Optimization problems of a microalgal raceway to enhance productivity

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November 4, 2020

Overview

Introduction

- Who?

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- Who? Microalgae

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- Who? Microalgae: photosynthetic organisms

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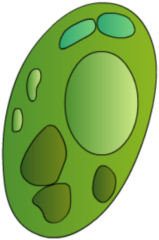

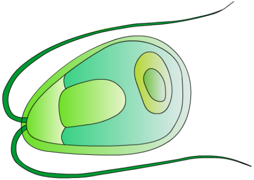

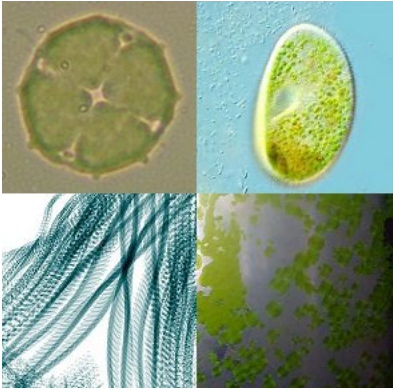

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- Why?

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  - Industrial cultivation - photobioreactors: Chemostats, RAB, Raceways, etc

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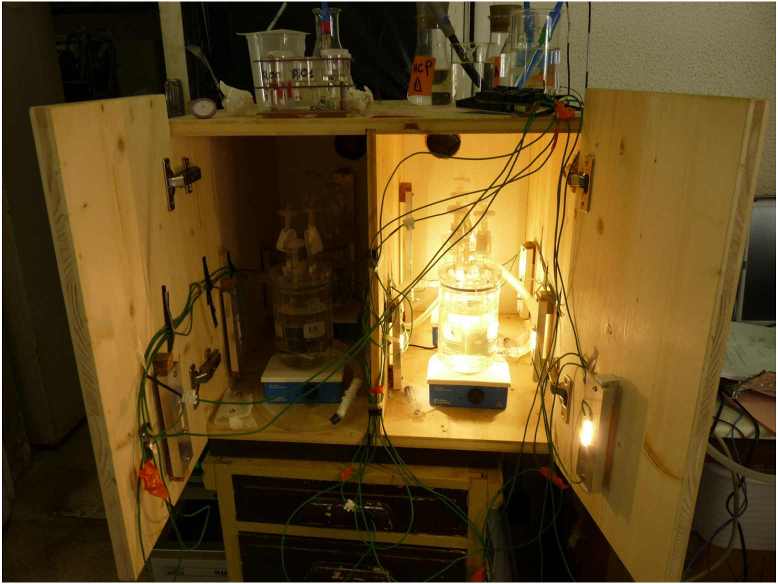

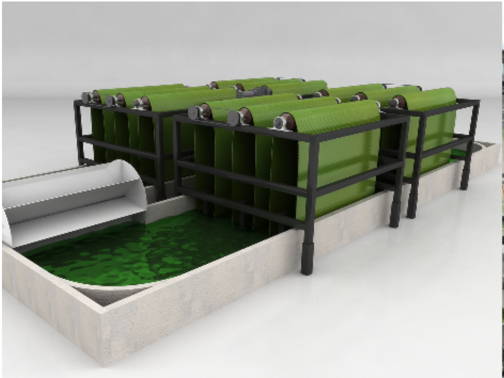


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Shallow Water Equations

- 1D steady state shallow water equation

$$\partial_x(hu) = 0, \tag{1}$$

$$\partial_x(hu^2 + g\frac{h^2}{2}) = -gh\partial_x z_b. \tag{2}$$

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- Free surface $\eta := h + z_b$, averaged discharge $Q = hu$.

Shallow Water Equations

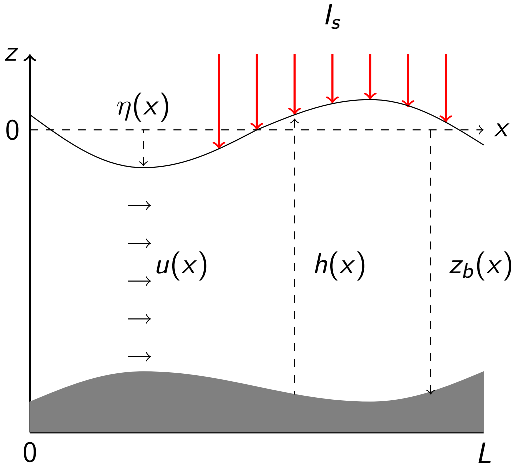

Figure: Representation of the hydrodynamic model.

Shallow Water Equations

1D steady state shallow water equation

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Integrating (1)

$$hu = Q_0,$$

for a fixed positive constant Q_0.

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Shallow Water Equations

$$hu = Q_0 \tag{1}$$

$$hu\partial_x u + h\partial_x gh + h\partial_x gz_b = 0 \tag{2}$$

Assume $h > 0$ and $Q_0 > 0$

Shallow Water Equations

$$hu = Q_0 \tag{1}$$

$$\partial_x\Big(\frac{Q_0^2}{2h^2} + g(h + z_b)\Big) = 0 \tag{2}$$

Consider two fixed constants $h(0), z_b(0) \in \mathbb{R}$

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$$\frac{Q_0^2}{2h^2} + g(h + z_b) = \frac{Q_0^2}{2h^2(0)} + g(h(0) + z_b(0)) =: M_0 \tag{2}$$

Consider two fixed constants $h(0), z_b(0) \in \mathbb{R}$

Shallow Water Equations

$$u = \frac{Q_0}{h}, \tag{1}$$

$$z_b = \frac{M_0}{g} - \frac{Q_0^2}{2gh^2} - h, \tag{2}$$

Shallow Water Equations

- u, z_b as a function of h

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- Froude number:

$$Fr := \frac{u}{\sqrt{gh}}$$

$Fr < 1$: subcritical case (i.e. the flow regime is fluvial)
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  $Fr < 1$: subcritical case (i.e. the flow regime is fluvial)
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- Given a smooth topography z_b, there exists a unique positive smooth solution of h which satisfies the subcritical flow condition [4, Lemma 1]

Lagrangian Trajectories

- Incompressibility of the flow: $\nabla \cdot \underline{\mathbf{u}} = 0$ with $\underline{\mathbf{u}} = (u(x), w(x,z))$

$$\partial_x u + \partial_z w = 0. \tag{3}$$

Lagrangian Trajectories

- Integrating (3) from z_b to z gives:

$$
\begin{aligned}
0 &= \int_{z_b}^{z} \big(\partial_x u(x) + \partial_z w(x,z)\big) \mathrm{d}z \\
&= \partial_x \int_{z_b}^{z} u(x) \mathrm{d}z + \int_{z_b}^{z} \partial_z w(x,z) \mathrm{d}z \\
&= \partial_x \big((z - z_b) u(x)\big) + w(x,z) - w(x,z_b) \\
&= (z - z_b)\partial_x u(x) - u(x)\partial_x z_b + w(x,z),
\end{aligned}
$$

where $w(x, z_b) = u(x)\partial_x z_b$ (the kinematic condition at the bottom).

Lagrangian Trajectories

- The vertical velocity:

$$w(x, z) = (\frac{M_0}{g} - \frac{3u^2(x)}{2g} - z)u'(x).$$

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- The Lagrangian trajectory is characterized by the system

$$\begin{pmatrix} \dot{x}(t) \\ \dot{z}(t) \end{pmatrix} = \begin{pmatrix} u(x(t)) \\ w(x(t), z(t)) \end{pmatrix}.$$

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- Recall $\eta = h + z_b = \frac{M_0}{g} - \frac{u^2}{2g}$

$$\begin{aligned} z' + z\frac{u'}{u} &= (\frac{M_0}{g} - \frac{3u^2}{2g})\frac{u'}{u} \\ &= (\eta + \frac{u^2}{g})\frac{u'}{u}. \end{aligned}$$

Lagrangian Trajectories

- The vertical velocity:

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- Note that $\eta' = -\frac{uu'}{g}$ and multiplying both sides by u

$$\begin{aligned} z'u + zu' &= \eta u' + \frac{u^2}{g}u' \\ &= \eta u' + \eta' u \end{aligned}$$

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- We find

$$\big(u(z-\eta)\big)' = 0$$

Since $h(0), z_b(0)$ are given constants, so does $u(0)$. For a given initial position $z(0)$, we have

$$u(x)(z(x)-\eta(x)) = u(0)(z(0)-\eta(0)).$$

Lagrangian Trajectories

- The vertical velocity:

$$w(x,z) = (\frac{M_0}{g} - \frac{3u^2(x)}{2g} - z)u'(x).$$

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$$z(x) = \eta(x) + \frac{u(0)}{u(x)}(z(0) - \eta(0)), \tag{3}$$

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$$z(x) = \eta(x) + \frac{u(0)}{u(x)}(z(0) - \eta(0)), \quad (3)$$

- If $z(0)$ belongs to $[z_b(0), \eta(0)]$, then $z(x)$ belongs to $[z_b(x), \eta(x)]$. In particular, choosing $z(0) = z_b(0)$ in (3) and using (1) gives $z(x) = z_b(x)$. In the same way, we find that $z(x) = \eta(x)$ when $z(0) = \eta(0)$.

Beer-Lambert Law

- The Beer-Lambert law describes how light is attenuated with depth:

$$I(x,z) = I_s \exp\Big(-\varepsilon(\eta(x) - z)\Big).$$

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- $$h \to u, z_b \to z \to I$$

Han model

- A: open and ready to harvest a photon,
  B: closed while processing the absorbed photon energy,
  C: inhibited if several photons have been absorbed simultaneously.

Han model

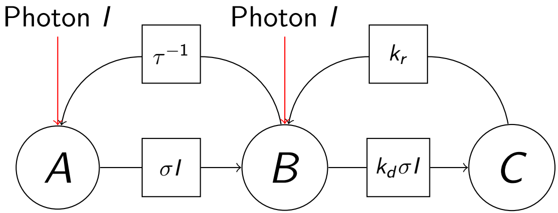

Figure: Scheme of the Han model, representing the probability of state transition, as a function of the photon flux density.

Han model

- A: open and ready to harvest a photon,
  B: closed while processing the absorbed photon energy,
  C: inhibited if several photons have been absorbed simultaneously.
- $$\begin{cases} \dot{A} = -\sigma I A + \frac{B}{\tau}, \\ \dot{B} = \sigma I A - \frac{B}{\tau} + k_r C - k_d \sigma I B, \\ \dot{C} = -k_r C + k_d \sigma I B. \end{cases}$$

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- A, B, C are the relative frequencies of the three possible states

$$A + B + C = 1,$$

Han model

- Using a fast-slow approximation and the singular perturbation theory(see [3]), this system can be reduced to one single evolution equation:

$$\dot{C} = -\alpha(I)C + \beta(I),$$

where

$$\alpha(I) = \beta(I) + k_r, \text{with } \beta(I) = k_d \tau \frac{(\sigma I)^2}{\tau \sigma I + 1}.$$

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- The net specific growth rate:

$$\mu(C, I) := -\gamma(I)C + \zeta(I),$$

where

$$\zeta(I) = \gamma(I) - R, \text{ with } \gamma(I) = \frac{k\sigma I}{\tau\sigma I + 1}.$$

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$$\bar{\mu} := \frac{1}{L} \int_0^L \frac{1}{h(x)} \int_{z_b(x)}^{\eta(x)} \mu\big(C(x,z), I(x,z)\big) \mathrm{d}z\mathrm{d}x.$$

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- In order to compute numerically, consider a uniform vertical discretization of the initial position $z(0)$ for $N_z + 1$ cells:

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- The semi-discrete average net specific growth rate:

$$\bar{\mu}_\Delta = \frac{1}{LN_z} \sum_{i=1}^{N_z} \int_0^L \mu(C_i(x), I_i(x)) \mathrm{d}x. \tag{4}$$

Mixing device

- Paddle wheel:
  - set this hydrodynamic-biologic coupling system in motion,
  - modifies the elevation of the algae passing through it, and giving successively access to light to all the population.

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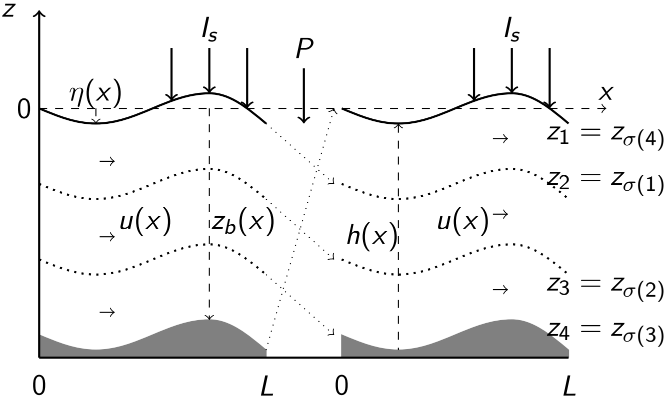

Figure: Representation of the hydrodynamic model with an example of mixing device (P). Here, P corresponds to the cyclic permutation $\sigma = (1\ 2\ 3\ 4)$.

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Theorem

The average growth rate of K laps equals to one lap (see [1]).

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- Periodic of C.
- Omit x in notations.

ε constant and no permutation

- Objective function:

$$\bar{\mu}_{\Delta}(a) = \frac{1}{LN_z} \sum_{i=1}^{N_z} \int_0^L \frac{-\gamma(I_i(a))C_i + \zeta(I_i(a))}{u(a)} \mathrm{d}x,$$

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- Constraints:

$$C_i' + \frac{\alpha(I_i(a))}{u(a)} C_i = \frac{\beta(I_i(a))}{u(a)}. \tag{6}$$

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- The optimization problem reads:
  Find a^* solving the maximization problem:

$$\max_{a \in \mathbb{R}^N} \bar{\mu}_\Delta(a).$$

ε constant and no permutation

- Lagrangian:

$$\mathcal{L}(C,p,a) = \frac{1}{LN_z}\sum_{i=1}^{N_z}\int_0^L \frac{-\gamma(I_i(a))C_i + \zeta(I_i(a))}{u(a)}\mathrm{d}x - \sum_{i=1}^{N_z}\int_0^L p_i\left(C_i' + \frac{\alpha(I_i(a))C_i - \beta(I_i(a))}{u(a)}\right)\mathrm{d}x$$

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- p_i the Lagrange multipliers associated with the constraint (6).

$$\begin{cases} \partial_{C_i}\mathcal{L} = p_i' - p_i\frac{\alpha(I_i(a))}{u(a)} - \frac{1}{LN_z}\frac{\gamma(I_i(a))}{u(a)} \\ \partial_{C_i(L)}\mathcal{L} = p_i(L). \end{cases}$$

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- If C is periodic (i.e. $C(0) = C(L)$), then $\partial_{C_i(L)}\mathcal{L} = p_i(L) - p_i(0)$.

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- where

$$\begin{aligned}
\partial_a \mathcal{L} = & \frac{1}{LN_z} \sum_{i=1}^{N_z} \int_0^L \frac{-\gamma'(I_i(a))C_i + \zeta'(I_i(a))}{u(a)} \partial_a I_i(a) \mathrm{d}x \\
& - \frac{1}{LN_z} \sum_{i=1}^{N_z} \int_0^L \frac{-\gamma(I_i(a))C_i + \zeta(I_i(a))}{u^2(a)} \partial_a u(a) \mathrm{d}x \\
& + \sum_{i=1}^{N_z} \int_0^L p_i \frac{-\alpha'(I_i(a))C_i + \beta'(I_i(a))}{u(a)} \partial_a I_i(a) \mathrm{d}x \\
& - \sum_{i=1}^{N_z} \int_0^L p_i \frac{-\alpha(I_i(a))C_i + \beta(I_i(a))}{u^2(a)} \partial_a u(a) \mathrm{d}x.
\end{aligned}$$

ε constant and no permutation

- The gradient $\nabla\bar{\mu}_\Delta(a)$ is obtained by

$$\nabla\bar{\mu}_\Delta(a) = \partial_a \mathcal{L},$$

Theorem

Under the parameterization (5), if C is periodic, then $\nabla\bar{\mu}_\Delta(0) = 0$.

ε constant with mixing device

- Objective function:

$$\bar{\mu}_{\Delta}^{P}(a) = \frac{1}{LN_z} \sum_{i=1}^{N_z} \int_0^L \frac{-\gamma(I_i(a))C_i^P + \zeta(I_i(a))}{u(a)} \mathrm{d}x,$$

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- Our optimization problem reads:
Find a permutation matrix $P_{\max}$ and a parameter vector a^* solving the maximization problem:

$$\max_{P\in\mathcal{P}}\max_{a\in\mathbb{R}^M}\bar{\mu}_{\Delta}^{P}(a).$$

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- Lagrangian:

$$\mathcal{L}^P(C,p,a) = \frac{1}{LN_z}\sum_{i=1}^{N_z}\int_0^L \frac{-\gamma(I_i(a))C_i^P + \zeta(I_i(a))}{u(a)}\mathrm{d}x$$
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- p_i^P is the Lagrange multiplier associated with the constraint (7).

$$\begin{cases} p_i^{P\prime} - p_i^P\frac{\alpha(I_i(a))}{u(a)} - \frac{1}{LN_z}\frac{\gamma(I_i(a))}{u(a)} & = 0 \\ p_i^P(L) - p_i^P(0)P & = 0. \end{cases}$$

ε constant with mixing device

$$\nabla \bar{\mu}_{\Delta}^{P}(a) = \partial_a \mathcal{L}^P,$$

where

$$\begin{aligned}
\partial_a \mathcal{L}^P = & \frac{1}{LN_z} \sum_{i=1}^{N_z} \int_0^L \frac{-\gamma'(I_i(a))C_i^P + \zeta'(I_i(a))}{u(a)} \partial_a I_i(a) \mathrm{d}x \\
& - \frac{1}{LN_z} \sum_{i=1}^{N_z} \int_0^L \frac{-\gamma(I_i(a))C_n^P + \zeta(I_i(a))}{u^2(a)} \partial_a u(a) \mathrm{d}x \\
& + \sum_{i=1}^{N_z} \int_0^L p_i^P \frac{-\alpha'(I_i(a))C_i^P + \beta'(I_i(a))}{u(a)} \partial_a I_i(a) \mathrm{d}x \\
& - \sum_{i=1}^{N_z} \int_0^L p_i^P \frac{-\alpha(I_i(a))C_i^P + \beta(I_i(a))}{u^2(a)} \partial_a u(a) \mathrm{d}x.
\end{aligned}$$

Overview

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- Numerical Algorithm: Gradient-based optimization algorithm, *fminunc*, *fmincon*, etc

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- Assume that only q percent of I_s is available at the bottom $q \in [0, 1]$

$$\varepsilon = (1/h(0, a))\,\text{ln}(1/q).$$

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- All the numerical parameters values for Han's model are taken from [2] and given in table 1.

Table: Parameter values for Han Model

k_r	$6.8\ 10^{-3}$	s^{-1}
k_d	$2.99\ 10^{-4}$	-
τ	0.25	s
σ	0.047	$\text{m}^2 \cdot (\mu\ \text{mol})^{-1}$
k	$8.7\ 10^{-6}$	-
R	$1.389\ 10^{-7}$	s^{-1}

Convergence of N_z

For 100 random a chosen, the average value of the functional $\bar{\mu}_\Delta$

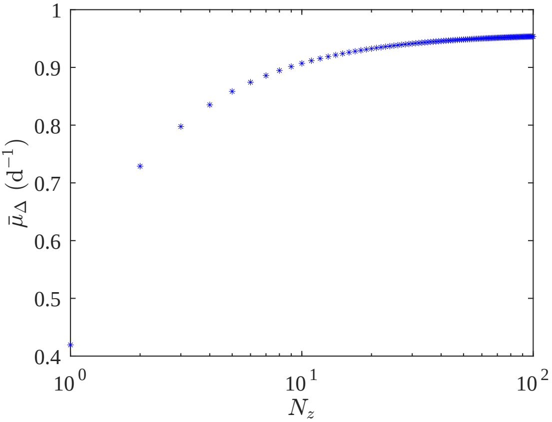

Figure: The value of the functional $\bar{\mu}_\Delta$ for $N_z = [1, 100]$.

C no periodic

The initial condition $C_0 = 0.1$

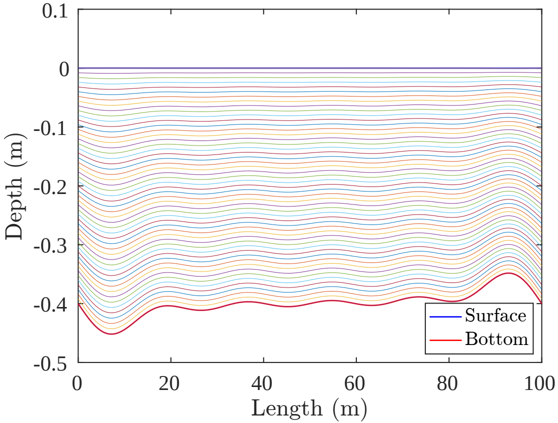

Figure: The optimal topography for $C_0 = 0.1$. The red thick line represents the topography (z_b), the blue thick line represents the free surface (η), and all the other curves between represent the different trajectories.

Optimal topography for a given permutation

The permutation: $\pi = (1\ N_z)(2\ N_z - 1)(3\ N_z - 2)\cdots$,

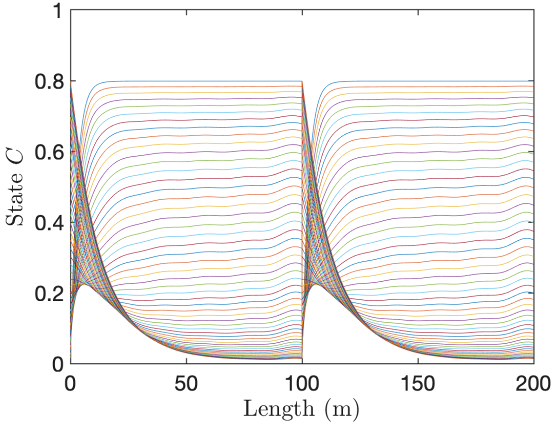

Figure: The evolution of the photo-inhibition state C for two laps.

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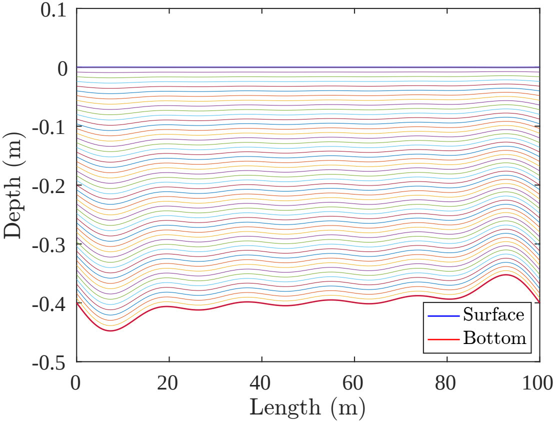

The increase in the optimal value of the objective function $\bar{\mu}_\Delta$ compared to a flat topography is around 0.228%, and compare to a flat topography and non permutation case is around 0.277%.

Optimal matrix and optimal topography

Set $N_z = 7$, the optimal matrix:

$$P_{\text{max}} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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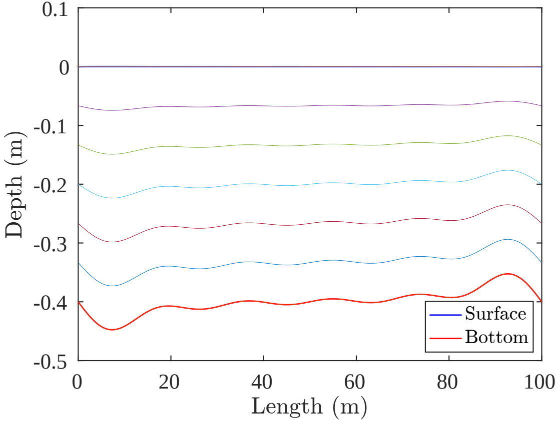

Compare to a flat topography with this $P_{\max}$, we have a gain of 0.224%, and a gain of 1.511% compare to the case a flat topography without permutation (i.e. $\mathcal{I}_{N_z}$).

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Permutation for flat topography

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- $$\bar{\mu}_\Delta = \frac{1}{N_z}\frac{1}{T}\Big(\langle \Gamma, C(0)\rangle + \langle \imath, Z\rangle\Big),$$
  - $\imath$ is a vector of size N_z whose coefficients equal 1
  - $\Gamma_i = \frac{\gamma(I_i)}{\alpha(I_i)}(e^{-\alpha(I_i)T} - 1)$
  - $Z_i = \frac{\gamma(I_i)}{\alpha(I_i)}\frac{\beta(I_i)}{\alpha(I_i)}(1 - e^{-\alpha(I_i)T}) - \frac{\gamma(I_i)\beta(I_i)}{\alpha(I_i)}T + \zeta(I_i)T$

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- The periodic condition of C

$$C(0) = (\mathcal{I}_{N_z} - PD)^{-1}PV.$$

  - D is a diagonal matrix $D_{ii} = e^{-\alpha(I_i)T}$
  - $V_i = \frac{\beta(I_i)}{\alpha(I_i)}(1 - e^{-\alpha(I_i)T})$

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- Since N, T and Z are independent of P, the objective function defined by

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- Expansion of $J(P)$
$$\begin{aligned}\langle \Gamma, (\mathcal{I}_{N_z} - PD)^{-1} PV \rangle &= \sum_{m=0}^{+\infty} \langle \Gamma, (PD)^m PV \rangle \\ &= \langle \Gamma, PV \rangle + \sum_{m=1}^{+\infty} \langle \Gamma, (PD)^m PV \rangle.\end{aligned}$$

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- The optimal solution $P_{\max}^{\text{approx}}$ of $J^{\text{approx}}(P)$ can be determined explicitly as the matrix corresponding to the permutation which associates the largest element of Γ with the largest element of V, the second largest element with the second largest, and so on.

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- For all three cases, $P_{\max}^{\text{approx}} = P_{\max}$

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- For all three cases, $P_{\max}^{\mathrm{approx}}$ is an anti-diagonal matrix.

Approximation

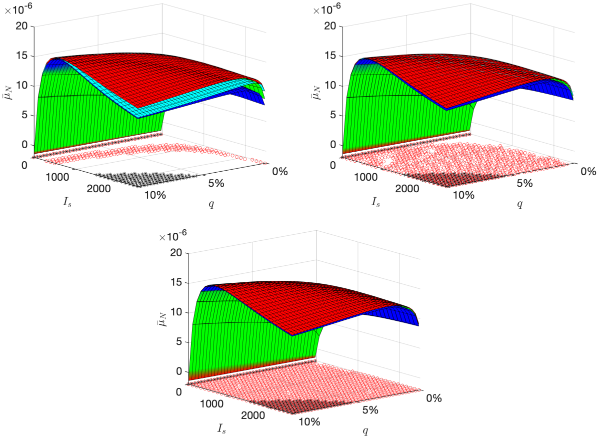

Figure: Average net specific growth rate $\bar{\mu}_N$ for $I_s \in [0, 2500]$ and $q \in [0.1\%, 10\%]$. In each figure, the red surface is obtained with P_{max}, the dark blue surface is obtained with P_{min}, the green surface is obtained with $\mathcal{I}_{N_z}$ and the light blue surface is obtained with $P_{\text{max}}^{\text{approx}}$. The black stars represent the cases

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