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 approach. These approaches are developed in the field of photo-reactive processes enabling to produce renewable third generation of biofuels or synthetic fuels (H2, CH4, Syngas, CH3OH) from solar energy. The example of a solar photobioreactor that produces Arthrospira platensis is presented here.

Multi-scale model

Biomass annual productivity < r_a > 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

\[ < r_a > = \int_{\Delta t}^{\Delta t} dt \rho_{\text{PA}}(t) \int_{\Delta t} d\lambda \rho_{\text{PA}}(\lambda) \int d^2 \lambda \int_{\lambda}^{\lambda_{\text{max}}} d k_{\lambda} e^{-\frac{\lambda}{\lambda_{\text{max}}}} P(\lambda) < V_{\lambda} > \]

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

\[ k_{\lambda} = C_\lambda \int d^2 \lambda \left( 1 - e^{-\sigma_{\lambda} \cdot \lambda_{\text{obs}}(\lambda)} \right) \]

- Refractive index given by the sum of pigments' contributions

\[ n = \sum p \sigma_{\lambda} \cdot C_p = \sum p \sigma_{\lambda} \cdot C_p \]

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

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)

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


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