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Coupling hydrodynamics and biology to model algae growth

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# October 16<sup>th</sup>

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# Motivations

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# Raceway modeling

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Biofu	lel				

Let us begin with several definitions:

**Biofuel** : fuel whose energy is derived from carbon fixation.

**Carbon fixation** : reduction of inorganic carbon to organic compounds by living organisms. *Example* : photosynthesis

$$6CO_2 + 6H_2O + light \to C_6H_{12}O_6 + 6O_2 \tag{1}$$

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Biof	uel generatio	ns			

# First generation : biofuels made from

- fermentation of sugars derived from wheat, corn... Produces alcohol : bioethanol, methanol...
- oil (sunflower, colza...)
   Produces biodiesel

Problem: biofuel production to the detriment of food production.

Second generation: derived from non-food lignocellulosic crops.

*Plants* = *lignin* + *cellulose* 

Problem: the conversion requires expensive technologies.

Third generation: algae !

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Alga	ae culture				

# Why algae?

- Capable of storing carbon under lipid form through photosynthesis
- Autotrophs species only need inorganic material
- Optimal conditions for the growth are easily reachable
- Natural techniques for the increase of oil production (nitrogen stress, thermal stress...)

# Actual barriers

- Compromise growth/oil production
- Cost of nutrients
- Need to find a way to use the other products of an algae
- Contamination hazard for outdoor raceways
- No economical study has been done yet

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A ra	ceway				

# Description: algae pool driven into motion by a paddlewheel



Figure: An industrial raceway (Innovalg, 85) Photo Olivier Darboux, Ifremer

**Goal**: optimize the biomass production by playing on the nutrients concentrations, water height, light intensity, agitation...

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2 The hydrodynamical model

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Shall	ow water	approximation	of Navier	<sup>.</sup> Stokes	

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**Starting point** : free surface Navier Stokes equation for incompressible fluids

$$\begin{cases} div(\mathbf{u}) = 0\\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = \mathbf{g} + div\mathbf{\Sigma} \end{cases}$$
(2)

valid for  $0 \le z \le h(t, x)$ .



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Hypothesis:

- Hydrostatic hypothesis (vertical pressure variation balanced only by gravity)
- Introduction of a small parameter  $\epsilon = \frac{H}{L}$ 
  - Rescaling in  $\epsilon$
  - Integration of NS equations along the vertical dimension

• 
$$u = \overline{u}$$



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Result : viscous Saint Venant system [Gerbeau, Perthame 2000]:

$$\begin{pmatrix} \partial_t H + \partial_x (H\bar{u}) = 0 \\ \partial_t H\bar{u} + \partial_x (H\bar{u}^2 + \frac{gH^2}{2}) = -gH\partial_x z_b + \partial_x (4\mu\partial_x\bar{u}) + \kappa(\bar{u})$$

$$(3)$$

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Bey	ond the Saint	-Venant sys	stem		

- $\bullet~\mbox{Reduced complexity}$  : 2D  $\rightarrow$  1D
- Hyperbolic conservation law
- Low computation cost

	The hydrodynamical model	The biological model	Numerical scheme		Raceway modeling
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Key idea :  $u = \sum_{\alpha=1}^{N} \mathbb{1}_{\alpha}(x, t) u_{\alpha}(x, t)$  instead of  $u = \bar{u}(x, t)$ .

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[Audusse, Bristeau, Perthame, Sainte-Marie, 2010] : a multilayer version with mass exchanges.

### 

From hydrostatic Euler equations

$$\begin{cases} \partial_{x}u + \partial_{z}w = 0\\ \partial_{t}u + \partial_{x}u^{2} + \partial_{z}uw + \partial_{x}p = 0\\ \partial_{z}p = -g \end{cases}$$
(4)

Two main steps:

• Galerkin approximation of every variable on

$$\mathbb{P}_{0,H}^{N,t} = \left\{ \mathbb{I}_{z \in L_{\alpha}(x,t)}(z), \quad \alpha \in \{1,\ldots,N\} \right\},\$$

• Vertical integration on each layer.



The Multilayer Saint Venant system writes

$$\begin{cases} \partial_t H + \sum_{\alpha=1}^{\alpha=N} \partial_x h_\alpha u_\alpha = 0\\ \partial_t h_\alpha u_\alpha + \partial_x (h_\alpha u_\alpha^2 + \frac{g}{2} H h_\alpha) = F_{\alpha+1/2} - F_{\alpha-1/2} \end{cases}$$
(5)

- Only one global continuity equation,  $H = \sum h_{lpha}$
- Exchange terms  $G_{\alpha+1/2}, F_{\alpha+1/2} = u_{\alpha+1/2}G_{\alpha+1/2} + P_{\alpha+1/2}$

The advantages of this formalism compared to Navier Stokes are:

- No more z-derivative
- H is a variable of the system: once it is known, the geometry is known.
- We get a system of conservation laws with source terms.

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# Motivations



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# Raceway modeling

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Phv	toplankton er	vironment			



We want to: study the combined influence of nitrate and light on algae growth.

Nutrient: Monod, Droop, mechanistic...?

Light: photoadaptation, photoinhibition...?

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Phy	toplankton er	vironment			



We choose: study the evolution of 3 variables:

- The phytoplanctonic carbon,  $C_1$
- The phytoplanctonic nitrogen,  $C_2$
- The extracellular nutrients,  $C_3$

We call  $q = C_2/C_1$  the internal nutrient quota.

#### 

We choose: a Droop model (the growth ratio is proportional to the internal nutrient quota)

$$\mu(q) = \bar{\mu}(1 - \frac{Q_0}{q}), \tag{6}$$

with photoinhibition (the growth can be weakened by excessive light exposure)

$$\bar{\mu}(I) = \tilde{\mu} \frac{I}{I + K_{sI} + \frac{I^2}{K_{iI}}},$$

and photoadaptation (the light sensitivity is proportional to the cell history)

$$I(z) = I_0 e^{-\int_0^z (aChI(z)+b)dz},$$
(7)

and Chl depends on the previous light exposure of the cell.

	The hydrodynamical model	The biological model	Numerical scheme	Kinetic interpretation	Raceway modeling
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Deriv	vation of the	model in 2	Π		

Add transport, diffusion, to reaction terms:

$$\begin{cases} \partial_t C_1 + \nabla \cdot (\mathbf{u}C_1) = \nu C_1 \Delta C_1 + \mu(q, I)C_1 - RC_1\\ \partial_t C_2 + \nabla \cdot (\mathbf{u}C_2) = \nu C_2 \Delta C_2 + \lambda(C_3, q)C_1 - RC_2\\ \partial_t C_3 + \nabla \cdot (\mathbf{u}C_3) = \nu C_3 \Delta C_3 - \lambda(C_3, q)C_1 \end{cases}$$
(8)

Integrate it in the multilayer model (Galerkin projection + integration):

$$\begin{aligned} \int \frac{\partial h_{\alpha} C_{\alpha}^{1}}{\partial t} &+ \frac{\partial}{\partial x} \left( h_{\alpha} C_{\alpha}^{1} u_{\alpha} \right) = C_{\alpha+1/2}^{1} G_{\alpha+1/2} - C_{\alpha-1/2}^{1} G_{\alpha-1/2} \\ &+ \nu \int_{z_{\alpha-1/2}}^{z_{\alpha-1/2}} \Delta C_{1} dz + h_{\alpha} (\mu(q_{\alpha}, l_{\alpha}) C_{\alpha}^{1} - R C_{\alpha}^{1}) \\ \frac{\partial h_{\alpha} C_{\alpha}^{2}}{\partial t} &+ \frac{\partial}{\partial x} \left( h_{\alpha} C_{\alpha}^{2} u_{\alpha} \right) = C_{\alpha+1/2}^{2} G_{\alpha+1/2} - C_{\alpha-1/2}^{2} G_{\alpha-1/2} \\ &+ \nu \int_{z_{\alpha-1/2}}^{z_{\alpha-1/2}} \Delta C_{2} dz + h_{\alpha} (\lambda(C_{\alpha}^{3}, q_{\alpha}) C_{\alpha}^{1} - R C_{\alpha}^{2}) \\ \frac{\partial h_{\alpha} C_{\alpha}^{3}}{\partial t} + \frac{\partial}{\partial x} \left( h_{\alpha} C_{\alpha}^{3} u_{\alpha} \right) = C_{\alpha+1/2}^{3} G_{\alpha+1/2} - C_{\alpha-1/2}^{3} G_{\alpha-1/2} \\ &+ \nu \int_{z_{\alpha-1/2}}^{z_{\alpha-1/2}} \Delta C_{3} dz - h_{\alpha} \lambda(C_{\alpha}^{3}, q_{\alpha}) C_{\alpha}^{1} \end{aligned}$$

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**Motivations** 

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Finit	e volume sch	eme			

Finally, we can summarize the hydro-bio system in:

$$\partial_t X + \partial_x F(X) = S_e + S_v + S_p + S_{bio}$$
(9)

Time discretization (splitting)

$$\begin{cases} \frac{\tilde{X}^{n+1} - X^{n}}{\Delta t} + \partial_{x}F(X^{n}) = S_{e}(X^{n}, \tilde{X}^{n+1}) + S_{p}(X^{n}) + S_{bio}(X^{n}) \\ \frac{X^{n+1} - \tilde{X}^{n+1}}{\Delta t} - S_{v}(X^{n}, X^{n+1}) = 0 \end{cases}$$
(10)

# Space discretization

- Division of the X-domain in N cells C<sub>i</sub>
- Integration of the system over  $[t_i, t_{i+1}] \times [x_i, x_{i+1}]$

$$\tilde{X}_{i}^{n+1} - X_{i}^{n} + \sigma_{i}^{n} [F_{i+1/2}^{n} - F_{i-1/2}^{n}] = \Delta t S_{e,i}^{n} + \Delta t S_{p,i}^{n} + \Delta t S_{bio,i}^{n}$$
(11)

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Kine	tic interpretat	ion				

# Particularity of the problem

No proof of MSV system being hyperbolic No analytical computation of the eigenvalues Riemann problem not possible

# Use of kinetic schemes

$$\mathsf{MSV}+\mathsf{Bio system} \Leftrightarrow \begin{cases} \partial_t M_\alpha + \xi \partial_x M_\alpha + N_{\alpha-\frac{1}{2}} - N_{\alpha+\frac{1}{2}} = Q_\alpha \\ \partial_t C^i M_\alpha + \xi \partial_x C^i M_\alpha + C^i N_{\alpha-\frac{1}{2}} - C^i N_{\alpha+\frac{1}{2}} = R_\alpha \end{cases}$$
(12)

- $(M_{\alpha}, C^{i}M_{\alpha})$  particle density,  $(Q_{\alpha}, R_{\alpha})$  collision term (= 0 a.e.)
- $\int_{B} \xi^{p} M d\xi$ ,  $\int_{B} \xi^{p} U d\xi$  give the macroscopic variables
- linear transport equation  $\Rightarrow$  upwind scheme

Idea

$$F_{i+1/2} = \int_R \xi M_{i+1/2} d\xi$$

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Anal	lytical validat	ion			

Analytical solution of Euler system with Biology [B., Sainte-Marie 2012]

- 2D and 3D hydro solutions for any topography  $z_b(x)$
- in 2D, stationary continuous solutions (u, H, T) satisfy

$$u(x, z) = \alpha \beta \frac{\cos(\beta(z - z_b))}{\sin(\beta H)}, \quad \left(g(H + z_b) + \frac{\alpha^2 \beta^2}{2\sin^2(\beta H)}\right)_x = 0$$
$$T(x, z) = e^{-(H - (z - z_b))}$$

(13)

where T is solution of the simple biological system  $\partial_t T + \partial_x uT + \partial_z wT = f(x, z)T(x, z)$ 

and

$$f(x,z) = \alpha \beta \frac{\cos(\beta(z-z_b))}{\sin(\beta H)} \left(\frac{\tan(\beta(z-z_b))}{\tan(\beta H)} - 1\right) \frac{\partial H}{\partial x}$$



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Rad	ceway modelin	g			

Geometry: a 2D rectangular pool along x and z axis (H = 50 cm and L = 20m )



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Race	eway modelin	g			

Agitation:

$$F_{x}(x,z,t) = F\left(\sqrt{(x-x_{wheel})^{2}+(z-z_{wheel})^{2}}\omega\right)^{2}\cos\theta \qquad (14)$$

$$F_z(x, z, t) = F\left(\sqrt{(x - x_{wheel})^2 + (z - z_{wheel})^2}\omega\right)^2 \sin\theta \qquad (15)$$

where F is a constant,  $\theta$  is the angle between the blade and the vertical direction,  $\omega = \dot{\theta}$ .



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Hyd	rodynamics				



Figure: (a): Velocities along vertical and horizontal axis in a cell located near from the wheel rotating at angular speed  $\omega = 0.8rad/s$ . The flow is very turbulent. (b): Velocities along vertical and horizontal axis in a cell located far from the wheel. An asymptotic value of  $0.48m.s^{-1}$  is reached.

$\mathbf{A} =$				
			200	

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Hydr	odynamics				



Figure: Snapshots of the tracer (pollutant) concentration in a raceway set into motion by a paddlwheel of angular velocity  $\omega = 0.85 rad/s$ . It is clear that after several minutes, the raceway is totally homogeneous. Therefore, the paddlewheel has indeed the required effect on the mixing.

	The hydrodynamical model	The biological model	Numerical scheme		Raceway modeling
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Lagr	rangian trajec	tories			



Figure: (a):Trajectories of three particles during the simulations. The large curve represents the water surface at the middle of the pool. The other plot is the height of a given particle through time. The algae undergo sudden changes of depth every time it meets the wheel.(b): Perceived light from the microalgae. Particles are subject to even greater irradiance changes since the light is exponentially decaying.

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Figure: (a): Carbon concentration; (b): Internal quota q; (c): nitrogen concentration; (d): substrate concentration( $NO_3$ ). Those plots illustrate the average concentrations in the raceway for 6 simulations. Three were carried out without agitation, and the other three had the agitation term. In each situation, agitation, leading to homogenization leads to a better productivity. However, for certain initial conditions, the improvement is quite slow (after several days), since the biological variables do not evolve as quickly as hydrodynamics does.

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3[	D investigation				

Simulation of a passive tracer in the raceway.

Passive tracer

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Exp	erimental vali	dation			

# Measurement points



Comparison (25 Hz, aligned blades, paths 2 and 3, H = 30 cm)



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Evn	erimental vali	dation			
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Comparison (25 Hz, aligned blades, paths 1 and 3, H = 20 cm)



Comparison (25 Hz, aligned blades, path 3, H = 30 cm)



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Figure: Y position of the particles

Figure: Depth of the particles

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Anin	nation				

**3D** Trajectories

$\mathbf{A} =$	124		67	

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6					
Cone	clusion				

- First order results in 2D are encouraging
- Job in 3D is in progress (hydrodynamics OK)
- Future work : data assimilation

	The hydrodynamical model	The biological model	Numerical scheme		Raceway modeling
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Tha	nk you for yo	ur attentior			

# Any questions ?