Monte Carlo Method For Multi-Scale Models: Application To A Solar Photobioreactor

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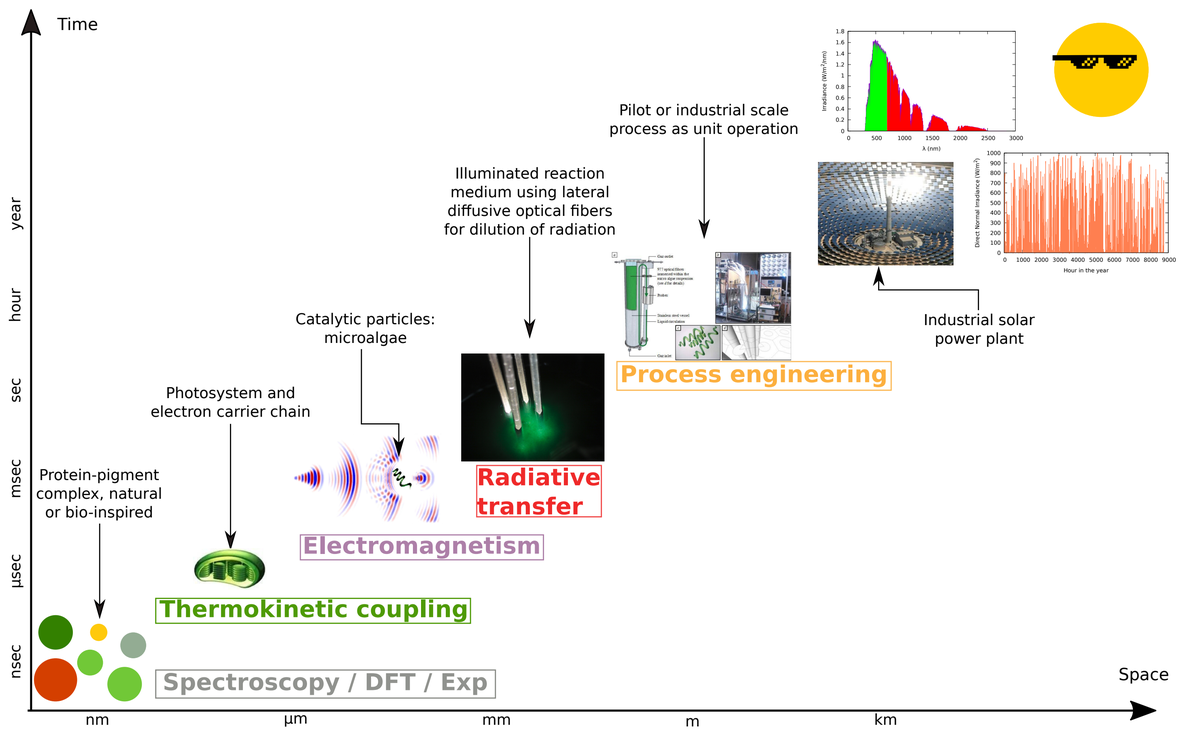
Introduction

Design and/or optimization of processes require the development of knowledge models. These models can involve several bodies of physics, chemistry and/or biology all coupled, sometimes non-linearly: this is generally referred to a multi-scale model (and sometimes also to a multiphysics model) [1]. Calculating a quantity at the scale of the process involves in general a sequential approach (the solution at a given level requires input data from the underlying level) that generates two difficulties involving calculation time issues:

- Geometry management at different scales
- Exchange of information between solvers using couplers

The main objective of this work is to develop statistical approaches to handle all scales through a single Monte Carlo algorithm. These approaches are developed in the field of photo-reactive processes enabling to produce renewable third generation of biofuels or synthetic fuels (H_2, CH_4 Syngas, CH_3OH) from solar energy. The example of a solar photobioreactor that produces *Arthrospira platensis* is presented here.

Multi-scale model



Biomass annual productivity $< r_x >$ is written as a path integral for the multi-scale model solution. At this state of our research, we use some approximations in order to tackle difficulties one by one:

- Linear thermokinetic coupling

$$< r_x > = \int_{\Delta t} dt\, p_{\Delta t}(t) \int_{\Delta \lambda} d\lambda\, p_{\Delta \lambda}(\lambda) \int_{\partial V} \frac{d\overrightarrow{x_s}}{S} \int_0^{\infty} dl\, k_{a,\lambda}\, e^{-k_{a,\lambda} l} H(\overrightarrow{x} \in V)\, \omega$$

- Purely absorbing medium (no scattering) with Schiff approximation of electromagnetism for the absorption coefficient

$$k_{a,\nu} = C_x \int_{4\pi} \frac{d\overrightarrow{e_0}}{4\pi} \int_{\Delta R} dR\, p_{\Delta R} \int\int_{\mathcal{P}} d\overrightarrow{x_m} \left[1 - e^{\left(-a_\nu L_m(\overrightarrow{x_m}; \overrightarrow{e_0}, R)\right)} \right]$$

- Refractive index given by the sum of pigments' contributions

$$a_\nu = \sum_p E_{a,\nu,p}\, C_p = \sum_p a_{\nu,pig,p}$$

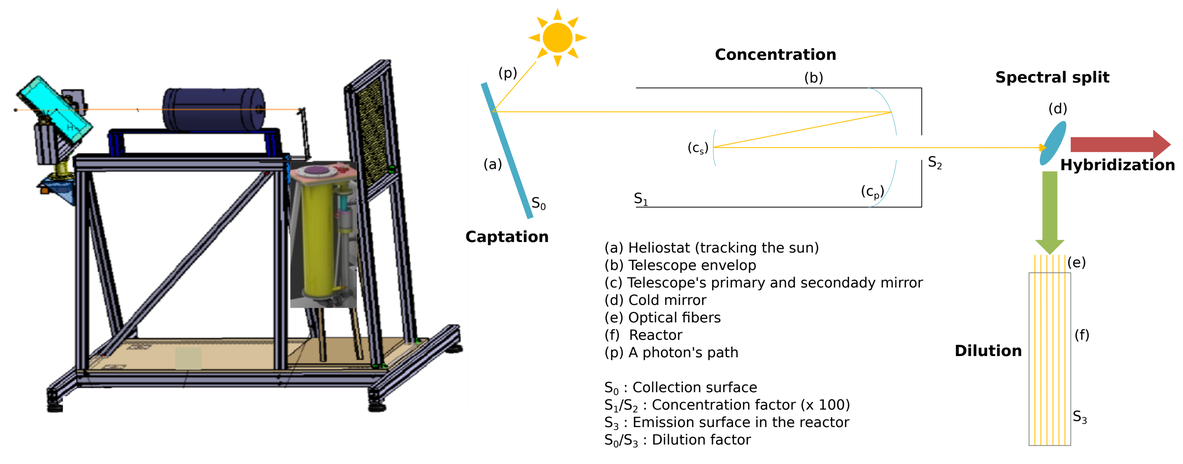
Monte Carlo (MC) method

Monte Carlo method is a statistical approach that offers suitable advantages:

- Management of infinite dimensions
- Meshless (in volume)
- Access to numerical error
- Possibility to compute sensitivities
- Complex geometries easily handled with advanced computer-graphics-tools [2]

An issue is to manage multi-scale non-linearities thanks to recent Monte Carlo advances (null collisions, ...) [3,4].

The developed DiCoFluV-Hy prototype



Main results

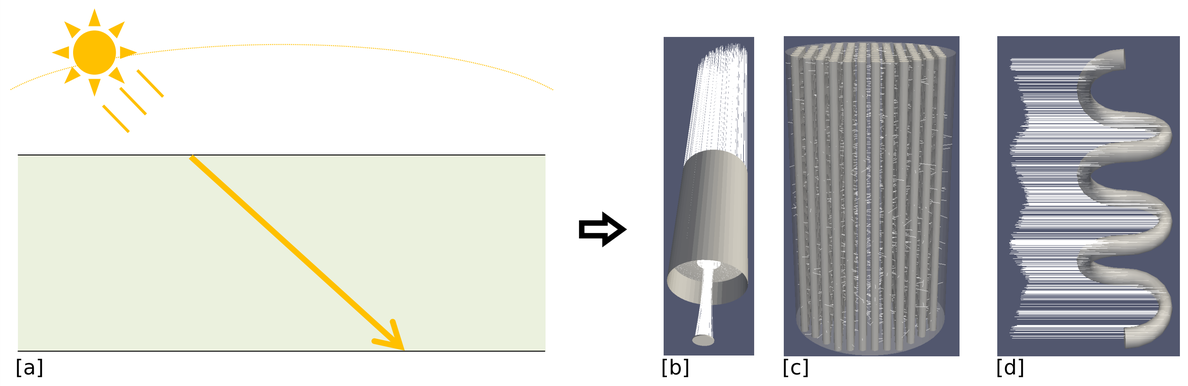


Figure 1: Development of algorithms in simple geometry and passage to complex geometry. [a] Reactor considered as a slab. [b] Ray tracing in a cassegrain telescope. [c] Ray tracing in a complex reactor with optical fibers. [d] Ray tracing on a microalgae with complex shape (*A. platensis*)

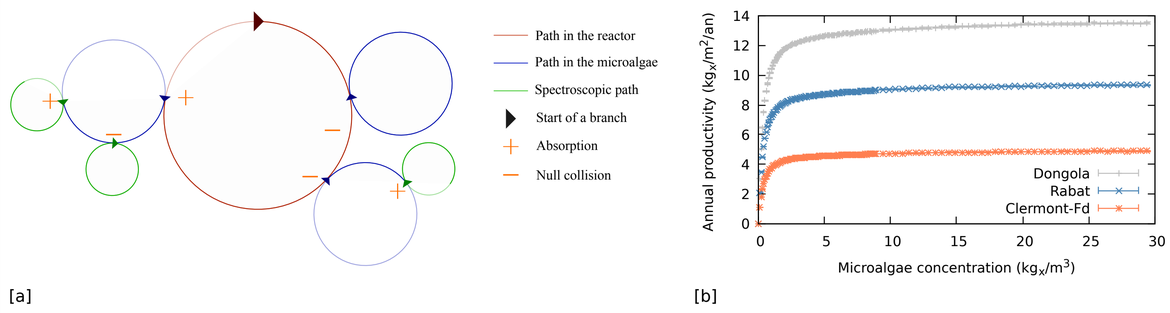


Figure 2: [a] A part of a MC realization (algorithm presented as a diagram). [b] Annual surface productivity according to the concentration of microalgae in Dongola, Rabat and Clermont-Fd (solar database www.meteonorm.com). The calculation of a point (10^7 samples on a Intel®Core™ i7-7820HQ CPU @ 2.90GHz) in complex geometry costs 1 minute.

Conclusion & perspectives

- The implementation of MC algorithms in complex geometry is conceptually simple and here validated
- MC method is a relevant and promising tool to tackle physical and engineering multi-scale problems
- Our kind of non-linear multi-scale model can be managed thanks to recent MC advances (null collision algorithm)

However, the management of non-linearities in any multi-scale model remains a bottleneck and requires further work.

References

[1] D. E. Keyes et al., *The International Journal of High Performance Computing Applications*, 27(1):483, February 2013.
[2] J. Delatorre et al., *Solar Energy*, 103:653681, May 2014.
[3] M. Galtier et al., *Journal of Quantitative Spectroscopy and Radiative Transfer*, 125:5768, August 2013.
[4] J. Dauchet et al., *Scientific Reports*, 8(1):13302, September 2018.

Acknowledgments

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