SOLSTICE	Name of the PhD: **CHARON Julien** Title of the PhD thesis: **Evaluation of radiative properties with Monte Carlo method for the optimisation of solar processes** Dates (start/end): 01/10/2014 – 31/09/2017
Supervisors	CALIOT C. – PROMES, Font-Romeu Odeillo (Advisor) EL HAFI M. – RAPSODEE, Albi CORNET J.-F. – Institut Pascal, Clermont-Ferrand (Co-advisor) DAUCHET J. – Institut Pascal, Clermont-Ferrand
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Context and objectives

Retrieving radiative properties of non-spherical particles is a significant difficulty encountered in many fields of physics and engineering. In particular, an accurate knowledge of these radiative properties is a major stake for the development of industrial processes producing solar fuels from only water and CO_2, using natural or artificial photosynthesis. Indeed, the conception, sizing, optimization and control of efficient photo(bio)reactors can only be achieved if predictive knowledge models are built and validated, which requires, at low modelling-scale, the resolution of the problem of an electromagnetic wave scattered by arbitrary shaped catalytic particles (micro-algae or doped semiconductor).

Approach

One way to solve this problem is to use integral equations of the electromagnetic field deduced from Maxwell's equations. In this work, we investigate for the first time the use of the Monte Carlo method (MCM) to solve these integral formulations of electromagnetic scattering. We use the most recent advances in MCM, such as systematic sensitivity estimation, variance reduction and ray tracing in complex geometry.

Main results

Thanks to this original and innovative way to solve Maxwell's equations, our algorithms allow 1) direct simulation of any particle geometry given in a CAD format, 2) exact solution of high-dimensional integrals including distributions over particle's sizes, orientations and shapes, with efficient CPU time, 3) computation of sensitivities to parameters of interest for the optimisation of the process. The tools developed here allow estimating radiative properties of any particle with low refractive index contrast (*e.g.* micro-algae, Figure 1); the treatment of particles with higher refractive index remains a challenging perspective. Based on this PhD work, Meso-Star SAS has developed an open-source software called *Star-Schiff* solving Schiff's approximation, that is widely used in the field of photobioreaction engineering.

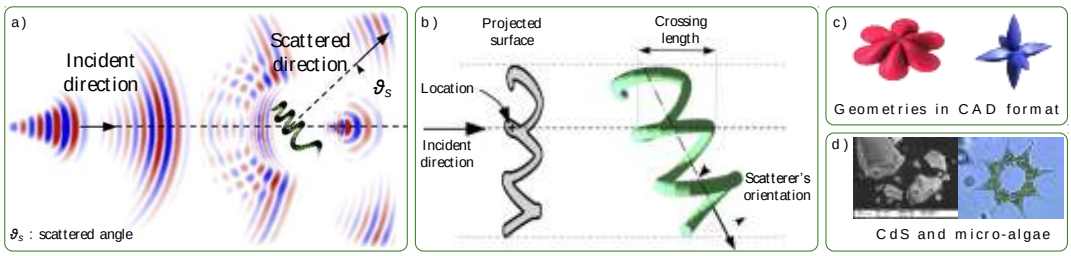

Figure 1: a) Illustration of the problem of an electromagnetic wave scattered by a micro-algae (*Spirulina*). b) Example of a Monte Carlo's algorithm: a location is sampled on the CAD projected surface and the crossing length is calculated before getting radiative properties. c) Geometries in CAD (Computer Aided Design) format. d) Example of semi-conductor catalyser used in artificial photosynthesis (CdS) and micro-organisms particles.

Publications in scientific journals

Charon J. and al, Monte Carlo implementation of Schiff's approximation for estimating radiative properties of homogeneous, simple-shaped and optically soft particles: applications to photosynthetic micro-organisms, *Journal of Quantitative Spectroscopy and Radiative Transfer,* 172 : 3-23, 2016.

Saleh H., Charon J., and al, Microwave analog experiments on optically soft spheroidal scatterers with weak electromagnetic signature, *Journal of Quantitative Spectroscopy and Radiative Transfer,* 196 : 1-9, 2017.

Weitz S. and al, Monte Carlo efficiency improvement by multiple sampling of conditioned integration variables, *Journal of Computational Physics*, 326 : 30-34, 2016

International conferences

EUROTHERM CTRPM-V – April 2015, Mines Albi, Albi, France: *Monte Carlo implementation of Schiff's approximation for the estimation of the radiative properties of photosynthetic micro-organisms.*

ELS-XVI (*Electromagnetic and Light Scattering*) – March 2017, Univ. of Maryland, College Park, United States: *A first investigation on solving integral equations of electromagnetic scattering with the Monte Carlo method: application to arbitrary shaped particles.*