

A Multi-Layers Method to Improve Optimization Algorithms. Application to the Design of Dispersive Bioreactors for Water Treatment.

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Outlines

- Outlines

- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives

- **Bioreactor Design Problem**
 - Industrial aspects
 - Mathematical model
 - Optimization problem
- **Optimization Method**
 - General method
 - Application to genetic algorithm
- **Numerical Results**
 - Original design
 - Optimized design
- **Conclusions and Perspectives**



Some Associated Articles

- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives

- Bello Rivas, J.M., Harmand, J., Ivorra, B., Ramos, A.M., Rapaport, A. *Bio reactor shape optimization Modeling, simulation, and shape optimization of a simple bioreactor for water treatment, Les STIC pour l'environnement 2011*, 125–130, Presses des MINES, 2011.
- Ivorra, B., Ramos, A.M., and Mohammadi., B., *Optimization strategies in credit portfolio management, Journal of Global Optimization*, 43(2), 415–427, 2009.
- Ivorra, B., Ramos, A.M. and Mohammadi., B. *Semideterministic global optimization method: Application to a control problem of the burgers equation, Journal of Optim. Theory and Applications*, 135(3), 549–561, 2007.



- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

- General Definition
- Considered Bioreactor
- Geometry Simplification
- Mathematical Model
- Numerical Scheme
- Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives

PART I: Bioreactor Design Problem



General Definition

- **Bioreactors** include various technologies (hydrodynamic, mechanic, etc.) to perform **chemical processes** for either **producing or degrading** biochemical substances.



- Basically, they involve **biomasses** (bacterias, enzymes, etc.) and **substrates** (glucose, sulfite, etc.).
- They are used for a **wide range** of applications (waste water treatment, drug conception, fermentation, etc.).

- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

● General Definition

- Considered Bioreactor
- Geometry Simplification
- Mathematical Model
- Numerical Scheme
- Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives



Considered Bioreactor

We focus here on **dispersive bioreactors** used for **water treatment**.

- Outlines
- Some Associated Articles

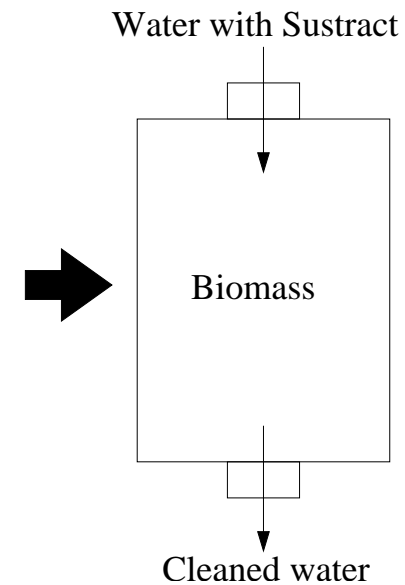
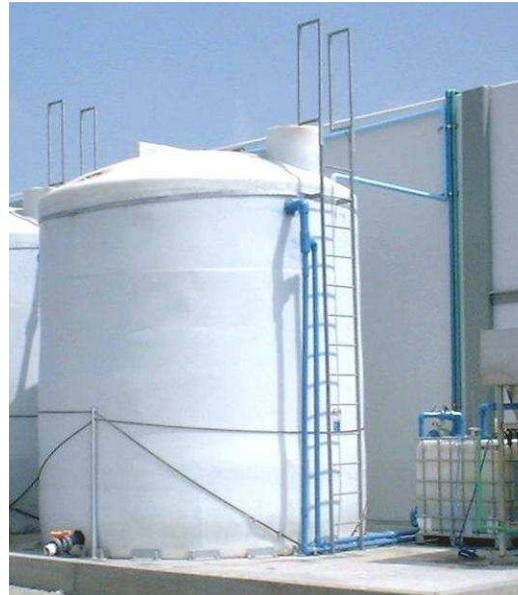
PART I: Bioreactor Design
Problem

- General Definition
- **Considered Bioreactor**
- Geometry Simplification
- Mathematical Model
- Numerical Scheme
- Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives





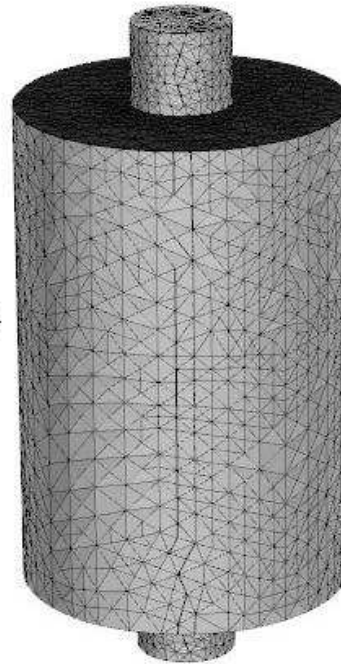
Geometry Simplification

We consider domains with **vertical axis symmetry** in order to simplify our problem.

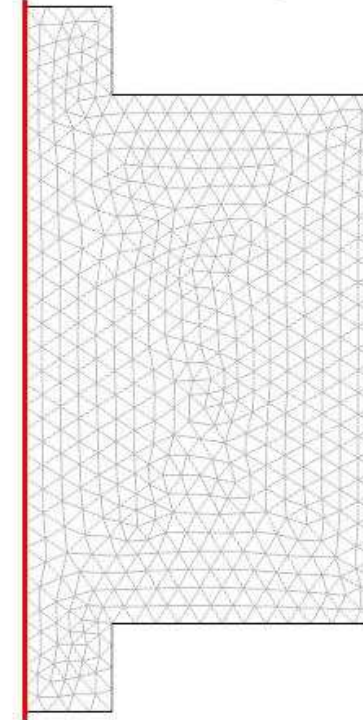
Real Geometry



3D Geometry



2D Geometry



- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

- General Definition
- Considered Bioreactor
- **Geometry Simplification**
- Mathematical Model
- Numerical Scheme
- Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives



Mathematical Model

The fluid flow is modeled by using the **Incompressible Navier-Stokes equations**:

$$\begin{cases} \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \eta \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] + \mathbf{F}, & \text{in } \Omega \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \end{cases} .$$

The process of **convection, diffusion and reaction** of the substrate (and biomass) concentration s (and b) is simulated by:

$$\frac{\partial s}{\partial t} + \nabla \cdot (-D \nabla s) - \mathbf{u} \cdot \nabla s = -\mu(s) b, \text{ in } \Omega.$$

The reaction rate μ is a **Monod** kinetic function of the form $\mu(s) = \mu_{\max} \frac{s}{K+s}$.

Those equations are completed by suitable **boundary conditions** and **coefficients**.

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

- General Definition
- Considered Bioreactor
- Geometry Simplification
- **Mathematical Model**
- Numerical Scheme
- Design Problem

PART II: Optimization Method

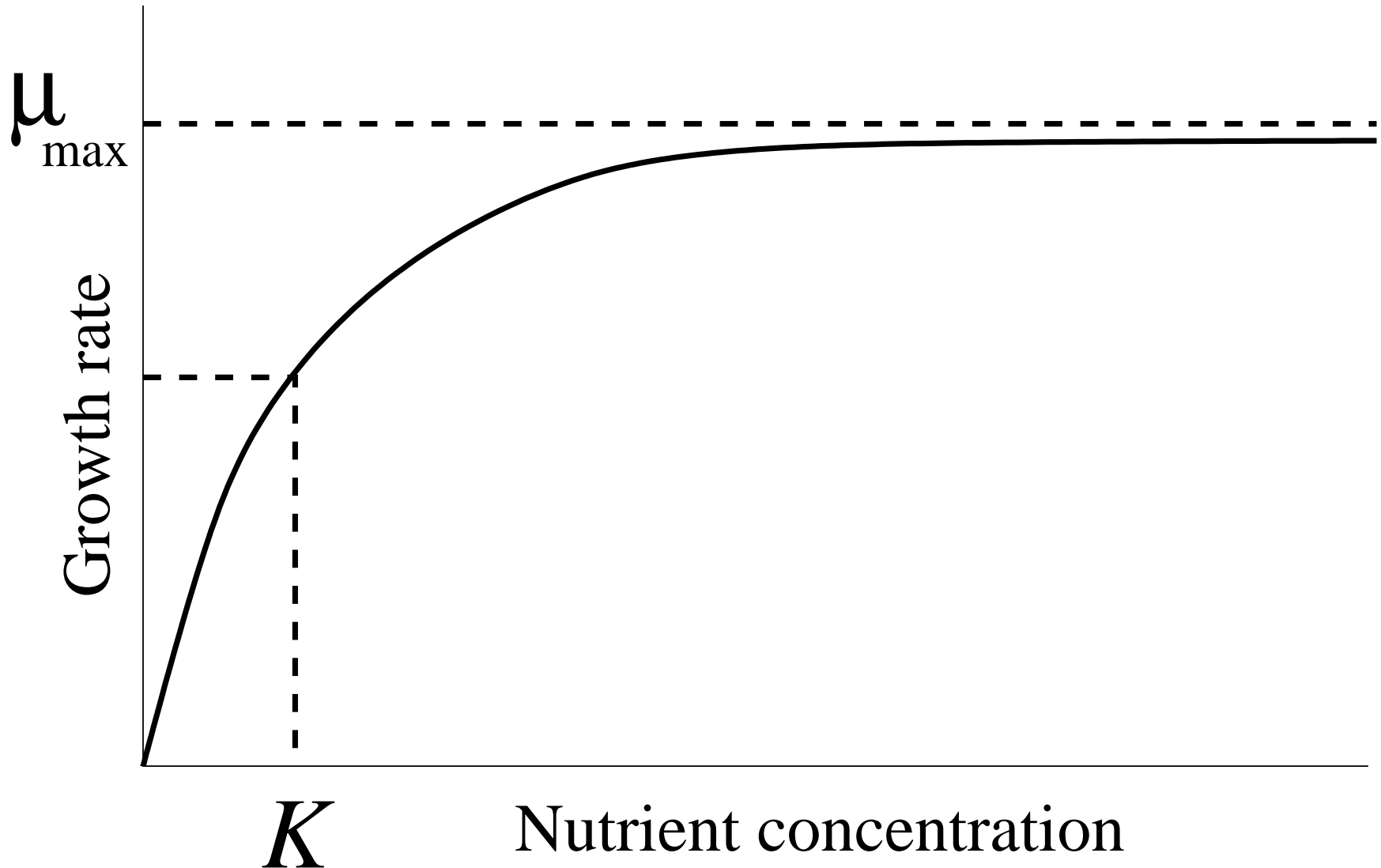
PART III: Numerical Results

Conclusion and perspectives



Mathematical Model

Monod kinetic:



- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

- General Definition
- Considered Bioreactor
- Geometry Simplification
- **Mathematical Model**
- Numerical Scheme
- Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives



Numerical Scheme

We use a **FEM** numerical approach:

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

- General Definition
- Considered Bioreactor
- Geometry Simplification
- Mathematical Model
- **Numerical Scheme**
- Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives



Numerical Scheme

We use a **FEM** numerical approach:

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

- General Definition
- Considered Bioreactor
- Geometry Simplification
- Mathematical Model
- **Numerical Scheme**
- Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives

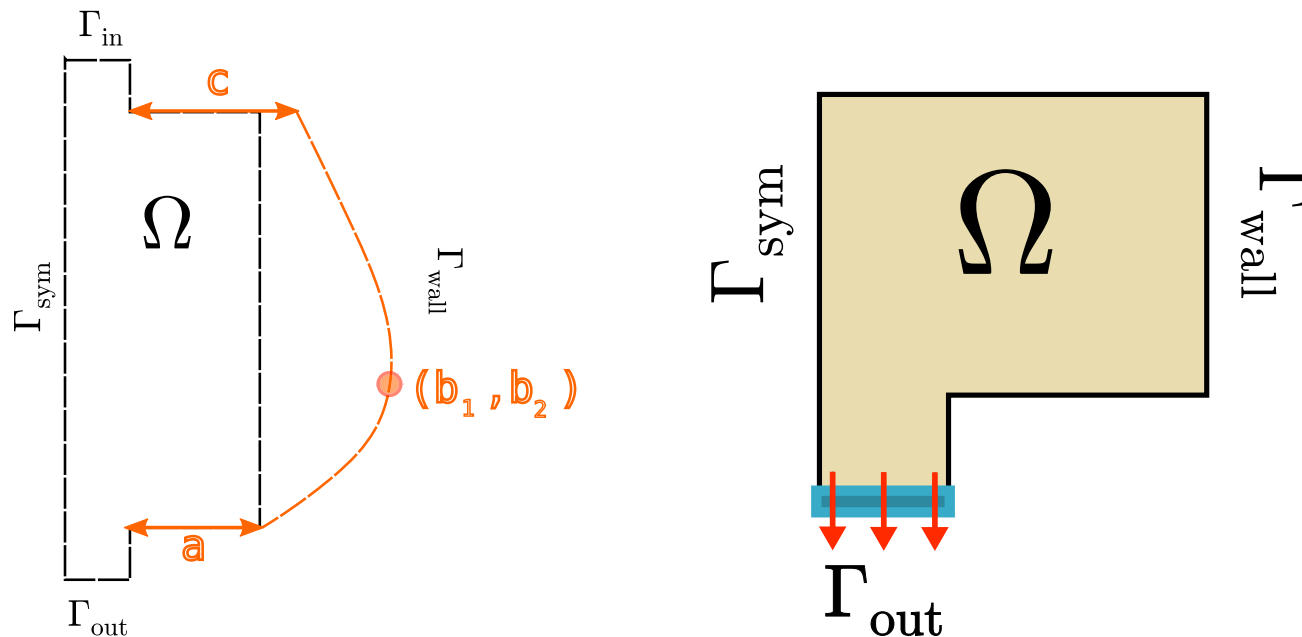


Design Problem

We are interested in **reducing** the **volume** of a particular bioreactor x_0 **keeping** its cleaning efficiency (at **equilibrium**).

$$\arg \min_{x \in \Omega} \text{Vol}(x) + P \max \left\{ 0, \int_{\Gamma_{out}} s(x) v(x) d\Gamma - \int_{\Gamma_{out}} s(x_0) v(x_0) d\Gamma \right\}$$

where Ω is the set of all admissible shapes.



This problem is solved with a **global optimization approach**.

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

- General Definition
- Considered Bioreactor
- Geometry Simplification
- Mathematical Model
- Numerical Scheme

● Design Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives



- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives

PART II: Optimization Method



General Optimization Problem

- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

● General Optimization Problem

- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives

$$\min_{x \in \Omega} J(x)$$

Where:

- x is the optimization parameter

- $\Omega \in \mathbb{R}^N$ is the admissible space

Assumption: J bounded on Ω .



Initial condition optimization

We consider an optimization algorithm $A_0 : V \rightarrow \Omega$, called '**core optimization algorithm**', to solve previous optimization problem. V is the space where we can choose the initial condition for A_0 . The other optimization parameters of A_0 are fixed.

Assumption: It exists a suitable initial condition $v \in V$ such that the output returned by $A_0(v)$ approaches a solution of optimization problem.

Solving numerically the optimization problem with $A_0 \Leftrightarrow$ Solve:

$$\begin{cases} \text{Find } v \in V \text{ such that} \\ A_0(v) \in \operatorname{argmin}_{x \in \Omega} J(x) \end{cases}$$

Idea: Use a **Multi-Layer Semi-Deterministic Algorithm** based on **line search methods** (collaboration with **B. Mohammadi**).

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

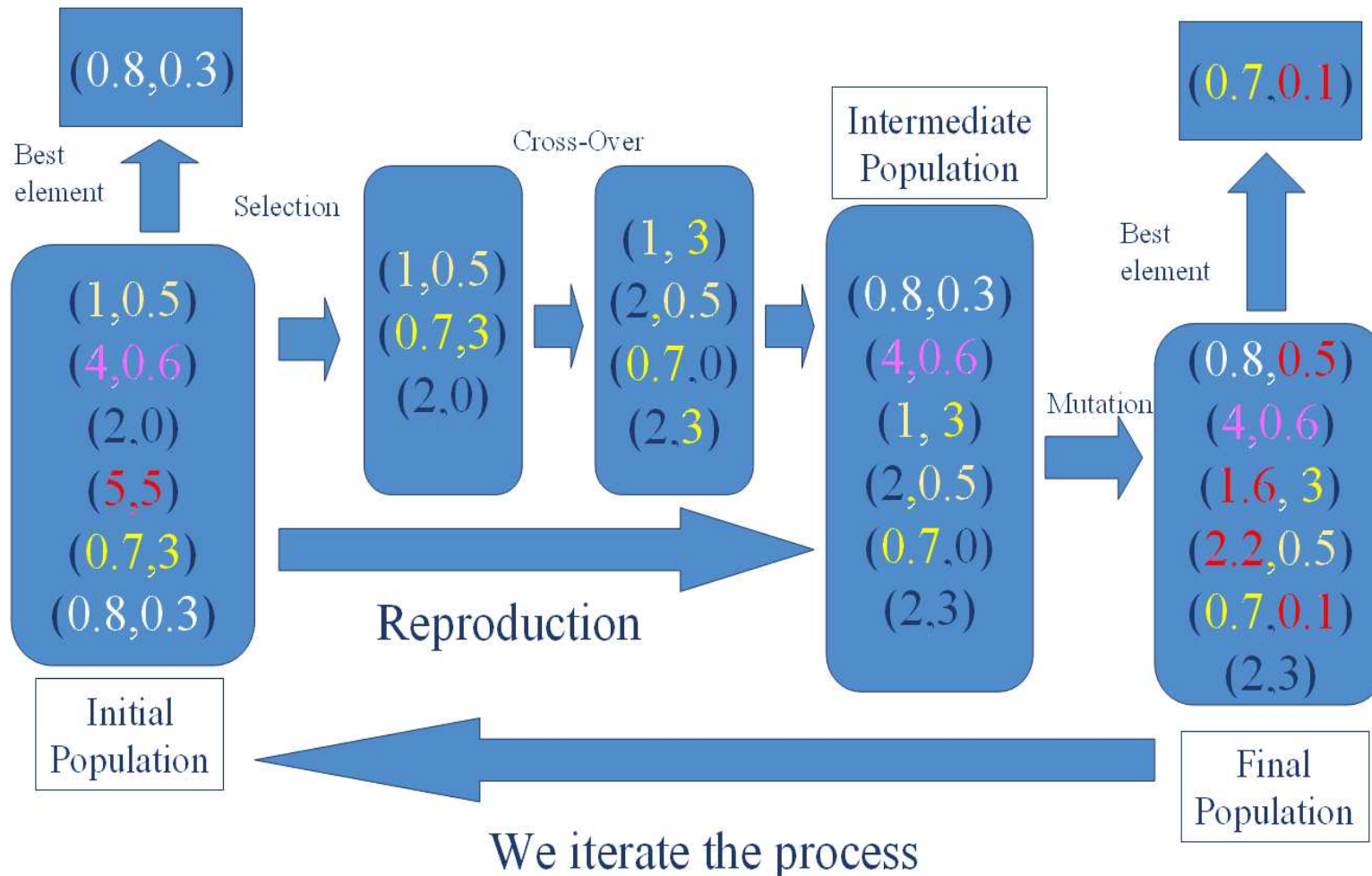
Conclusion and perspectives



Implementation with Genetic Algorithm

General overview of GAs:

We want to minimize: $J(x) = x_1^2 + x_2^2$



- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives



Implementation with Genetic Algorithm

Matrix representation of GAs:

i^{th} Population: $X^i = \{x_l^i \in \Omega, l = 1, \dots, N_p\}$

Selection: \mathcal{S}^i , Crossover: \mathcal{C}^i , Mutation: \mathcal{E}^i

The new population can be written as:

$$X^{i+1} = \mathcal{C}^i \mathcal{S}^i X^i + \mathcal{E}^i$$

Optimization problem reformulation:

$$\left\{ \begin{array}{l} \text{Find } X^0 \in \Omega^{N_p} \text{ such that:} \\ X(0) = X^0 \\ X^{i+1} = \mathcal{C}^i \mathcal{S}^i X^i + \mathcal{E}^i, i = 0, \dots, N_{gen} - 1 \\ \hat{J}(X^{N_{gen}}) < \epsilon \end{array} \right.$$

where $N_{gen} \in \mathbb{N}$ is fixed and $\hat{J}(X) = \min(J(x_i) | x_i \in X)$.

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives



Implementation with Genetic Algorithm

- Outlines
- Some Associated Articles

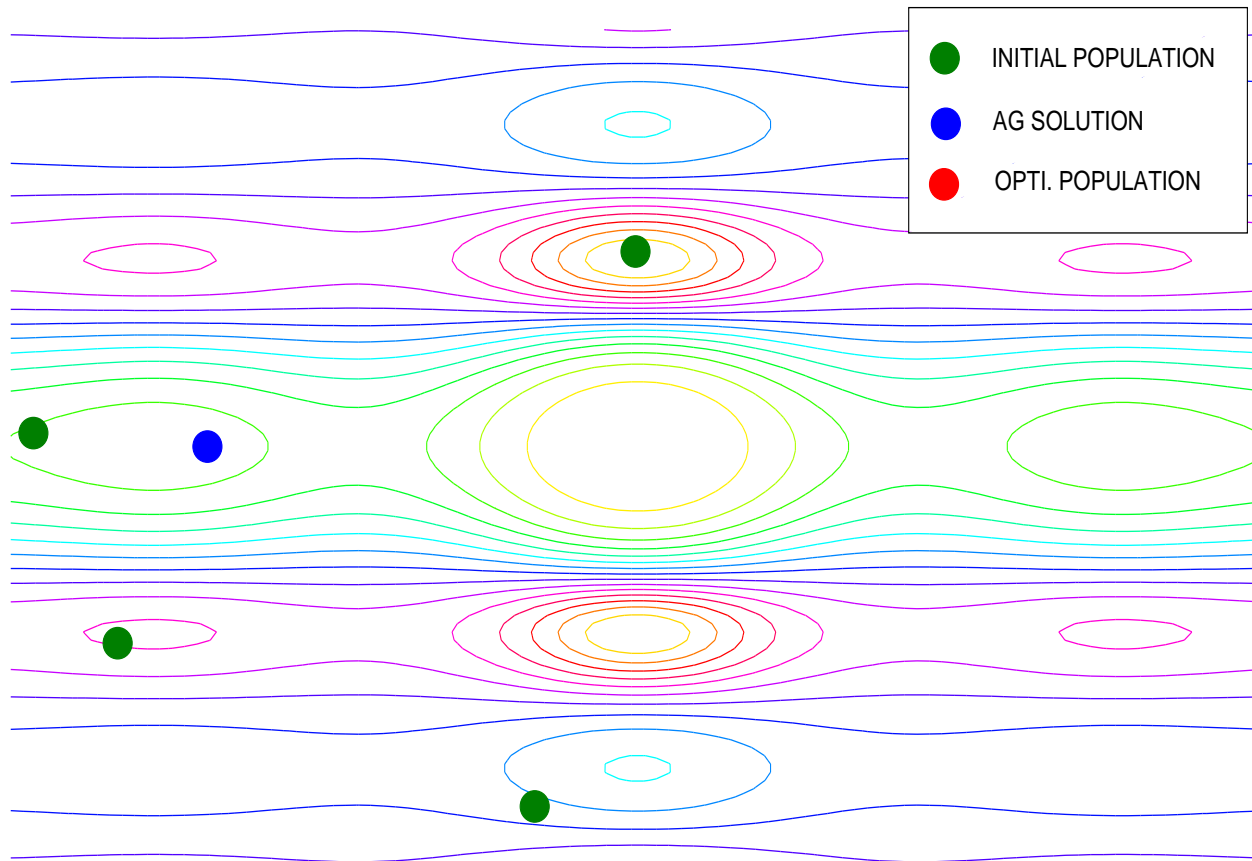
PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives





Implementation with Genetic Algorithm

- Outlines
- Some Associated Articles

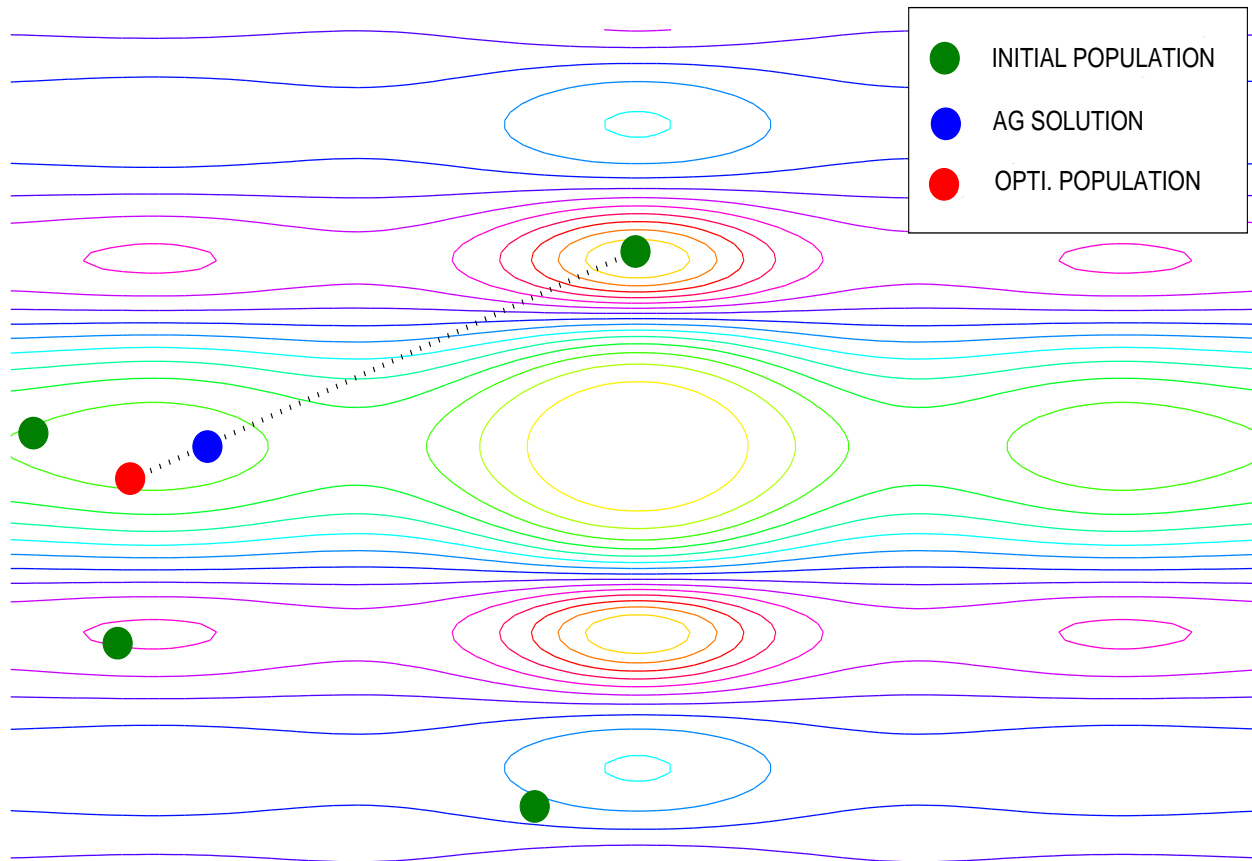
PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives





Implementation with Genetic Algorithm

- Outlines
- Some Associated Articles

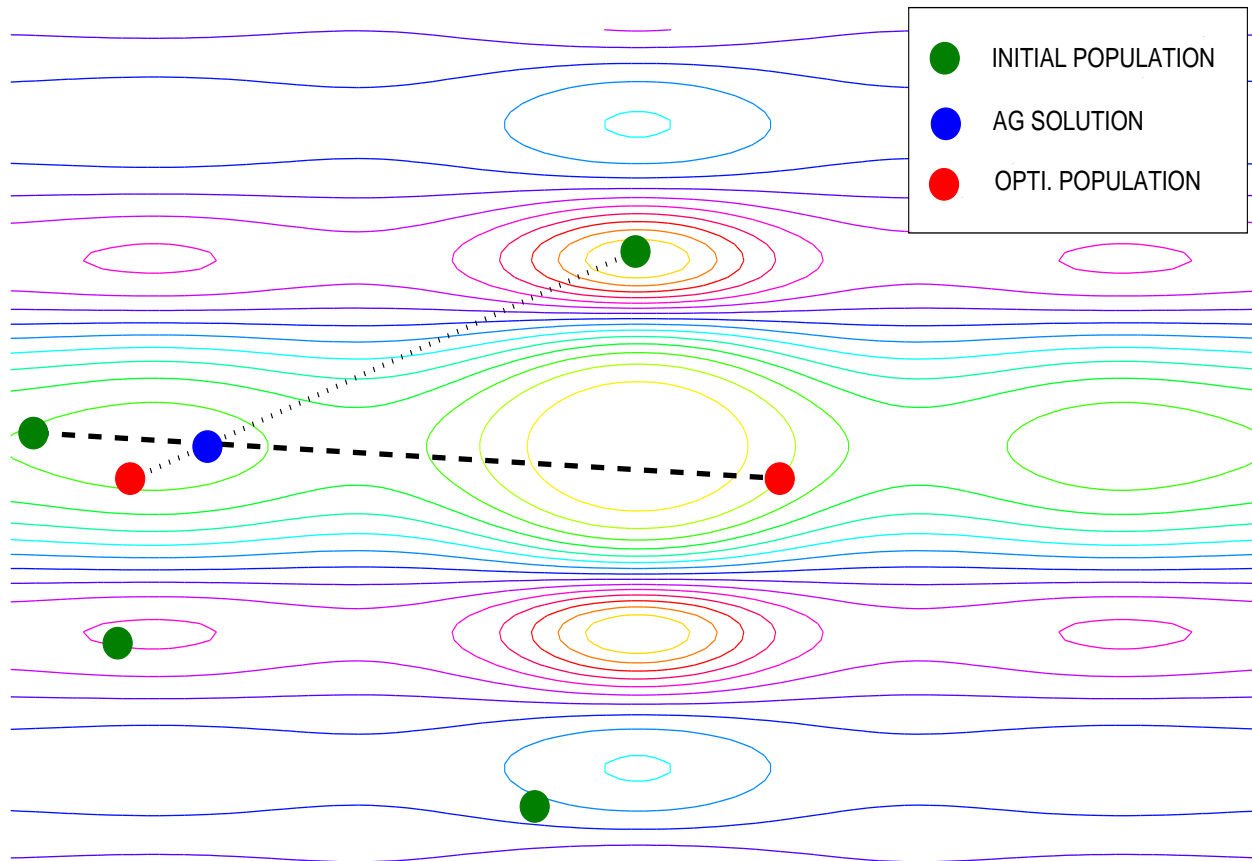
PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives





Implementation with Genetic Algorithm

- Outlines
- Some Associated Articles

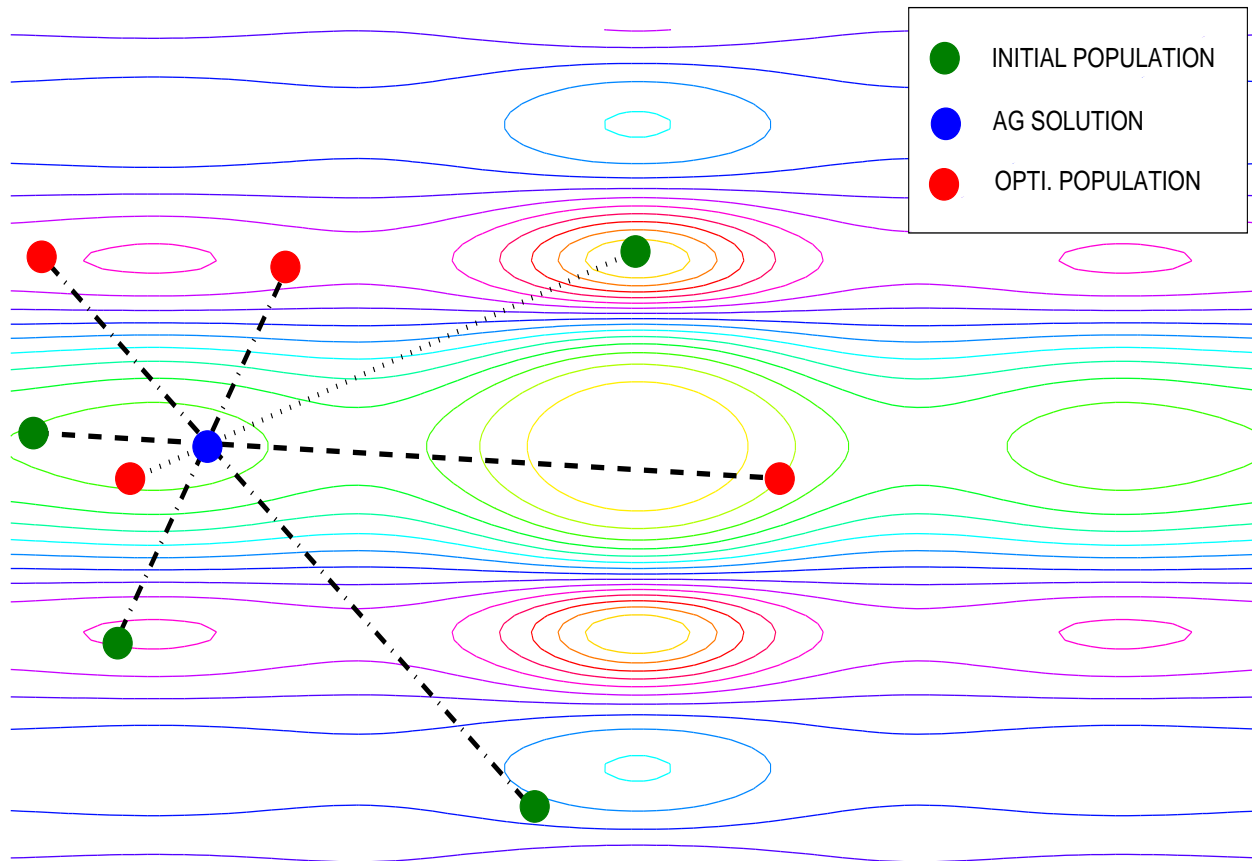
PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

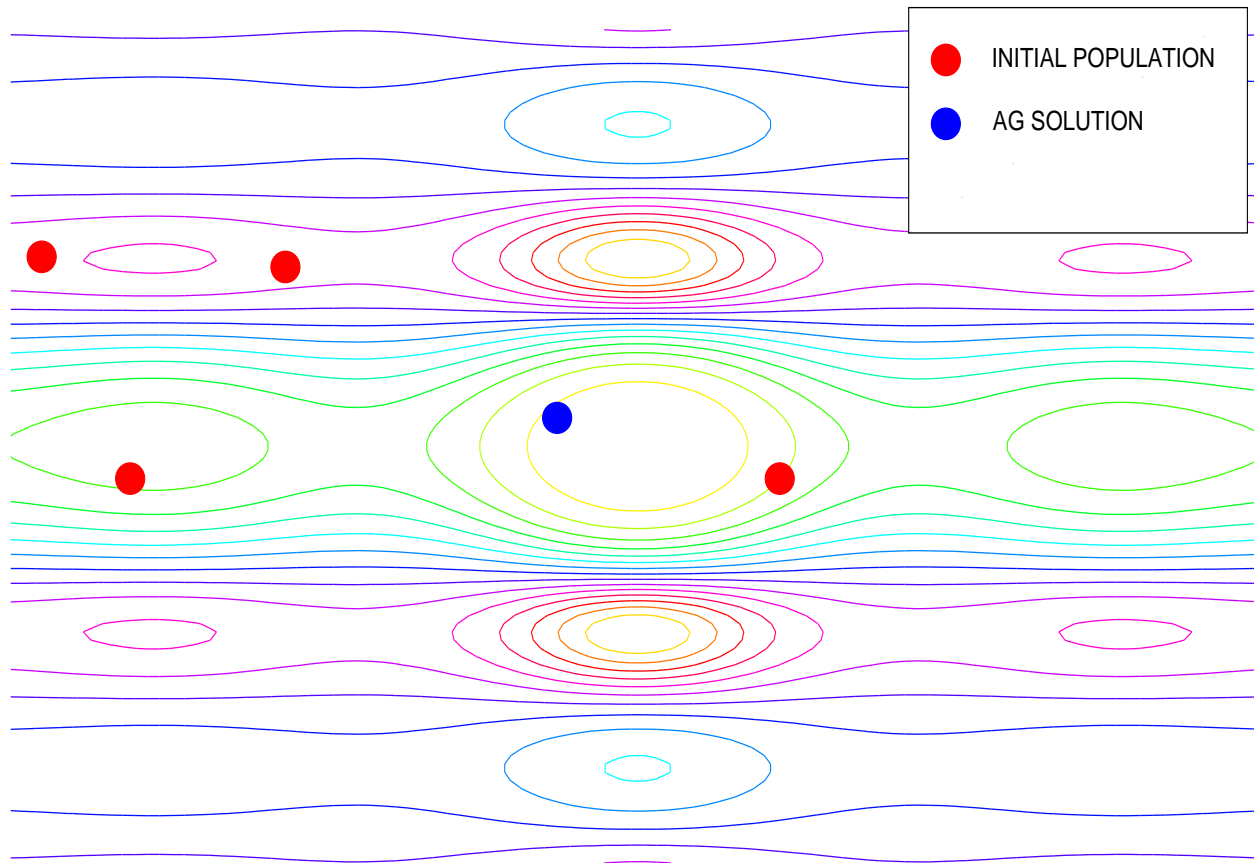
PART III: Numerical Results

Conclusion and perspectives





Implementation with Genetic Algorithm



- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives



Implementation with Genetic Algorithm

Example:

- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

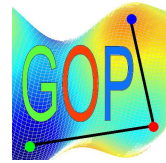
- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives

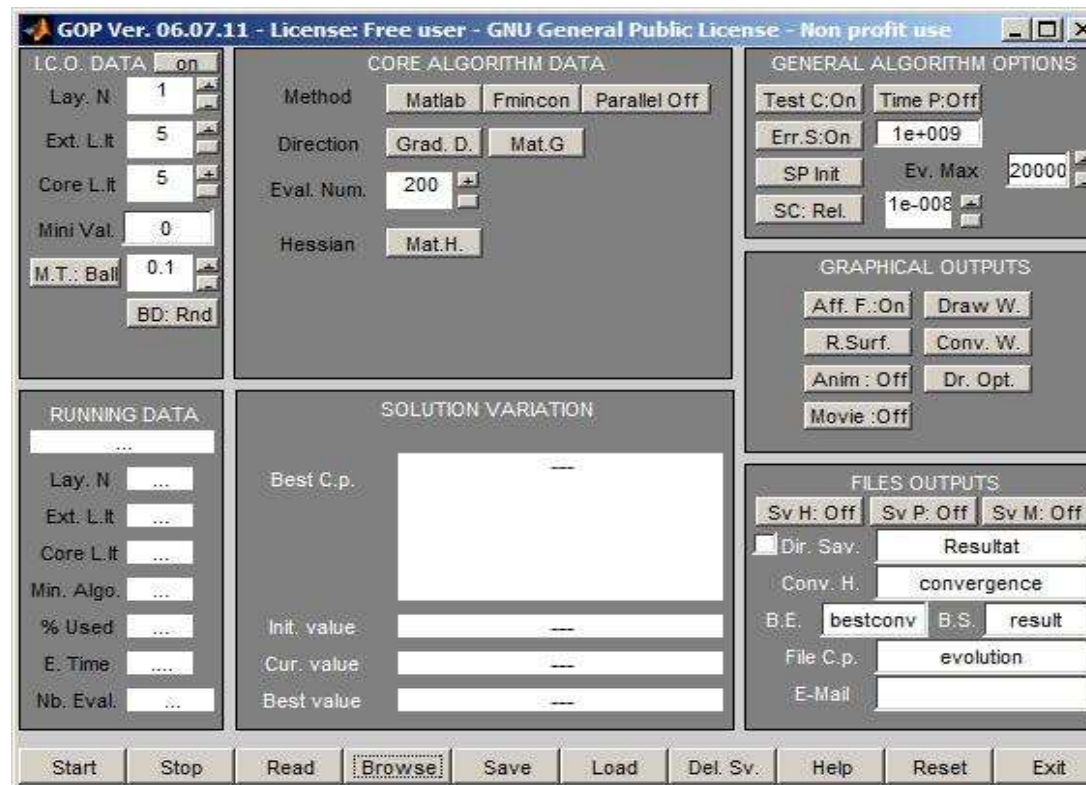


A MATLAB implementation: GOP



Global Optimization Platform

<http://www.mat.ucm.es/momat/software.htm>



- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- Some benchmark Results

PART III: Numerical Results

Conclusion and perspectives



Some benchmark Results

Number of evaluations:

Function	GA	DTS	C-GRASP	SDDA-2L	GSDA
Branin	1304	212	59857	140	252
Easom	40125	223	189630	7085	3488
Goldstein-Price	465	230	29	312	439
Shubert	7748	274	82363	4274	1270
Hartmann-3	1119	438	20743	347	425
Hartmann-6	4418	1787	79685	369	1054
Rosenbrock-2	3918	254	1158350	945	1675
Rosenbrock-10	44557	9037	20282529	2657	44828
Shekel-(4,5)	37328	819	5545982	1123	6991
Shekel-(4,7)	36046	812	4052800	936	4619
Shekel-(4,10)	40217	6828	4701358	3159	1637
Zakharov-5	24988	1003	959	152	267
Zakharov-10	40489	4032	3607653	309	20719

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- **Some benchmark Results**

PART III: Numerical Results

Conclusion and perspectives



Some benchmark Results

Success rate:

Function	GA	DTS	C-GRASP	SDDA-2L	GSDA
Branin	100	100	100	100	100
Easom	100	82	100	100	100
Goldstein-Price	100	100	100	100	100
Shubert	100	92	100	100	100
Hartmann-3	100	100	100	100	100
Hartmann-6	100	83	100	100	100
Rosenbrock-2	92	100	100	100	92
Rosenbrock-10	89	85	99	100	95
Shekel-(4,5)	95	57	100	100	97
Shekel-(4,7)	96	65	100	100	98
Shekel-(4,10)	96	52	100	100	97
Zakharov-5	100	100	100	100	100
Zakharov-10	100	100	100	100	100

- Outlines
- Some Associated Articles

PART I: Bioreactor Design Problem

PART II: Optimization Method

- General Optimization Problem
- Initial condition optimization
- Implementation with Genetic Algorithm
- A MATLAB implementation: GOP
- **Some benchmark Results**

PART III: Numerical Results

Conclusion and perspectives



- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

PART III: Numerical Results

- Original Bioreactor
- Optimized Bioreactor
- Volume Reduction

Conclusion and perspectives

PART III: Numerical Results



Original Bioreactor

- Outlines
- Some Associated Articles

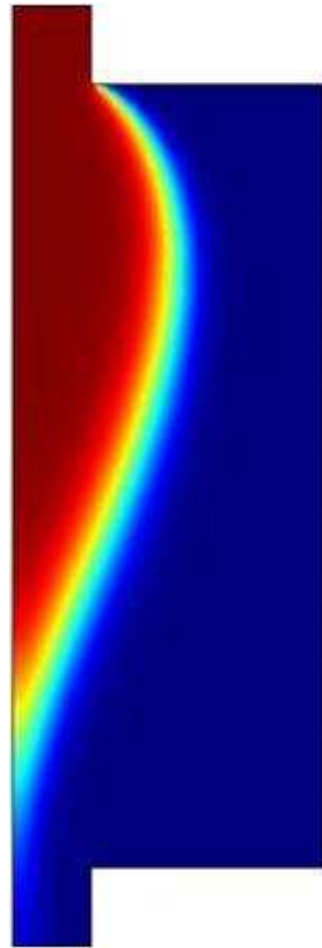
PART I: Bioreactor Design Problem

PART II: Optimization Method

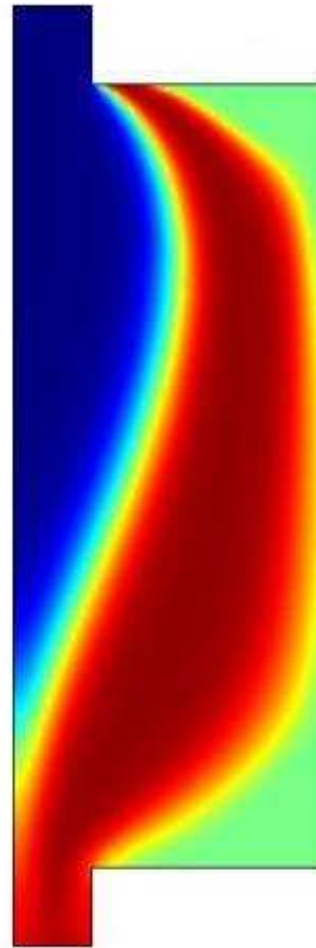
PART III: Numerical Results

- Original Bioreactor
- Optimized Bioreactor
- Volume Reduction

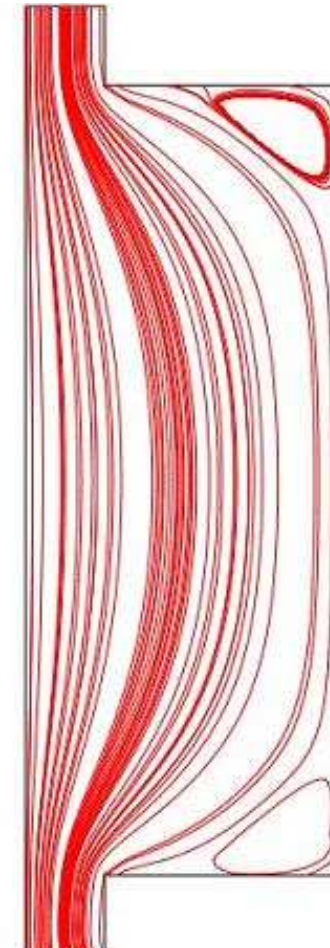
Conclusion and perspectives



Sustrate



Biomass



Flow



Optimized Bioreactor

- Outlines
- Some Associated Articles

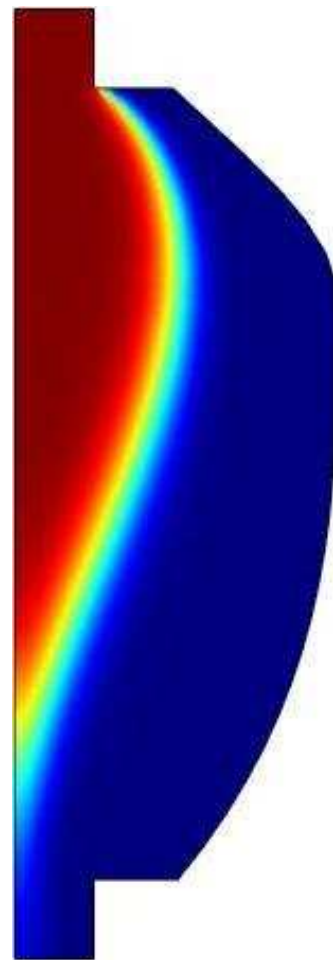
PART I: Bioreactor Design Problem

PART II: Optimization Method

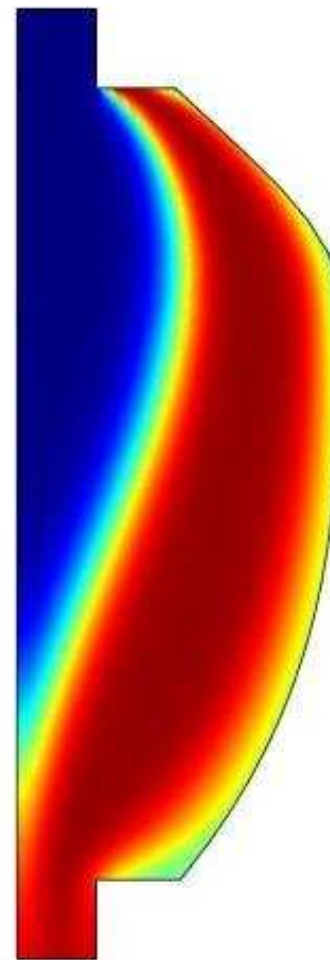
PART III: Numerical Results

- Original Bioreactor
- **Optimized Bioreactor**
- Volume Reduction

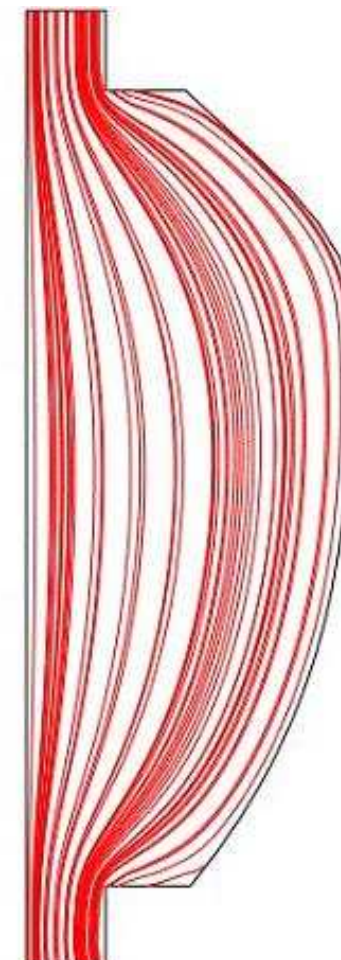
Conclusion and perspectives



Sustrate



Biomass

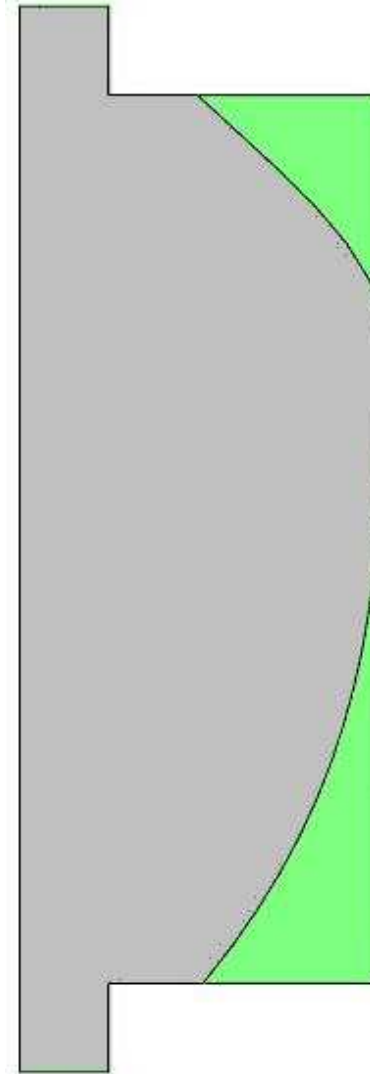


Flow



Volume Reduction

We have obtained a volume reduction by **20%**:



- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

PART III: Numerical Results

- Original Bioreactor
- Optimized Bioreactor
- Volume Reduction

Conclusion and perspectives



- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives

- Conclusions and perspectives
- Thank You

Conclusion and perspectives



Conclusions and perspectives

- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives

- Conclusions and perspectives
- Thank You

- Presented a **Time/Spatial** PDE model to simulate the behavior of a diffusive bioreactor.
- Obtained **encouraging** optimized results.

Perspectives:

- Study **different** optimization problems.
- Consider a **ODE simplified model** for the optimized bioreactors to obtain some theoretical behaviors.
- Add other technologies to diffusive bioreactor, such as **central channel** and **recirculation flow**, to improve cleaning efficiency
- **Couple** this model with a contaminated lake (collaboration: **H. Ramirez, P. Gajardo** and **A. Rousseau**)



Thank You

!!! Thank you for your attention !!!



- Outlines
- Some Associated Articles

PART I: Bioreactor Design
Problem

PART II: Optimization Method

PART III: Numerical Results

Conclusion and perspectives

● Conclusions and perspectives

● Thank You