Solving industrial design problems by using COMSOL Multiphysics with MATLAB

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Outline

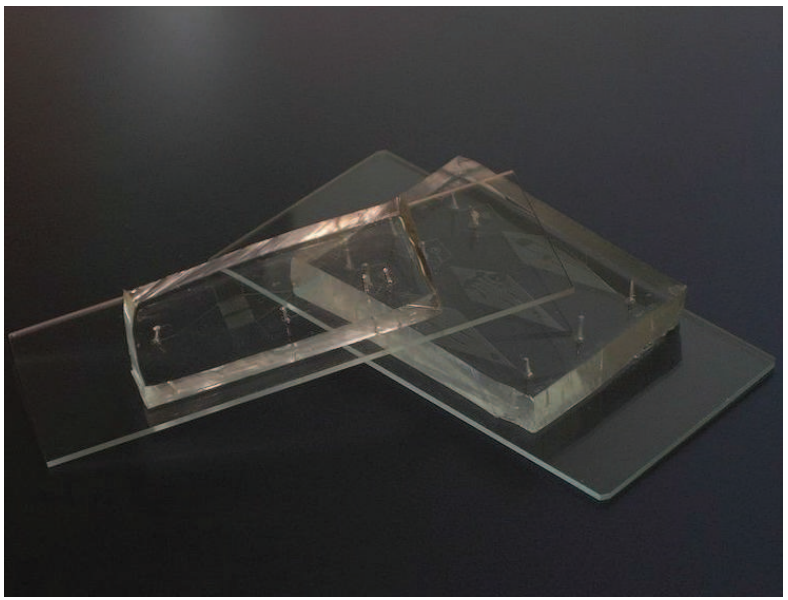
- Industrial examples
  - Microfluidic mixer
  - Toy problem
- COMSOL Multiphysics
  - Creation of the model
  - Conversion to MATLAB
- MATLAB
  - Structure of the M-script
  - Useful commands
  - Creating a function
- Conclusions

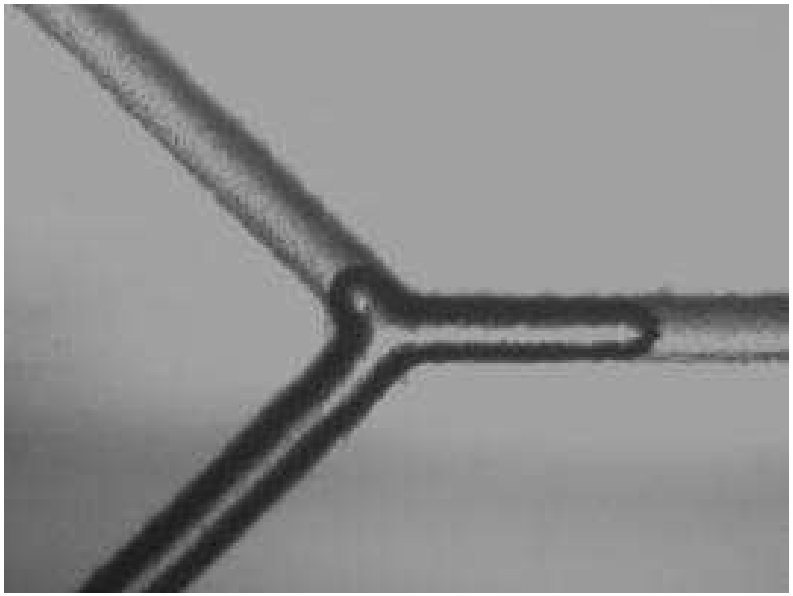
Part I: Industrial examples

Device: Microfluidic mixer

Application: Microfluidic mixers are used to quickly mix a protein solution with a solvent provoking a rapid change in chemical potential resulting in the unfold of certain proteins.

Example of microfluidic mixer: There exist a wide range of techniques to create microfluidic mixers. For instance:

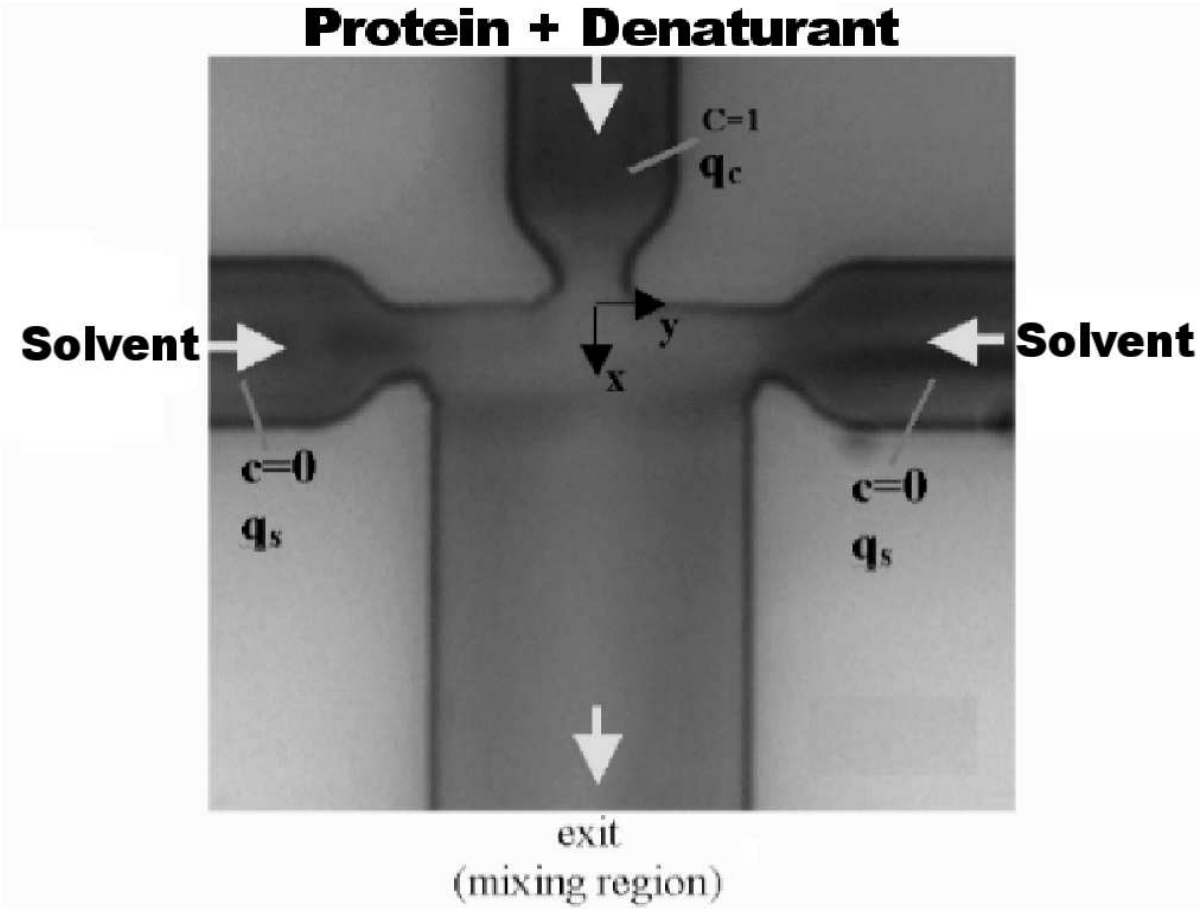




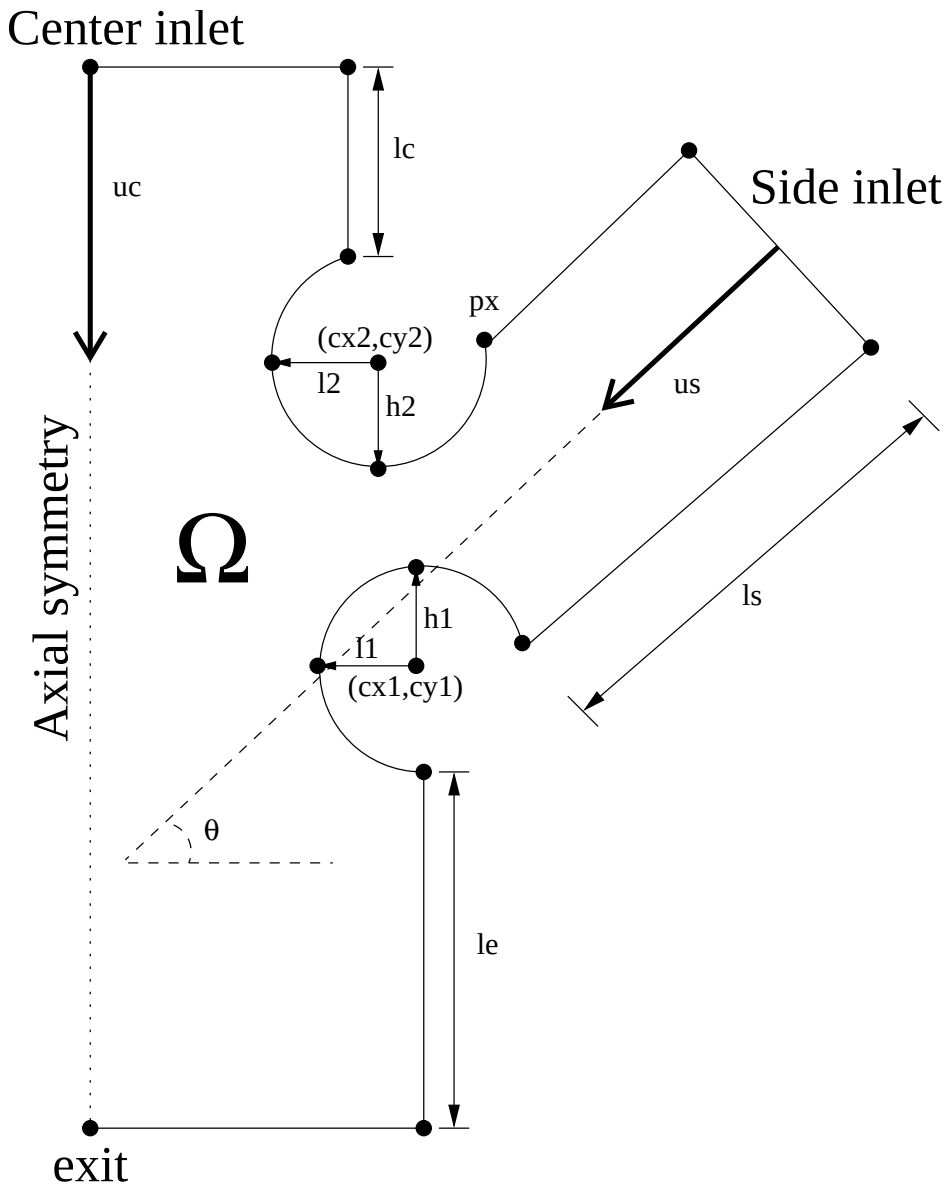
Industrial problem

Objective: optimize the mixer to reduce the time needed to reach a certain protein concentration.

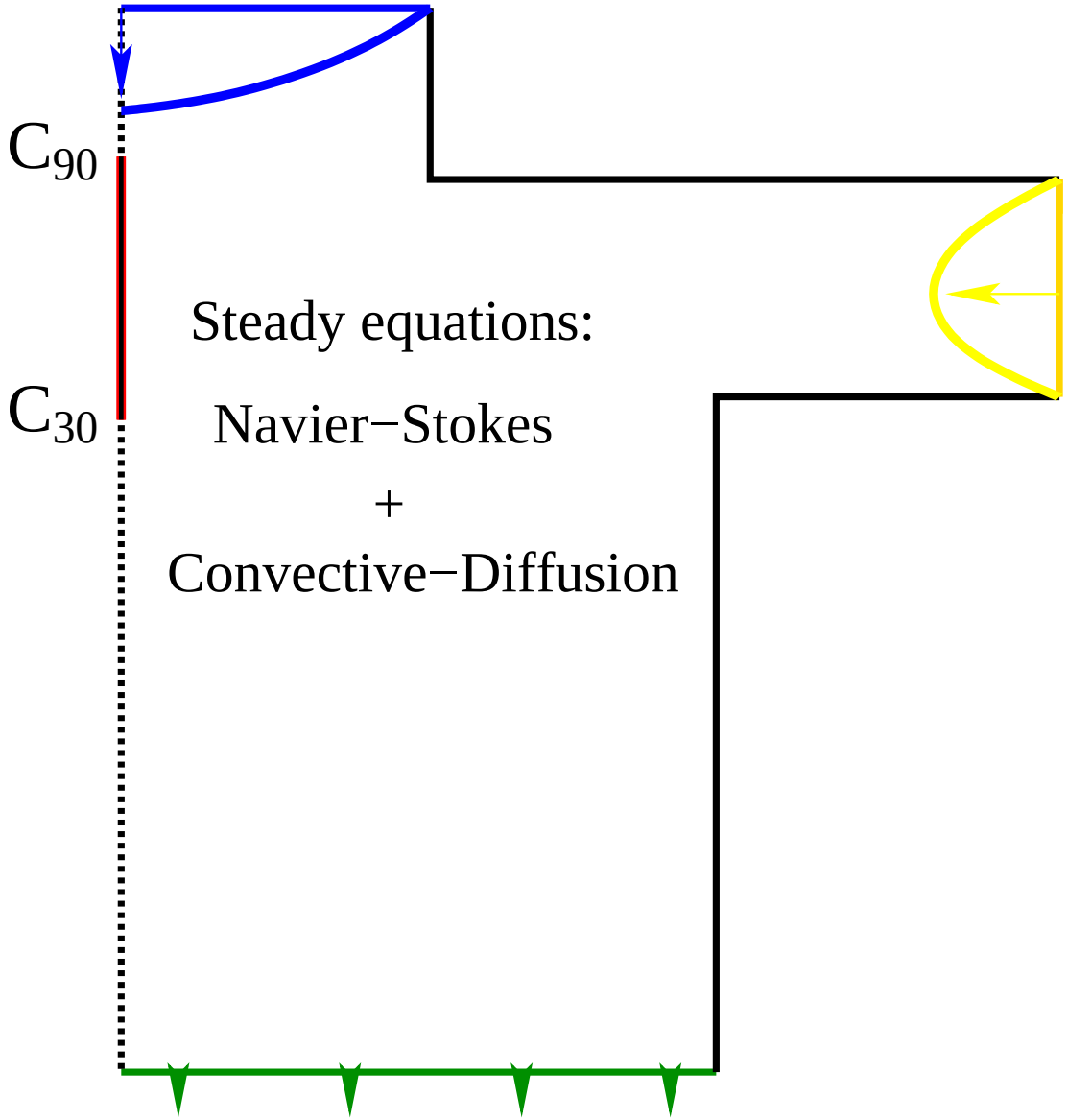
Considered mixer: Knight mixer



Parameters



Mathematical Modeling



Design Problem

We are interested in minimizing:

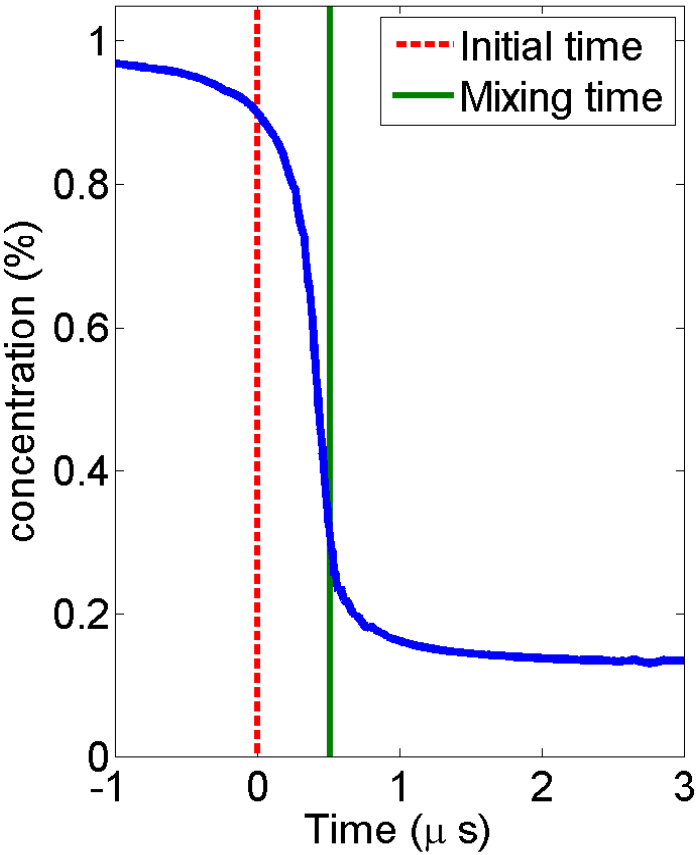
$$J(x_{\text{param}}) = \int_{c_{90}^{x_{\text{param}}}}^{c_{30}^{x_{\text{param}}}} \frac{\mathrm{d}y}{\mathbf{u}^{x_{\text{param}}}(y) \cdot t},$$

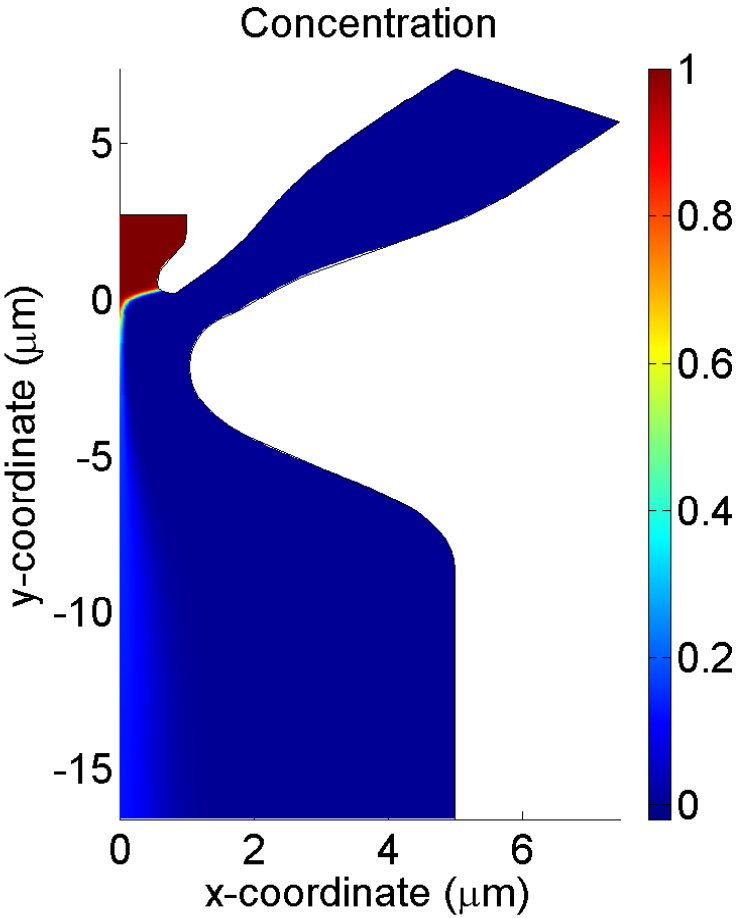
where $c_{90}^{x_{\text{param}}}$, $c_{30}^{x_{\text{param}}}$ and $\mathbf{u}^{x_{\text{param}}}$ are computed by solving numerically (COMSOL) the following system:

$$\begin{cases} -\nabla \cdot (\eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^\top)) + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = 0 & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega, \\ \nabla \cdot (-D\nabla c + c\mathbf{u}) = 0 & \text{in } \Omega, \\ + \text{ boundary conditions.} \end{cases}$$

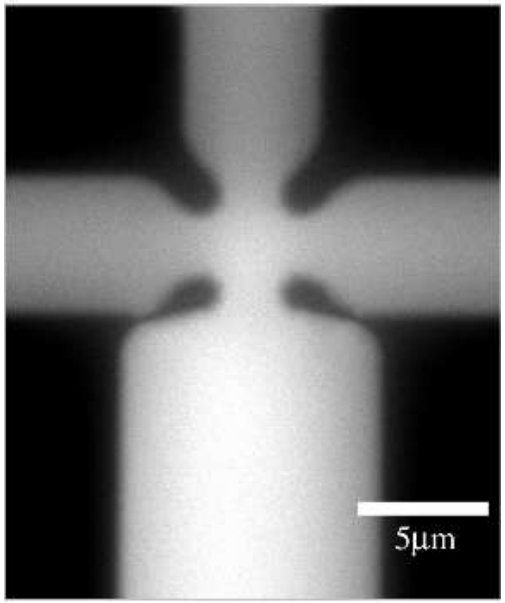
This optimization problem is solved by using the Global Optimization Platform software (MATLAB):
`http://www.mat.ucm.es/momat/software.htm`

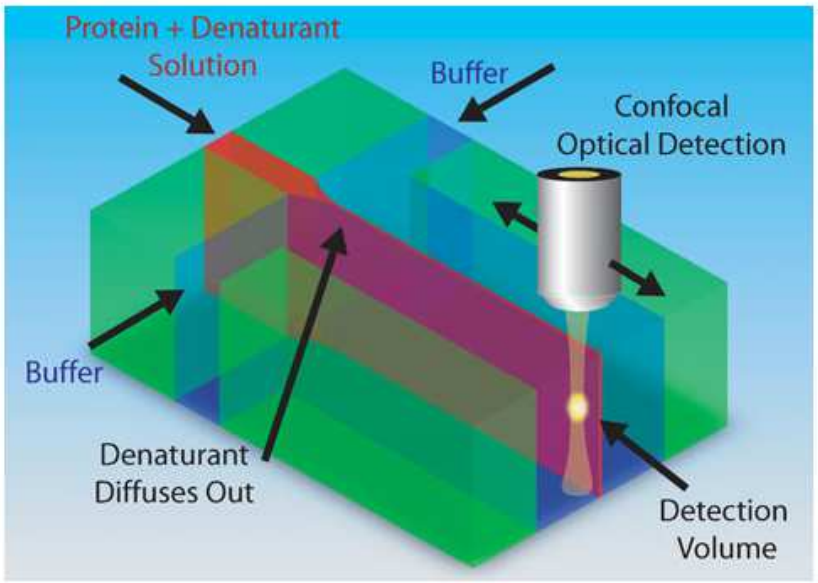
Some Results





Experimental implementation





Bibliography

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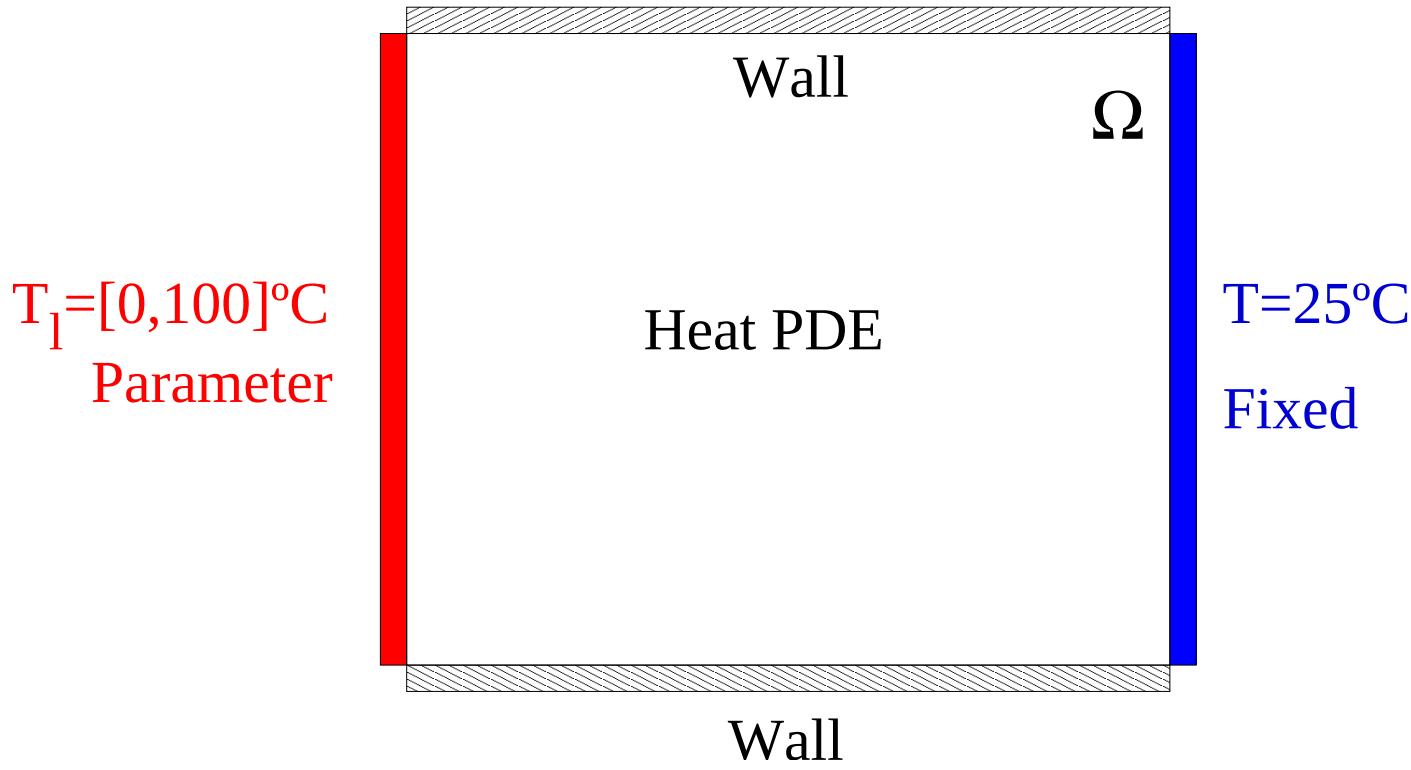
- David E. Hertzog, Benjamin Ivorra, Bijan Mohammadi, Olgica Bakajin, Juan G. Santiago. *Optimization of a Fast Microfluidic Mixer for Studying Protein Folding Kinetics.* Analytical chemistry, 78(13), 4299-4306, 2006.
- Benjamin Ivorra, David E. Hertzog, Bijan Mohammadi, Juan G. Santiago. *Semi-deterministic and genetic algorithms for global optimization of microfluidic protein-folding devices.* International Journal for Numerical Methods in Engineering , 66(2), 319-333, 2006.

Toy problem

We want to optimize the temperature of the left wall (T_l) of a given rectangular heat chamber such that the mean spatial temperature is 50°C:

$$\min_{T_l \in [0,100]} J(T_l) = \left| \left(\int_\Omega T(T_l) dx / \int_\Omega 1 dx \right) - 50 \right|$$



Part II: COMSOL Multiphysics

Main steps

- Use the COMSOL GUI to easily create the model.
- Identify and isolate all the parameters to be modified by the MATLAB code.
- Compress history before exporting the model to MATLAB format.

Part III: MATLAB

Useful MATLAB commands

- mphgeom(model,'geom1')
- mphmesh(model,'mesh1')
- model.result.table('tbl1').getReal
- mphint(model,'u','T',tf,'edim',2,'selection',[1])
- mphinterp(model,'u','T',tf,'coord',[0.2;0.2])
- mphsave(model,'optimum')
- model=mphload('optimum')
- model.variable('var1').set('Tmax', num2str(x(1)))

Conclusions

Extended courses

- Course (10H): **Método de Elementos Finitos: Aplicaciones y Optimización con COMSOL MULTIPHYSICS.** Doctorado en Ingeniería Matemática, Estadística e Investigación Operativa. **Universidad Complutense de Madrid**. February.

- Seminary (2H): **Simulación numérica en Ingeniería y Ciencias con MATLAB + COMSOL Multiphysics.** Departamento de Física Aplicada II y Vicerrectorado de Investigación. **Universidad de Málaga**. May.

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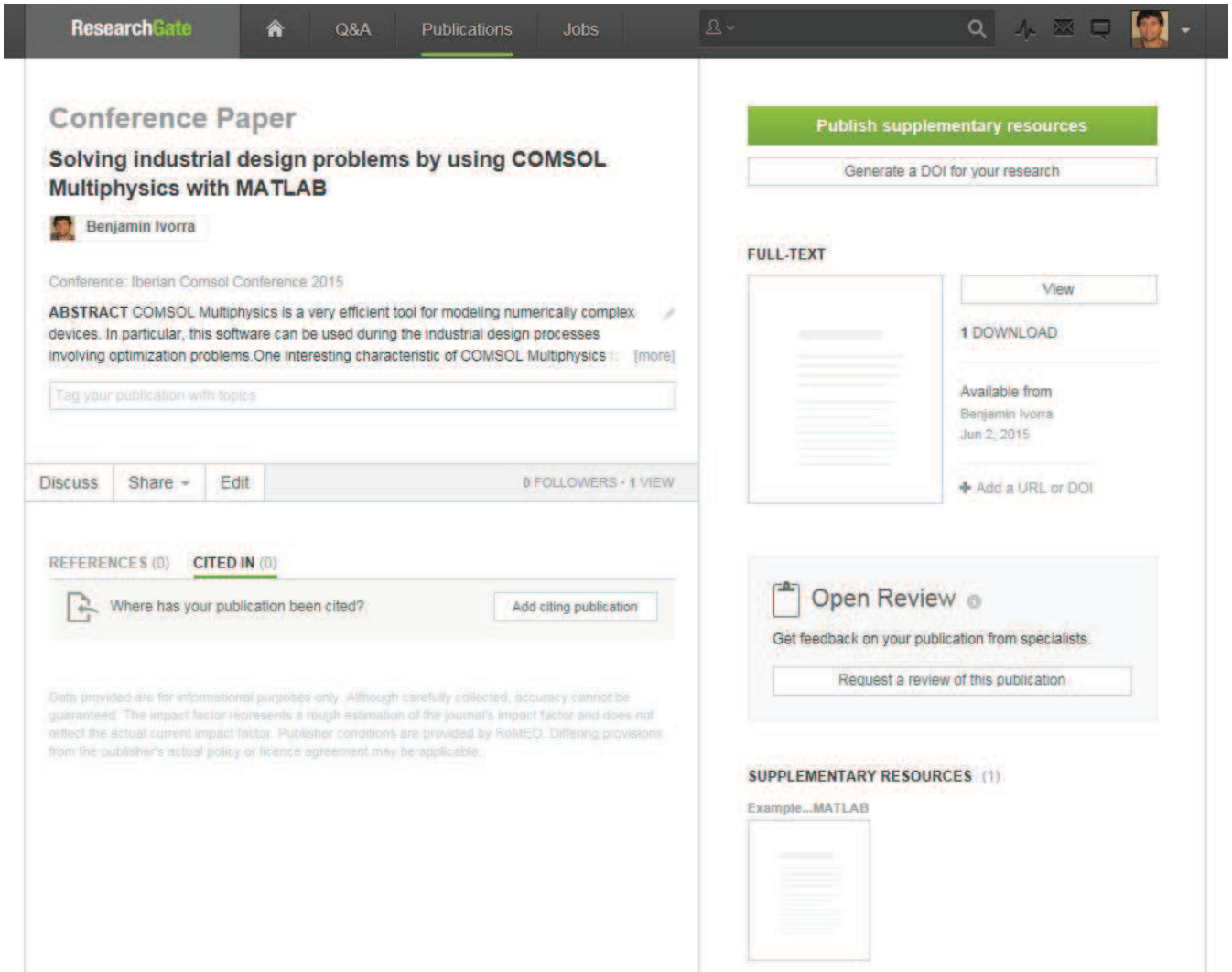
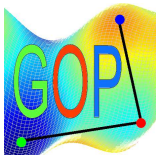


Thank you

!!! Thank you for your attention!!!



Global **O**ptimization **P**latform

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