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Funded by:
Outlines

- 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


PART I: Bioreactor Design Problem
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.).
Considered Bioreactor

We focus here on dispersive bioreactors used for water treatment.
Geometry Simplification

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

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

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

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

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

The reaction rate \( \mu \) is a Monod kinetic function of the form

\[
\mu(s) = \mu_{\text{max}} \frac{s}{K + s}.
\]

Those equations are completed by suitable boundary conditions and coefficients.
Mathematical Model

Monod kinetic:

\[
\mu = \begin{cases} 
\frac{\mu_{\text{max}}}{1 + \frac{K}{C}} & \text{if } C < K \\
\mu_{\text{max}} & \text{if } C \geq K 
\end{cases}
\]
Numerical Scheme

We use a FEM numerical approach:
We use a **FEM** numerical approach:
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 $\Omega$ is the set of all admissible shapes.

This problem is solved with a global optimization approach.
PART II: Optimization Method
General Optimization Problem

\[
\min_{x \in \Omega} J(x)
\]

Where:
- \( x \) is the optimization parameter
- \( \Omega \subset \mathbb{R}^N \) is the admissible space

Assumption: \( J \) bounded on \( \Omega \).
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:

$$\left\{ \begin{array}{l}
\text{Find } v \in V \text{ such that } \\
A_0(v) \in \arg\min_{x \in \Omega} J(x)
\end{array} \right.$$ 

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

General overview of GAs:

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

Initial Population

<table>
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<tr>
<th>(1.0, 0.5)</th>
<th>(4.0, 0.6)</th>
<th>(2.0)</th>
<th>(5.5)</th>
<th>(0.7, 3)</th>
<th>(0.8, 0.3)</th>
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Best element

Selection

(1.0, 0.5) | (0.7, 3) | (2.0) | (2.0) |

Cross-Over

Intermediate Population

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<td>(1.6, 3)</td>
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Reproduction

Final Population

| (0.8, 0.1) |

We iterate the process
Implementation with Genetic Algorithm

Matrix representation of GAs:

$\text{\textit{i}th \ Population: } X^i = \{x^i_l \in \Omega, l = 1, ..., N_p\}$

Selection: $S^i$, Crossover: $C^i$, Mutation: $E^i$

The new population can be written as:

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

Optimization problem reformulation:

\[
\begin{cases} 
\text{Find } X^0 \in \Omega^{N_p} \text{ such that:} \\
X(0) = X^0 \\
X^{i+1} = C^i S^i X^i + E^i, i = 0, ..., N_{gen} - 1 \\
\hat{J}(X^{N_{gen}}) < \epsilon
\end{cases}
\]

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

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

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Conclusion and perspectives
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- Initial Population
- Optimized Population
- AG Solution

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PART III: Numerical Results

Conclusion and perspectives
Implementation with Genetic Algorithm

- Initial population
- AG solution
Example:
A MATLAB implementation: GOP

http://www.mat.ucm.es/momat/software.htm
### Some benchmark Results

#### Number of evaluations:

<table>
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<th>Function</th>
<th>GA</th>
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<th>SDDA-2L</th>
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### Some benchmark Results

#### Success rate:

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PART III: Numerical Results
Optimized Bioreactor

- Sustrate
- Biomass
- Flow
Volume Reduction

We have obtained a volume reduction by 20%:
Conclusion and perspectives
Conclusions and perspectives

- Present a **Time/Spatial** PDE model to simulate the behavior of a diffusive bioreactor.

- Obtain **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 for your attention !!!