Computational Fluid Dynamics Simulations of Fluid Flow with Algae at IMH

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IMH - Institute of Modelling and High-Performance Computing, Hochschule Niederrhein - University of Applied Sciences, Krefeld, Germany

The IMH in a Few Words - 1

- People:
  - 4 professors (Parallel Systems, Robust Design Optimization, Mathematics, Optimization, FEM, FSI and CFD)
  - 2 scientific assistants
    Computer Science, Parallel Computing, Process Engineering, CFD
  - 2 PhD students
    Robust Design Optimization, FEM, FSI
  - 1 assistant for finance and organisation

The IMH in a Few Words - 2

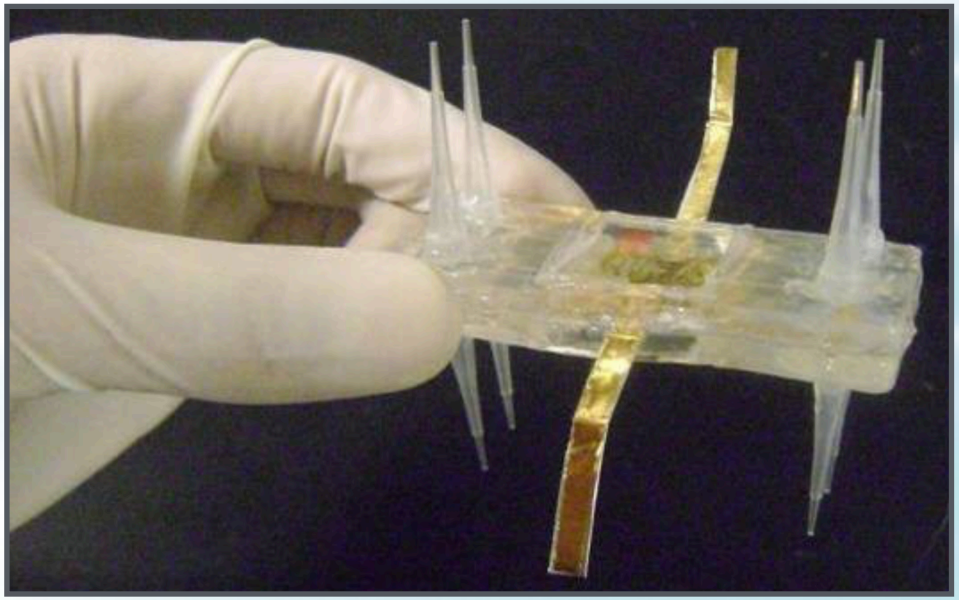
- Computer:
  - Several compute cluster, the newest has 1200 CPU cores and 38 Nvidia A100 GPU
  - Workstation up to 128 GB RAM and 16 cores / high-end GPU's
- This stands for the possibility of modelling and simulating complex geometries and complex physics

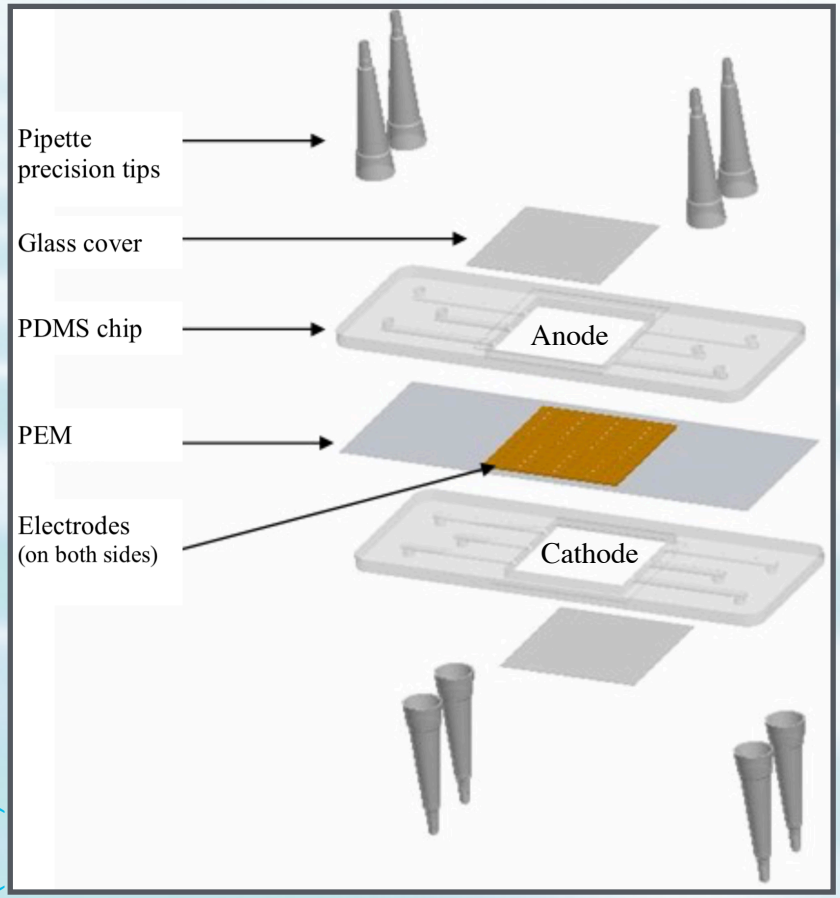
The IMH in a Few Words - 3

- 77 permanent licenses Ansys Multiphysics,
  512 permanent parallel licenses Ansys Multiphysics
- DSMC OpenFOAM, incl. self established coupling with Fluent
- Self established program extensions to Fluent and DSMC OpenFoam
- 106 permanent licenses optiSLang/optiPLug
- 4 licenses Diffpack
- 50 licenses Matlab

Fluid Flow with Algae: Starting point - 1

- **Micro-photosynthetic solar cell experiments by Shahparnia (2011) and Shahparnia et al. (2015)**
- **New means of electricity generation by algae**

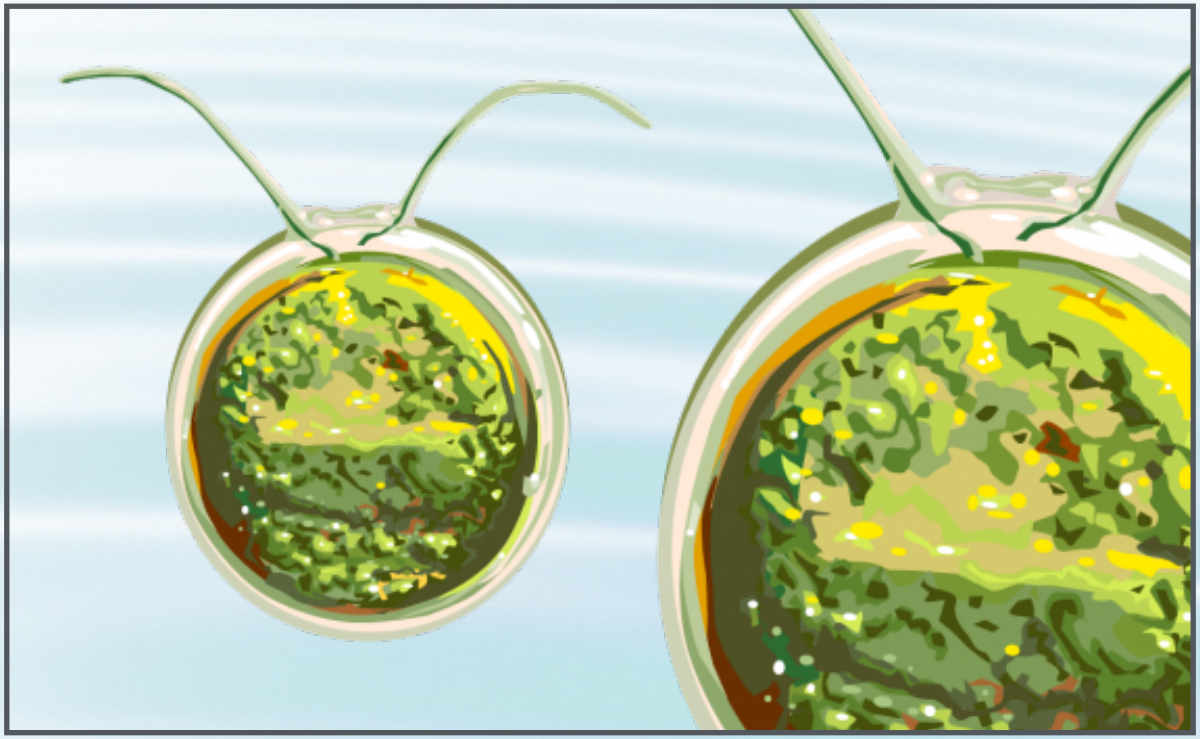




Shahparnia (2011)

Fluid Flow with Algae: Starting point - 2

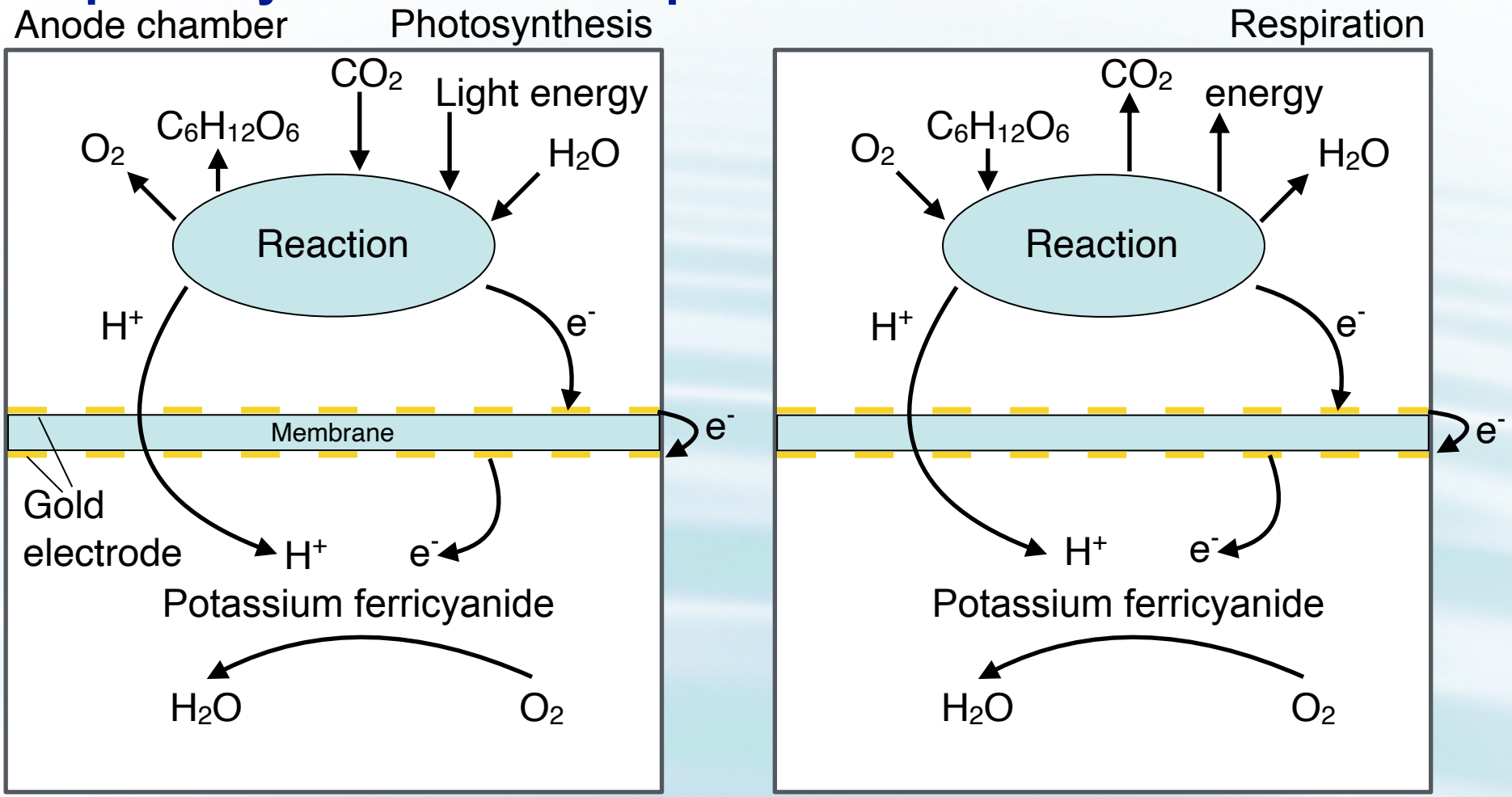
- **Algae *Chlamydomonas reinhardtii* is used in the experiments of Shahparnia (2011) and Shahparnia et al. (2015)**
- **Diameter approx. 8 micrometer**



http://www.pflanzenforschung.de/de/themen/pflanzen-im-fokus/chlamydomonas 27.2.2018

Principle of Operation

- **Electrons are produced and utilised during photosynthesis and respiration**

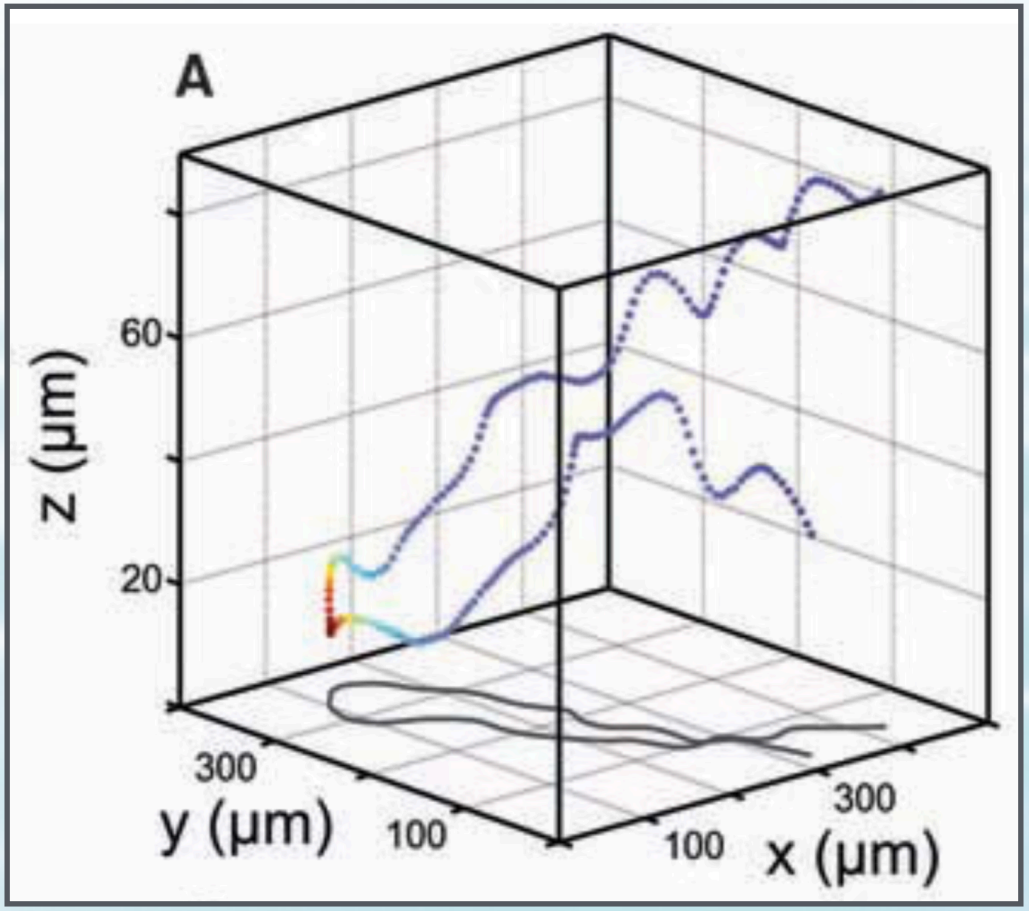


Targets of the Project

- Overall goal is a model of the bio-solar cell and an optimization of the electrical current
- Current aim is the modelling and simulation of the algal movement
- Algae react with orientation on
  - the gravitational field: Gravitaxis
  - the gravitational field and the vorticity of the surrounding fluid: Gyrotaxis
  - the intensity of the incident light: Phototaxis
  - the concentration gradient of air: Aerotaxis
  - the concentration gradient of chemical substances: Chemotaxis

Gravitaxis

- **Algae mostly swim in the opposite direction of the gradient of the gravitational field in helices with sudden turns**



Polin et al. (2009)

Mathematical Model of the Gravitaxis - 1

- **In the mathematical model the fluid (water) is modeled in Eulerian description**

Total mass balance equation

Total momentum balance equation ← Two-way coupling

and the algal cells are modeled as a sphere of diameter of 8 micrometer in Lagrangian description

Sum of forces on the particle = mass of particle * acceleration of particles

Sum of torques on the particle = tensor of inertia of the particle * angular acceleration

Mathematical Model of the Gravitaxis - 2

- **In the mathematical model the fluid (water) is modeled in Eulerian description**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{v} \right) = 0$$

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot \left(\rho \vec{v} \otimes \vec{v} \right) = -\nabla p + \nabla \cdot \vec{\vec{T}} + \vec{F}_p \qquad \vec{F}_p = -\frac{1}{V_c} \sum \left(\frac{\vec{v} - \vec{v}_p}{\tau_r} \right) m_p$$

and the algal cells are modeled as a sphere of diameter of 8 micrometer in Lagrangian description

$$\frac{\partial \vec{v}_p}{\partial t} = \frac{\vec{v} - \vec{v}_p}{\tau_r} + \frac{\vec{g}\left(\rho_p - \rho \right)}{\rho_p} \qquad \tau_r = \frac{\rho_p d_p^2}{18\mu} \frac{24}{C_d \mathrm{Re}_p} \qquad \mathrm{Re}_p = \frac{\rho d_p \left| \vec{v}_p - \vec{v} \right|}{\mu} \qquad C_d = \frac{24.0}{\mathrm{Re}_p}$$

($Re_p < 0.1$)

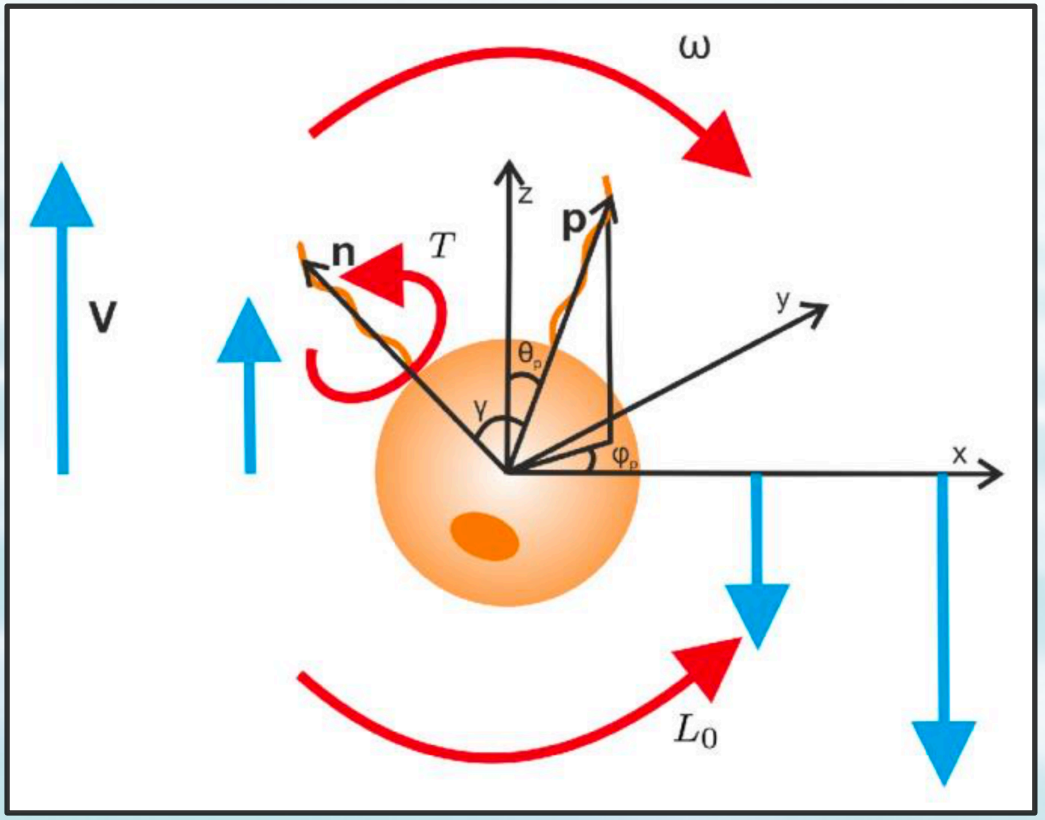
Sum of torques on the particle =
tensor of inertia of the particle * angular acceleration

Next slide

Mathematical Model of the Gravitaxis - 3

- **The term:** tensor of inertia of the particle * angular acceleration **is very much smaller than the term:** Sum of torques on the particle **(Hopkins, 2002)**
- **This leads to an equation for the angular velocity vector $\vec{\Omega}$ (Alqarni, 2016)**

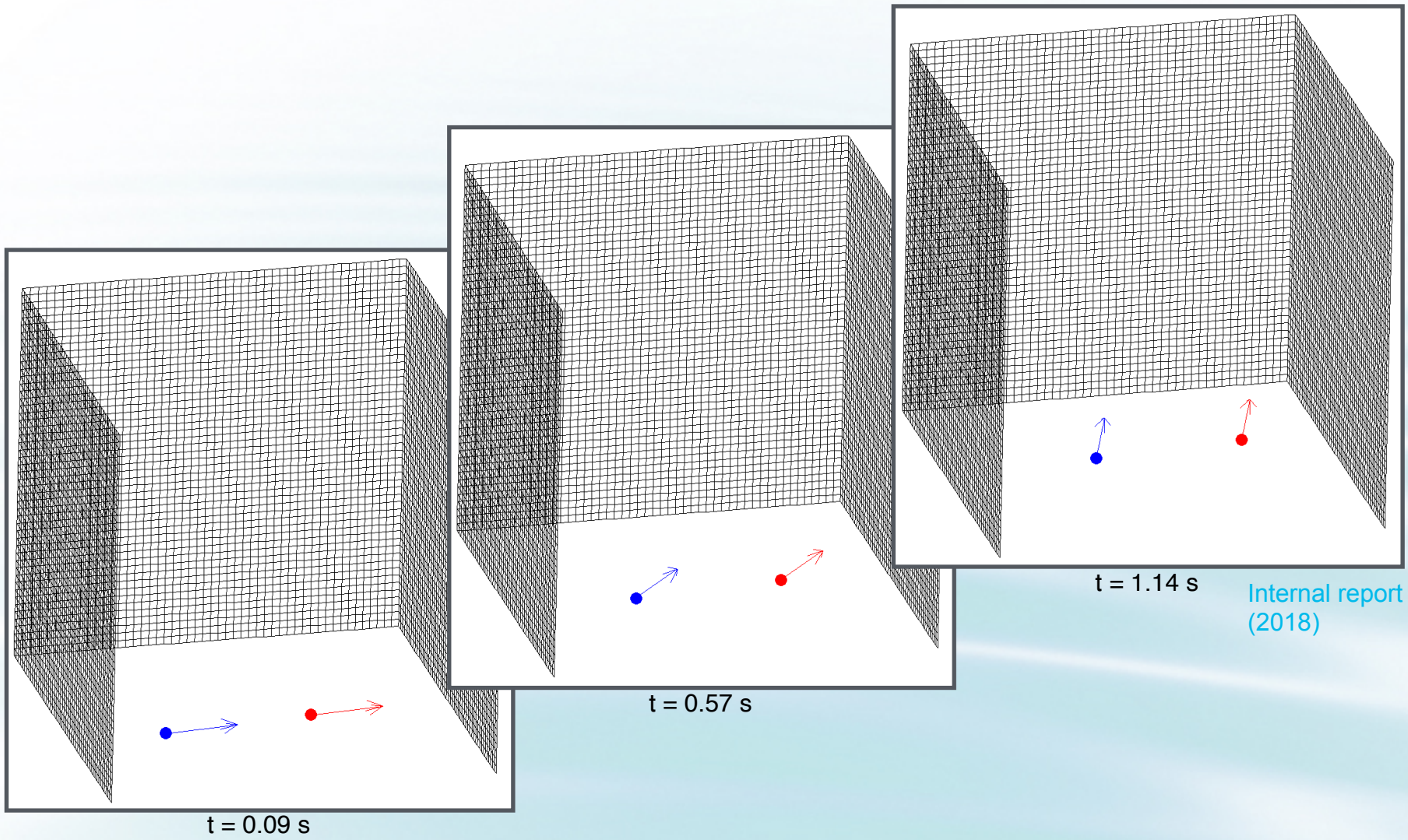
$$\vec{\Omega} = \frac{L_0}{8\pi\mu\left(\frac{d_p}{2}\right)^3}\vec{p}\times\vec{k} + \frac{T}{8\pi\mu\left(\frac{d_p}{2}\right)^3}\vec{n} + \frac{1}{2}f\cdot\vec{j}$$



Maraun (2018)

Simulation of Gravitaxis - 1

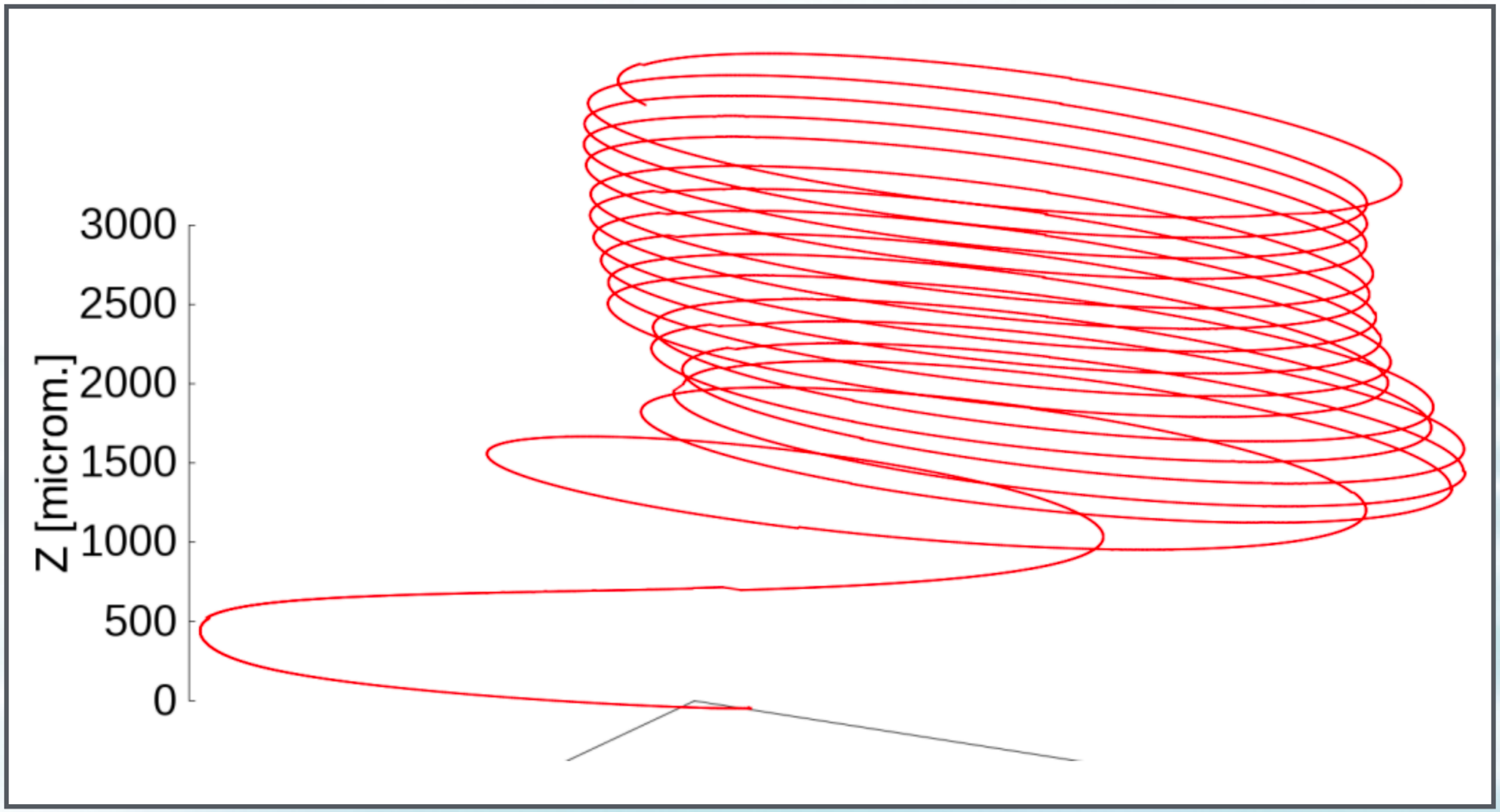
- **The helical movement was modeled and simulated**



Internal report (2018)

Simulation of Gravitaxis - 2

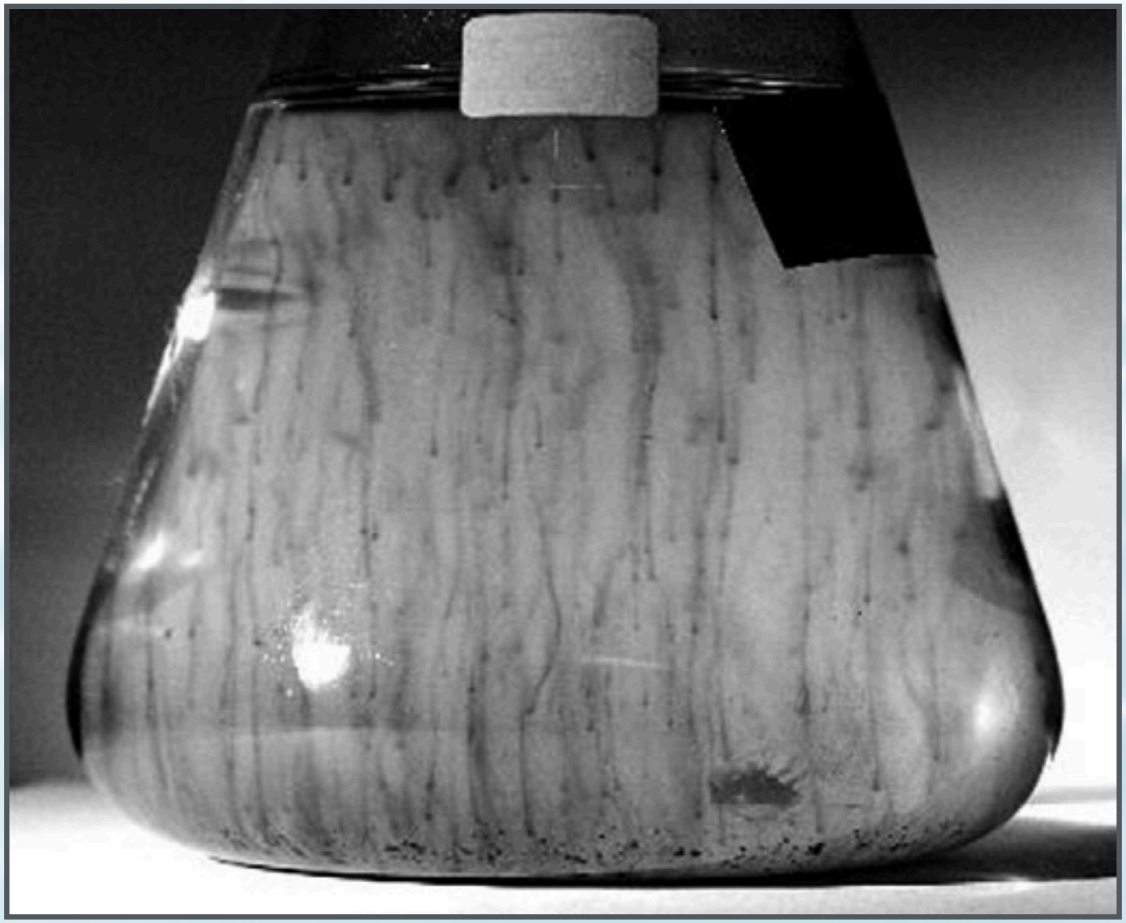
- **The helical movement was modeled and simulated**



Maraun (2018)

Downward Oriented Plumes

- **Due to density differences between algae and fluid the algae and the fluid together form downward oriented plumes**



Williams and Bees (2011)

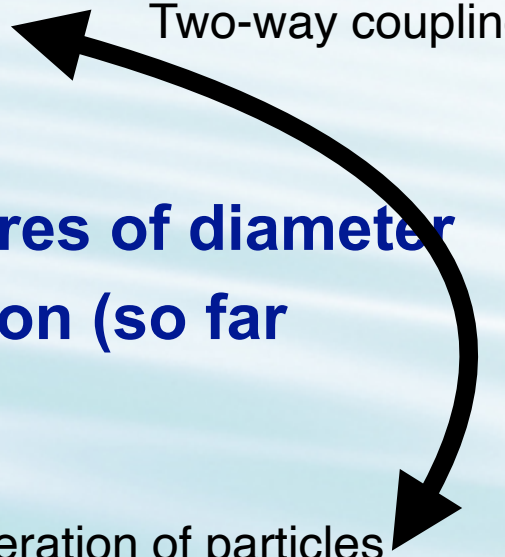
Model of the Downward Oriented Plumes - 1

- **In the mathematical model**
  the fluid (water) is modeled in Eulerian description

Total mass balance equation

Total momentum balance equation

Two-way coupling

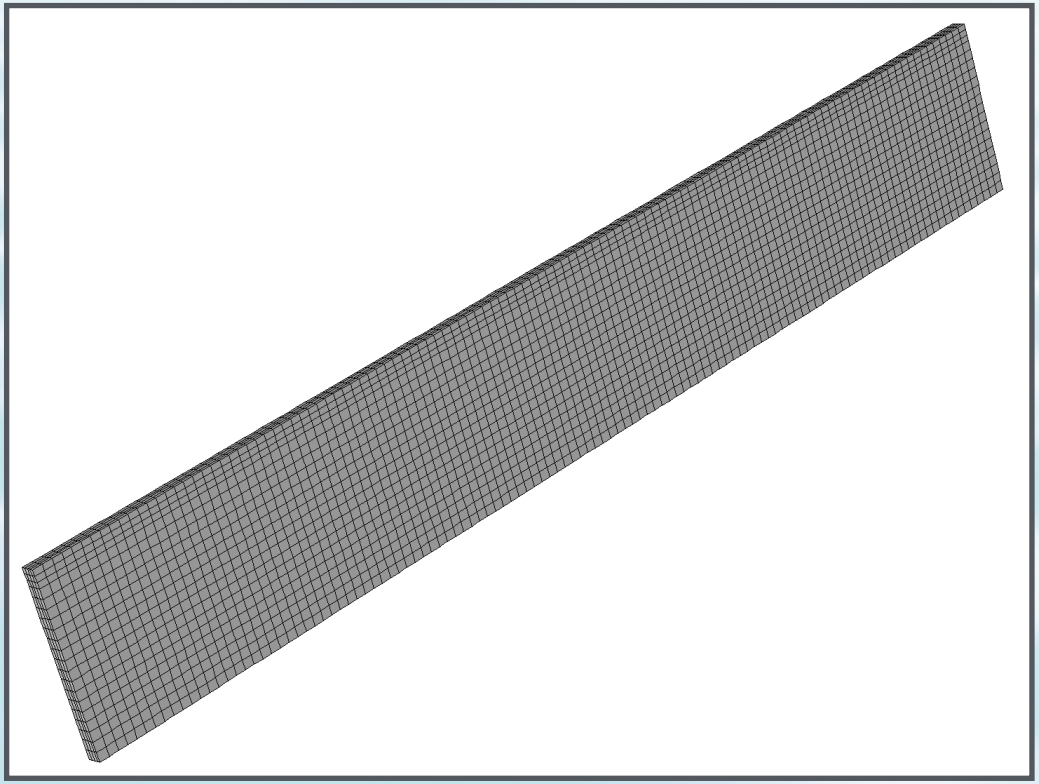


and the algal cells are modeled as spheres of diameter of 8 micrometer in Lagrangian description (so far without torque balance equation)

Sum of forces on the particle = mass of particle * acceleration of particles

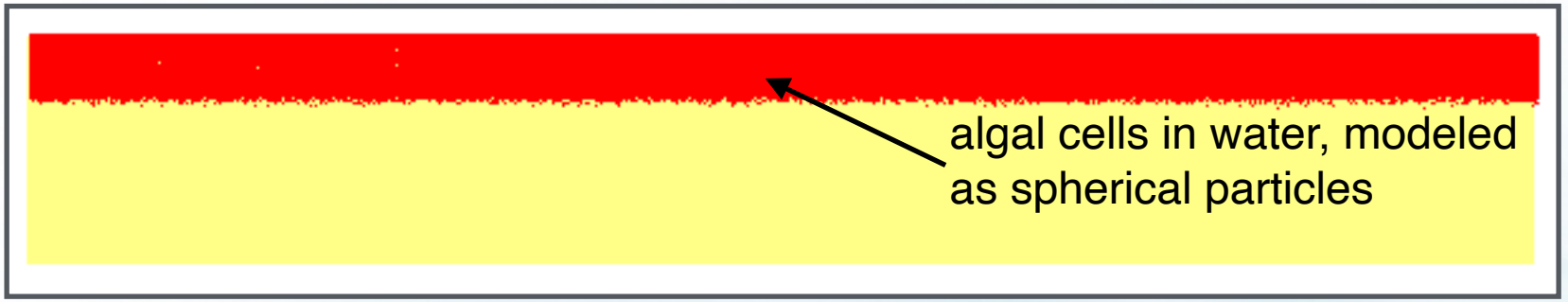
Model of the Downward Oriented Plumes - 2

- Geometrical model: Width 80 mm, height 12 mm and depth 1 mm
- Boundary conditions: top wall - no stress, side walls - symmetry, bottom wall - no slip, front and back wall- symmetry

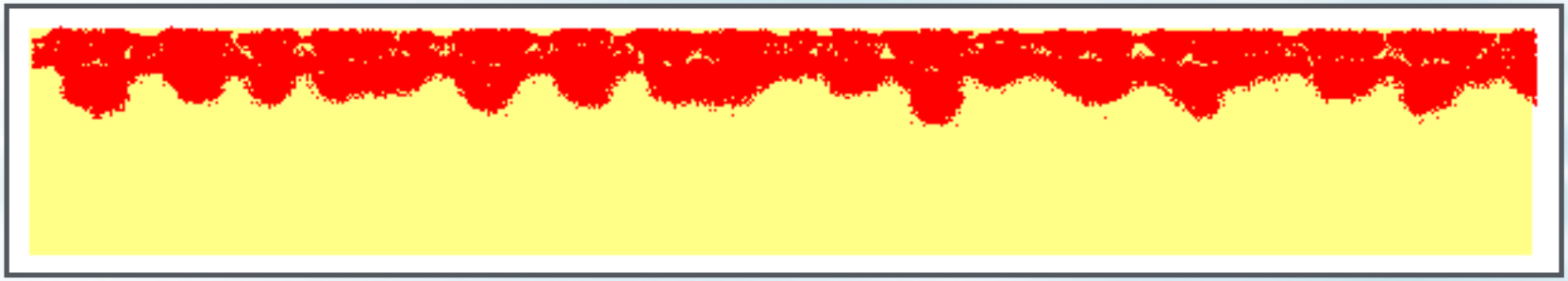


Model of the Downward Oriented Plumes - 3

- **The formation of plumes was modeled**



t = 0.2 s



t = 60 s

t = 80 s

Conclusion and Outlook - 1

- Mathematical models for the gravitaxis and plume formation were developed
- The models will be extended to modelling the gyrotaxis and tested for numerical accuracy
- The comparison with experiments will come in the near future
- The other taxi like e.g. phototaxis will be incorporated next
- Then the generation of electrons will be included in the mathematical model and the comparison with experiments will be conducted

Conclusion and Outlook - 2

- **Long-term aim is the optimization of the bio-solar cell, e.g.**
  - **optimise the geometry of the cell**
  - **realise a flow through the cell**
  - **optimise the volume flow rate**
  - **optimise the filling degree**
  - **optimise the density of cells**
  - **…**

References - 1

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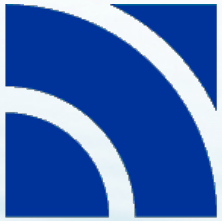

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