Controlling eutrophication in a moving domain

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Concept of eutrophication

Eutrophication

- From Greek: *eú* (= well) + *trophé* (= nourished)
- Oxford English Dictionary: *The process of nutrient enrichment (usually by nitrogen and/or phosphorus) in aquatic ecosystems such that the productivity of the system ceases to be limited by the availability of nutrients.*
- Environmental sciences: *The enrichment of water by nutrients causing an accelerated growth of algae and higher forms of plant life to produce an undesirable disturbance to the balance of organisms present in the water and to the quality of the water concerned. It refers to the undesirable effects resulting from anthropogenic enrichment by nutrients: It occurs naturally over geological time, but may be accelerated by human activities (sewage, land drainage...)*

Concept of eutrophication

Effects

- Decrease in light availability
- Change in algal dominance (phytoplankton blooms)
- Reduction of oxygen concentration
- Increase in inorganic matter production
- Reduction of biodiversity...

Sources

- Fertilizers
- Deposition from atmosphere
- Phosphate detergents
- Erosion of soils
- Discharges from sewage treatment plants...

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Examples

Real-world problem

Aims

- Controlling eutrophication processes along a time interval $[0, T]$ inside a sensitive zone from a moving water body $\Omega(t)$, where a wastewater outfall discharges polluted water with a high concentration of nutrients, coming, for instance, from a sewage treatment plant.
- In particular, we try to keep the level of eutrophication inside this zone $G(t) \subset \Omega(t)$ under safety thresholds, and with an economic cost (due to wastewater purification processes) as low as possible.
- From a mathematical viewpoint, this problem can be formulated as an optimal control problem with state and control constraints.

Mathematical model

State variables

- u^1 (Generic nutrient, for instance, N or P)
- u^2 (Phytoplankton)
- u^3 (Zooplankton)
- u^4 (Organic detritus)
- u^5 (Dissolved oxygen)

State $\vec{u} = (u^1, u^2, u^3, u^4, u^5)$

$u^i(x,t), \quad i = 1, \ldots, 5, \quad$ with:

- $t \in I = [0, T]$ (time interval under study)
- $x \in \Omega(t) \subset \mathbb{R}^3$ (moving water domain)

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State system: Advection-diffusion-reaction PDEs with Michaelis-Menten kinetics

$$\frac{\partial u^1}{\partial t} + \vec{v}\cdot\nabla u^1 - \nabla\cdot(\mu_1\nabla u^1) + C_{nc}L\frac{u^1}{K_N+u^1}u^2 - C_{nc}K_r u^2 - C_{nc}K_{rd}\Theta^{\theta-20}u^4 = g^1$$
$$\frac{\partial u^2}{\partial t} + \vec{v}\cdot\nabla u^2 - \nabla\cdot(\mu_2\nabla u^2) - L\frac{u^1}{K_N+u^1}u^2 + K_r u^2 + K_{mf}u^2 + K_z\frac{u^2}{K_F+u^2}u^3 = g^2$$
$$\frac{\partial u^3}{\partial t} + \vec{v}\cdot\nabla u^3 - \nabla\cdot(\mu_3\nabla u^3) - C_{fz}K_z\frac{u^2}{K_F+u^2}u^3 + K_{mz}u^3 = g^3$$
$$\frac{\partial u^4}{\partial t} + \vec{v}\cdot\nabla u^4 - \nabla\cdot(\mu_4\nabla u^4) - K_{mf}u^2 - K_{mz}u^3 + K_{rd}\Theta^{\theta-20}u^4 - W_{fd}\frac{\partial u^4}{\partial z} = g^4$$
$$\frac{\partial u^5}{\partial t} + \vec{v}\cdot\nabla u^5 - \nabla\cdot(\mu_5\nabla u^5) - C_{oc}L\frac{u^1}{K_N+u^1}u^2 + C_{oc}K_r u^2 + C_{oc}K_{rd}\Theta^{\theta-20}u^4 = g^5$$

+ Boundary / Initial Conditions

where:
- $L(x,t)$: Luminosity function
- $\theta(x,t)$: Water temperature
- W_{fd} : Falling velocity of organic detritus
- C_α, K_α : Constants (stoichiometric, regeneration, death, predation...)

State system: Advection-diffusion-reaction PDEs with Michaelis-Menten kinetics

- $\vec{v}(x,t) = (v^1, v^2, v^3)$: Water velocity, solution of classical Navier-Stokes equations:

$$\left\{ \begin{array}{l} \frac{\partial \vec{v}}{\partial t} + \nabla \vec{v}\, \vec{v} - \nabla \cdot (\nu \nabla \vec{v}) + \nabla p = \vec{f} \\ \nabla \cdot \vec{v} = 0 \\ + \text{ Boundary / Initial Conditions} \end{array} \right.$$

with:
- $p(x,t)$: pressure
- $\vec{f}(x,t)$: body forces
- ν : dynamic viscosity

[1] L.J. Alvarez-Vázquez, F.J. Fernández, and R. Muñoz-Sola, Mathematical analysis of a three-dimensional eutrophication model. *J. Math. Anal. Appl.*, 349 (2009), 135–155.

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Control variable

The control $g(t)$

The source term for nutrients g^1 in state system is modelled with a Dirac measure $g^1(x,t) = g(t)\delta(x-b)$, where $g(t)$ represents the pollutant concentration (nitrogen and/or phosphorus in our case) discharged through the outfall, and b is the outfall location.

The other source terms $g^2, \ldots, g^5$ will be considered null, since no other species (but nutrients) are discharged from the wastewater outfall.

Constraints

Control constraints

Technological constraints on g (related, for instance, to purification capacities of the sewage treatment plant).
In this way, we assume that the control g belongs to a convex, closed, bounded subset $\mathcal{U}_{ad}$ of $L^2(0,T)$, that is, $g \in \mathcal{U}_{ad}$.

State constraints

To guarantee water quality inside the sensitive zone $G(t)$ all along the time interval $[0,T]$, we need that the averaged concentrations of the five species remain between some desired thresholds:

$$\eta^i \leq \frac{1}{\|G(t)\|} \int_{G(t)} u^i(t,x)\, dx \leq \tau^i, \quad \forall t \in I, \quad \forall i = 1,\ldots,5$$

where η^i and τ^i denote the lower and upper bounds, and $\|G(t)\|$ represents the volume occupied by domain $G(t)$ at time t.

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Optimal control problem

Cost function

We are interested in reducing the global economic cost of the purification process, i.e., minimizing the cost function:

$$J(g) = \int_0^T m(g(t))dt$$

where $m(g)$ denotes the depuration cost in the treatment plant.

Summarizing, our control/state constrained optimal control problem $(\mathcal{P})$ consists of minimizing the cost function J such that the control g verifies the control constraint, and the state $\vec{u}$ satisfies the state constraints.

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Existence results for state system

Theorem

Under suitable hypotheses on the data for the state system, then there exists a unique weak solution

$$\vec{u} \in [L^2(I; H^1(\Omega(t))) \cap L^\infty(I; L^2(\Omega(t)))]^5$$

of the state system satisfying:

- $\|\vec{u}\|_{[L^2(I;H^1(\Omega(t)))\cap L^\infty(I;L^2(\Omega(t)))]^5} \leq C(T,M)$
- $0 \leq u^i(t,x) \leq C(T,M)$, a.e. $x \in \Omega(t),\ t \in I,\ \forall i = 1,\ldots,4$
- $|u^5(t,x)| \leq C(T,M)$, a.e. $x \in \Omega(t),\ t \in I$

[2] L.J. Alvarez-Vázquez, F.J. Fernández, I. López and A. Martínez, An Arbitrary Lagrangian Eulerian formulation for a 3D eutrophication model in a moving domain. *J. Math. Anal. Appl.*, 366 (2010), 319–334.

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Existence results for state system

Theorem

Under stronger hypotheses on the data for the state system, then there exists a unique strong solution

$$\vec{u} \in [L^q(I; W^{2,q}(\Omega(t))) \cap W^{1,q}(I; L^q(\Omega(t))) \cap \mathcal{C}(\overline{\cup_{t\in I}\{t\} \times \Omega(t)})]^5$$

that verifies the estimate:

$$\|\vec{u}\|_{[L^q(I;W^{2,q}(\Omega(t)))\cap W^{1,q}(I;L^q(\Omega(t)))\cap \mathcal{C}(\overline{\cup_{t\in I}\{t\}\times\Omega(t)})]^5} \leq C(T, M)$$

for $q > 5/2$.

[3] L.J. Alvarez-Vázquez, F.J. Fernández and A. Martínez, Optimal control of eutrophication processes in a moving domain. *J. Franklin Institute*, 351 (2014), 4142–4182.

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Existence of optimal solutions

Theorem

Under the hypotheses of previous theorems, if we also assume that

- *the admissible set*

$$\mathcal{U}_{ad} \subset \{g \in L^2(I) \; : \; 0 \leq g(t) \leq M, \; a.e. \; t \in I\}$$

  is convex, closed, bounded, and nonempty

- *the function*

$$m : [0, M] \subset \mathbb{R} \longrightarrow \mathbb{R}$$

  is continuous

then, the optimal control problem $(\mathcal{P})$ *admits, at least, a solution.*

Characterization of the optimal solutions

Theorem

Under the hypotheses of previous theorems, if we also assume that the function $m : L^2(I) \to \mathbb{R}$ *is differentiable, let* $\tilde{\rho} \in \mathcal{U}_{ad}$ *be a solution of the control problem* $(\mathcal{P})$*, with associated state* $\vec{u}_{\tilde{\rho}} \in [L^q(I;W^{2,q}(\Omega(t))) \cap W^{1,q}(I;L^q(\Omega(t))) \cap \mathcal{C}(\overline{\cup_{t\in I}\{t\} \times \Omega(t)})]^5$*. Then, there exist element* $\gamma \geq 0$ *and Borel measures* $\lambda^i \in M(I)$*,* $i = 1, \ldots, 5$*, such that:*

$$\gamma + \sum_{i=1}^{5} \|\lambda^i\|_{M(I)} > 0,$$

$$\sum_{i=1}^{5} \langle \lambda_i, g^i - \frac{1}{\|G(t)\|} \int_{G(t)} u^i_{\tilde{\rho}}\, dx \rangle_{M(I),\mathcal{C}(I)} \leq 0, \quad \forall \vec{g} \in E,$$

with $E = \{\vec{g} \in [\mathcal{C}(I)]^5 \ : \ \eta^i \leq g^i(t) \leq \tau^i, \ \forall t \in I, \ \forall i = 1, \ldots, 5\}$ *...*

Characterization of the optimal solutions

Theorem (continuation)

... satisfying the following optimality condition:

$$\gamma \int_0^T m'(\widetilde{\rho})(\rho - \widetilde{\rho})dt + \int_0^T (\rho - \widetilde{\rho})q^1(b)\, dxdt \leq 0, \quad \forall \rho \in \mathcal{U}_{ad}$$

with $\vec{q} \in [L^2(I; H^1(\Omega(t))) \cap L^\infty(I; L^2(\Omega(t)))]^5$ the unique solution of a suitably defined adjoint system.

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Numerical resolution

In order to obtain the numerical solution of the control problem, we will proceed to a full discretization of the problem $(\mathcal{P})$:

- The space semi-discretization of the state system will be done by the well-known method of finite elements
- The time semi-discretization will use the method of characteristics, using a partition $\{t_0, t_1, \ldots, t_N\}$ of the time interval $I = [0, T]$ for a time step $\Delta t = T/N$
- Moving domain will be solved with Arbitrary Lagrangian Eulerian (ALE) techniques referred to a fixed domain $\widehat{\Omega}$
- Delta distributions $\delta(x - b)$ are regularized by smooth $R_{b,\epsilon}$
- The nonlinearities in the problem will be treated with fixed-point techniques
- The optimization of the discretized problem will be addressed by an interior-point algorithm

Numerical resolution

So, we consider the following discretization for the different elements conforming the optimal control problem:

- Discretization of the space of admissible controls:

$$\mathcal{U}_{ad}^{\Delta t} = \{\rho \in \mathbb{R}^N \ : \ N_{min} \leq \rho_n \leq N_{max}, \ \forall n = 1, \ldots, N\}$$

for $\rho_n \simeq \rho(t_n)$, and where N_{min} and N_{max} represent, respectively, allowed minimal and maximal discharges.

- Discretization of the cost functional:

$$F^{\Delta t}(\rho) = \sum_{n=1}^{N} m(\rho_n)$$

Numerical resolution

- Discretization of the state system:

$$\left\{\begin{array}{l} u_0^i \simeq u^i(t_0) \in H^1(\Omega(0)),\ \ i=1,\ldots,5, \text{ given.} \\ \\ \text{For } n=0,\ldots,N-1,\ u_{n+1}^i \simeq u^i(t_{n+1}) \in H^1(\Omega(t_n)), \\ i=1,\ldots,5, \text{ is the solution of:} \\ \\ \alpha \displaystyle\int_{\Omega(t_n)} u_{n+1}^i z\,dx + \int_{\Omega(t_n)} \mu_i \nabla_x u_{n+1}^i \cdot \nabla_x z\,dxdx \\ \quad = \displaystyle\int_{\Omega(t_n)} A_{n+1}^i(\mathbf{u}_{n+1}) z dx + \int_{\Omega(t_n)} \delta_{i,1} R_{\mathbf{b},\epsilon}(\rho_{n+1}) z\,dx \\ \quad +\alpha \displaystyle\int_{\Omega(t_n)} u_n^i(X_{\mathbf{r}_n}(t_n)) z\,dx, \\ \quad \forall z \in H^1(\Omega(t_n)), \quad i=1,\ldots,5. \qquad\qquad (\alpha = \frac{1}{\Delta t}) \end{array}\right.$$

Numerical resolution

- Discretization of the state constraints: Given

$$\mathbf{G} : \rho \in \mathcal{U}_{ad}^{\Delta t} \longrightarrow \mathbf{G}(\rho) = [\mathbf{G}_1(\rho), \mathbf{G}_2(\rho), \ldots, \mathbf{G}_N(\rho)]^T \in \mathbb{R}^{N\times 5}$$

where, for any $n = 1, \ldots, N$,

$$\mathbf{G}_n(\rho) = \frac{1}{\|G(t_n)\|}\Big(\int_{G(t_n)} u_n^1\, dx,\ \ldots,\ \int_{G(t_n)} u_n^5\, dx\Big)^T$$

then the state constraints

$$\eta^i \leq \frac{1}{\|G(t_n)\|}\int_{G(t_n)} u_n^i\, dx \leq \tau^i,\ \forall n = 1, \ldots, N,\ \forall i = 1, \ldots, 5$$

can be rewritten in an equivalent way as $\mathbf{G}(\rho) \in E^{\Delta t}$, with

$$E^{\Delta t} = \{\mathbf{g} \in \mathbb{R}^{N\times 5}\ :\ \eta^i \leq g_n^i \leq \tau^i,\ \forall n = 1, \ldots, N,\ \forall i = 1, \ldots, 5\}$$

Numerical resolution

So, the discretized optimal control problem reads now as the nonlinear constrained optimization problem:

$$(\mathcal{P}^{\Delta t}) \qquad \begin{array}{l} \text{minimize } F^{\Delta t}(\rho) \\ \text{such that } \rho \in \mathcal{U}_{ad}^{\Delta t} \\ \text{and } \mathbf{G}(\rho) \in E^{\Delta t} \end{array}$$

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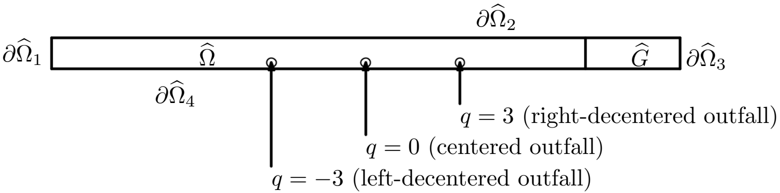
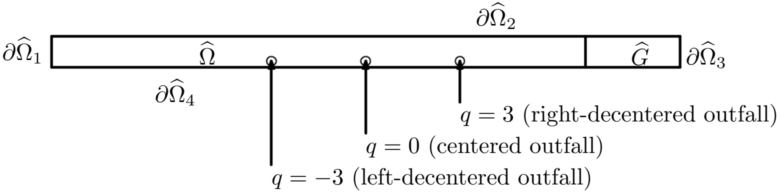
Numerical results



Reference domain : $\widehat{\Omega} = [-10h, 10h] \times [0, h]$ $(h = 10 \text{ m})$
Control domain : $\widehat{G} = [7h, 10h] \times [0, h]$
Time : $T = 48$ hours $(\simeq 4$ tidal cycles)
3 possible outfall locations : $b = (qh, 2)$, with $q \in \{-3, 0, 3\}$

Numerical results

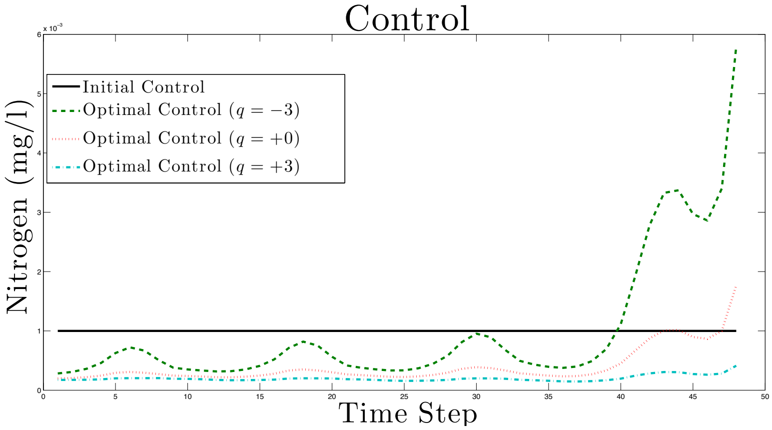


$\mathcal{P}_2 - \mathcal{P}_1$ FEM for Navier-Stokes, $\mathcal{P}_1$ for eutrophication system (triangular mesh of 800 elements, time step of 20 s) Freefem++

Time semi-discretization with $\Delta T = 1$ h ($N = 48$ steps)

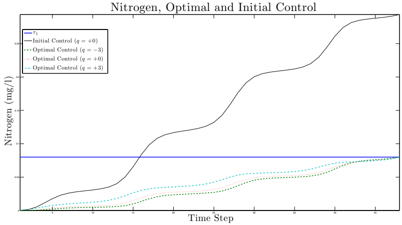
Minimization by interior-point optimization algorithm IPOPT

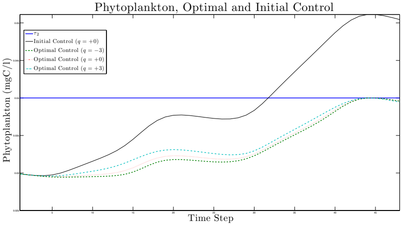
Numerical results



Uncontrolled nitrogen discharge, and optimal nitrogen discharges for the three scenarios (wastewater locations) under study

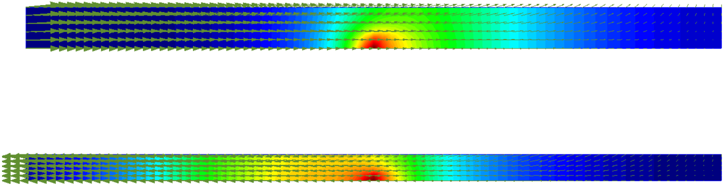
Numerical results





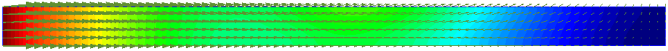
Evolution along the whole time interval of the initial and optimal concentrations with respect to the corresponding upper bounds for the cases of nitrogen and phytoplankton (active constraints)

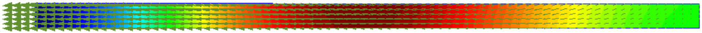
Numerical results



Concentrations of nitrogen for time steps $n = 5$ (up) and $n = 21$ (down), corresponding to high and low tides for the case $q = 0$. Water velocities represented by proportional arrows at mesh nodes

Numerical results





Concentrations of phytoplankton for time steps $n = 5$ (up) and $n = 21$ (down), corresponding to high and low tides

Conclusions

- We have shown the usefulness of a combination of optimal control theory and mathematical simulation in the resolution of environmental control problems
- We have developed a theoretical analysis of the problem (existence of optimal solutions, characterization of solutions by a first order optimality system)
- We have proposed a complete numerical algorithm for its numerical solution (resolution of the hydrodynamical problem, computation of the concentrations for the different species, numerical optimization of the fully discretized problem)
- We have solved a simplified realistic problem under different scenarios