}$$

Rotation by quaternions [5]

$$K' = RKR^T \tag{10}$$

$$R = \begin{bmatrix} 1 - 2(q_2^2 - q_3^2) & 2 \times (q_1 \times q_2 + q_0 q_3) & 2(q_1 q_3 - q_0 q_2) \\ 2(q_1 q_2 - q_0 q_3) & 1 - 2(q_1^2 + q_3^2) & 2(q_2 q_3 + q_0 q_1) \\ 2(q_1 q_3 + q_0 q_2) & 2(q_2 q_3 - q_0 q_1) & 1 - 2(q_1^2 + q_2^2) \end{bmatrix} \tag{11}$$

- Integration method

$$\dot{q} = \frac{1}{2} q \times \omega \tag{12}$$

5. Betsch, P. and Siebert, R. (2009). Rigid body dynamics in terms of quaternions : Hamiltonian formulation and conserving numerical integration. International Journal for Numerical Methods in Engineering, 79(4), 444(473)

Simpler approach

What is the simplified way to approach this problem ?

- Introducing the problem by neglecting inertia.

$$\frac{dx}{dt} = u \tag{13}$$

u – is the velocity of fluid.

Jeffery equation (1922)

$$\dot{p}_i = \Omega_{ij} p_j + \frac{\alpha^2 - 1}{\alpha^2 + 1} \left(S_{ij} p_j - p_i p_k S_{kl} p_l \right) \tag{14}$$

where,

$\alpha = l/d$ ....is the aspect ratio

Ω_{ij}............... is the rate of rotation tensor

S_{ij}............... is the rate of strain tensor

$\dot{p}_i$ .... is the component of orientation vector which is along the axis of symmetry of particle

- These will produce particle with complex dynamics.

6. [**Parsa**, **Calzavarini et al PRL 2012**,
Rotation rate of rods in turbuennt fluid flow]

Simpler approach

- These will produce particle with complex dynamics.
- Particles distribute homogeneously,so is need to use inertia, also the orientation is not reveled.
- Particles gets aligned to the vorticity vector.

6. [**Parsa**, **Calzavarini et al PRL 2012**,
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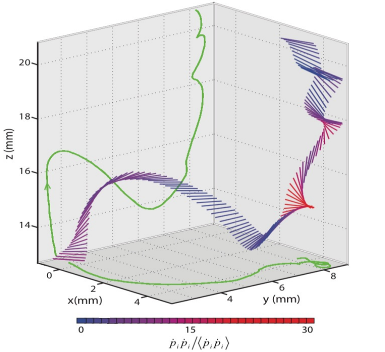
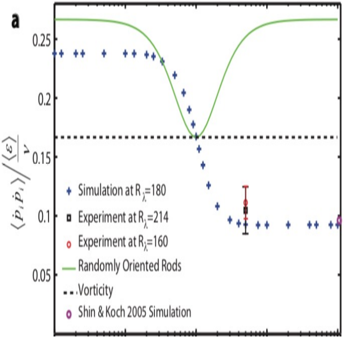
Simpler approach

- These will produce particle with complex dynamics.
- Particles distribute homogeneously,so is need to use inertia, also the orientation is not reveled.
- Particles gets aligned to the vorticity vector.
- Disks like particle rotate much faster then elongated particles.





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6. [**Parsa**, **Calzavarini et al PRL 2012**, **Rotation rate of rods in turbuennt fluid flow**]

Simpler approach,(with gravity)

- Another approach could be account for inertia only in center of mass.
- Based on observation that rotational relaxation time, are shorter then transnational relaxation time.It is not known in general,but few papers reveals this key information.

In recent works on diatoms obeys :[7]

$$\frac{dx}{dt} = u|_x + v_s(p) \tag{15}$$

$$v_s(p) = v_s^{min}\hat{e}_g + \left(v_s^{max} - v_s^{min}\right)\left(\hat{e}_g \cdot p\right) p \tag{16}$$

where,

x .... is the spheroid position

$u|x$ ....is the fluid velocity at spheriod position.

v_s ....is the Stokes settling velocity.

p .... is the spheroid orientation position.

7. [**M.Niazi Ardekani et al J.Fluid Mech. 2017**, **Sedimentation of inertialess prolate**, **spheroid in HIT with application to non motile phytoplankton**]

Simpler approach,(with drag)

The fact that $\tau_R < \tau_T$ [8] allows us to propose this model.

- Newton equation

$$m \cdot \frac{dv_p}{dt} = F \tag{17}$$

- Drag force

$$\mathbf{F} = \mu\pi a \cdot \mathbf{R}K^b\mathbf{R}^T \left(u_f - v_p\right) \tag{18}$$

where, K is the resistance tensor.
For the rotation we use Jeffery equation. [9]

$$\dot{p}_i = \Omega_{ij}p_j + \frac{\alpha^2 - 1}{\alpha^2 + 1}\left(S_{ij}p_j - p_i p_k S_{kl} p_l\right) \tag{19}$$

8. Zhao et al, PRL 2015,Rotation of non spherical particles in turbulent channel flow
9. Jeffery,1922, The motion of ellipsoidal particle immersed in viscous fluid

Summary and Perspectives

- Summary
  - Proposed a model in turbulent environment with nutrients
  - The model is Eulerian and Lagrangian
  - We proposed a simplified model based on the idea that $\tau_R < \tau_T$
- Perspective
  - Parametric study of aspect ratio and Stokes number
  - Study the difference between two models (select better model)
  - Draw ecological conclusion

Questions

Thank you for your attention.

Do you have any questions ?