KNOWLEDGE MODELS OF PHOTOBIOREACTORS AND THEIR PATH-INTEGRAL FORMULATION

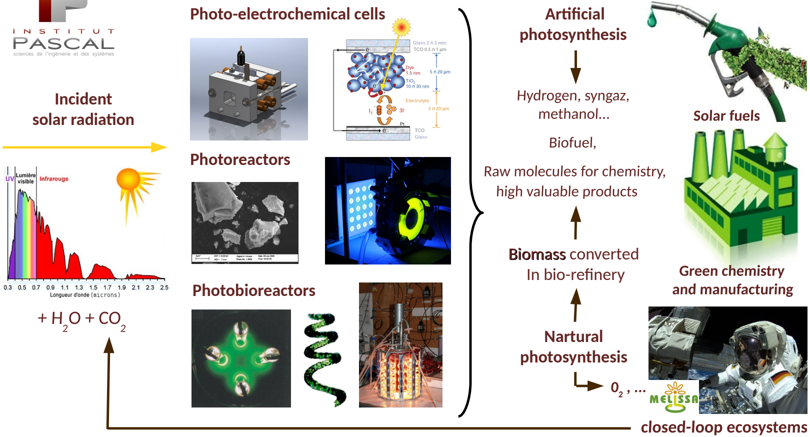
Jérémi DAUCHET, Jean-François CORNET, C.-Gilles DUSSAP,
Guillaume FOIN, Fabrice GROS, Céline LAROCHE, Laurent POUGHON,
Thomas VOURC'H, Daniel YAACOUB

MELISSA conference, 8-10/11 2022

Institut Pascal

GEPEB : génie des procédés, énergétique et biosystèmes

Photo-reactive Systems Engineering research group



Incident solar radiation

$+ H_2O + CO_2$

Photo-electrochemical cells

Photoreactors

Photobioreactors

Artificial photosynthesis

Hydrogen, syngaz, methanol...

Biofuel,

Raw molecules for chemistry, high valuable products

Biomass converted In bio-refinery

Nartural photosynthesis

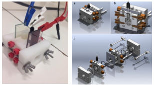
0_2 , ...

Solar fuels

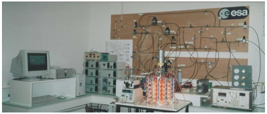
Green chemistry and manufacturing

closed-loop ecosystems

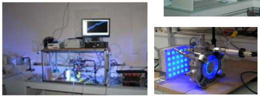
Methodology



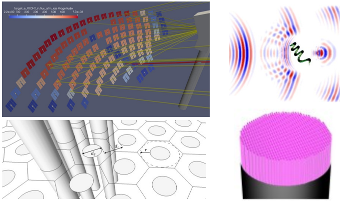
Photoelectrochemical cell

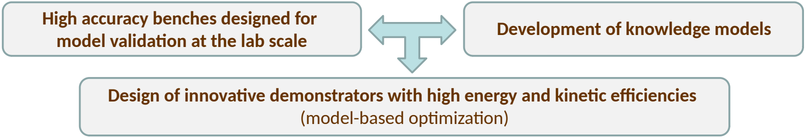


Photobioreactor



Photoreactor



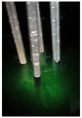


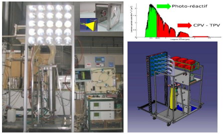
High accuracy benches designed for model validation at the lab scale

Development of knowledge models

Design of innovative demonstrators with high energy and kinetic efficiencies
(model-based optimization)

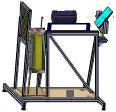
Dilution





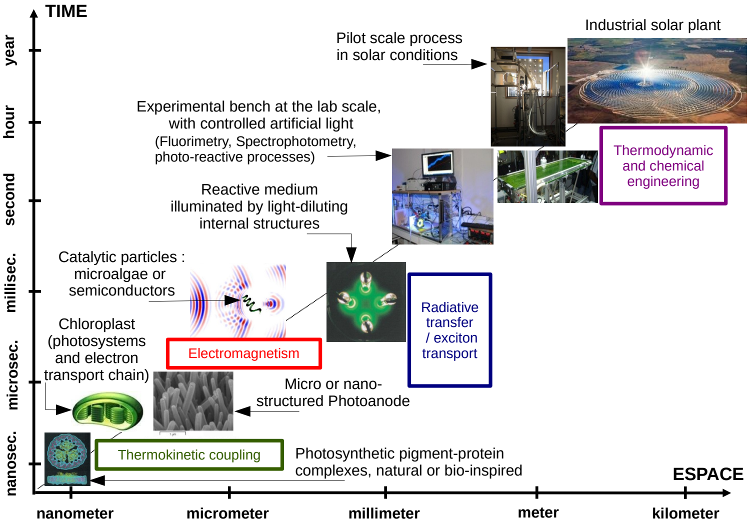
DiCoFluV – solar dilution photoreactor
(30 L - 1 m² - héliostat 2 m²)

Hybridization



DiCoFluV-Hy - hybrid solar reactor
(2 L - 0,03 m² - héliostat 0,1 m²)

Phenomenological, geometric and temporal complexity



Industrial solar plant

Pilot scale process in solar conditions

Experimental bench at the lab scale, with controlled artificial light (Fluorimetry, Spectrophotometry, photo-reactive processes)

Thermodynamic and chemical engineering

Reactive medium illuminated by light-diluting internal structures

Catalytic particles : microalgae or semiconductors

Radiative transfer / exciton transport

Electromagnetism

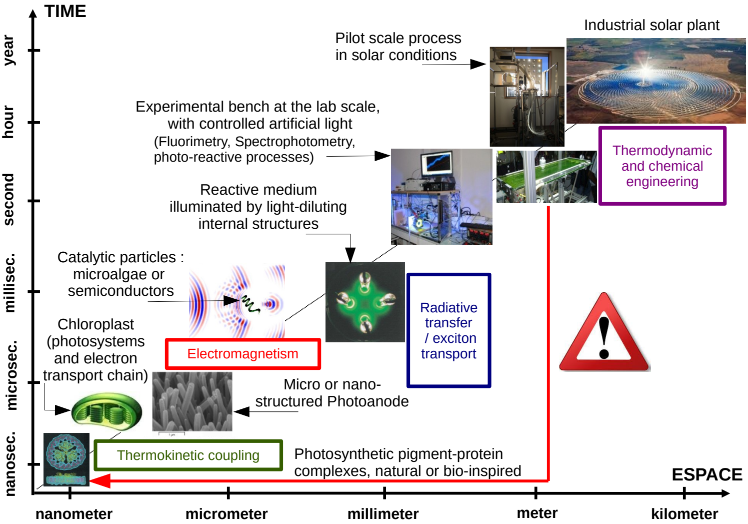
Chloroplast (photosystems and electron transport chain)

Micro or nano-structured Photoanode

Thermokinetic coupling

Photosynthetic pigment-protein complexes, natural or bio-inspired

Feedback loop on radiative properties



TIME

year

hour

second

millisec.

microsec.

nanosec.

Industrial solar plant

Pilot scale process
in solar conditions

Experimental bench at the lab scale,
with controlled artificial light
(Fluorimetry, Spectrophotometry,
photo-reactive processes)

Thermodynamic
and chemical
engineering

Reactive medium
illuminated by light-diluting
internal structures

Catalytic particles :
microalgae or
semiconductors

Radiative
transfer
/ exciton
transport

Chloroplast
(photosystems
and electron
transport chain)

Electromagnetism

Micro or nano-
structured Photoanode

Thermokinetic coupling

Photosynthetic pigment-protein
complexes, natural or bio-inspired

ESPACE

nanometer

micrometer

millimeter

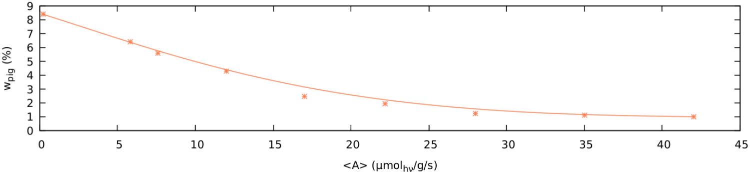
meter

kilometer

Feedback loop on radiative properties

- *via* pigment content

varies as a function of photon absorption rate



Experimental results from Arnaud ARTU, PhD at GEPEA (chlorella vulgaris)

- *via* micro-organism geometry

shape and size distribution vary as a function of mixing

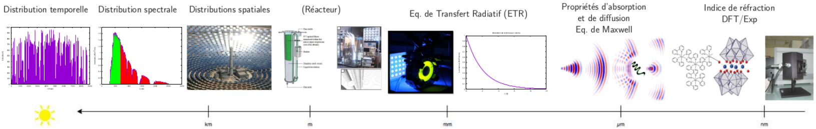
Size distribution,
fixed average aspect ratio

Optical microscopy

size and aspect ratio
distribution

Experimental results from Vincent Rochatte, PhD at Institut Pascal (Arthrospira platensis)

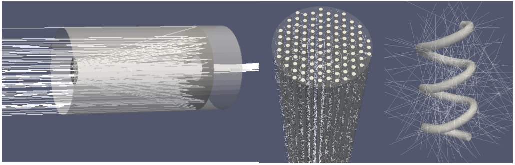
Extending Feynmann-Kac path integral formulation

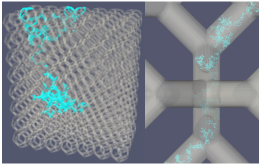


$$< \bar{r}_{O_2} >= \phi \int_{\Delta t} DNI(t)\, dt \int_{\Delta\nu} p_\nu(\nu)\, d\nu \int_V \frac{1}{V} dr\; r_{O_2} \left(r, \int_{\mathcal{D}_\Gamma} p_\Gamma(\gamma)\, d\gamma\; k_{a,\nu}\, e^{-C \int_{\mathcal{G}} p_{\mathcal{G}}(g)\, dg\; \sigma_{a,\nu} \left(\sum_n k_{s,n,\nu}\right) l(\gamma)} \right)$$

Renewed interpretation of the process:

1. highlighting the scales, phenomenon and their hierarchical coupling
2. bringing random walks that propagate in a multi-physics multi-scales path-space



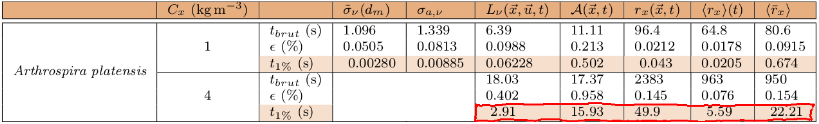


A research topic in the french consortium EDStar (www.edstar.cnrs.fr/prod/fr/):
recent advances to handle couplings, including nonlinearities

Monte Carlo method

Numerical simulations benefit from path-integral formulations:

- convergence rates is independent of the number of nested integrals
  → *phenomenological complexity*

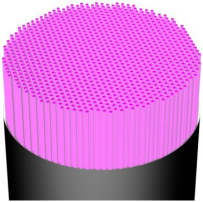


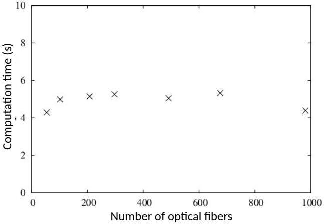
	C_x (kg m^{-3})		$\tilde{\sigma}_\nu(d_m)$	$\sigma_{a,\nu}$	$L_\nu(\vec{x},\vec{u},t)$	$\mathcal{A}(\vec{x},t)$	$r_x(\vec{x},t)$	$\langle r_x\rangle(t)$	$\langle \bar{r}_x\rangle$
Arthrospira platensis	1	t_{brut} (s)	1.096	1.339	6.39	11.11	96.4	64.8	80.6
		ϵ (%)	0.0505	0.0813	0.0988	0.213	0.0212	0.0178	0.0915
		$t_{1\%}$ (s)	0.00280	0.00885	0.06228	0.502	0.043	0.0205	0.674
	4	t_{brut} (s)			18.03	17.37	2383	963	950
		ϵ (%)			0.402	0.958	0.145	0.076	0.154
		$t_{1\%}$ (s)			2.91	15.93	49.9	5.59	22.21

Monte Carlo method

Numerical simulations benefit from path-integral formulations:

- convergence rates is independent of the number of nested integrals
  → *phenomenological complexity*
- computer graphics tools for orthogonal handling of the geometric data
  → *fast path-tracing insensitive to geometric complexity*





Monte Carlo method

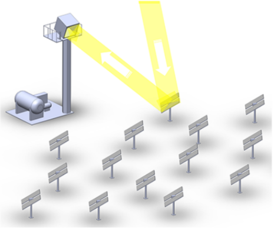
Numerical simulations benefit from path-integral formulations:

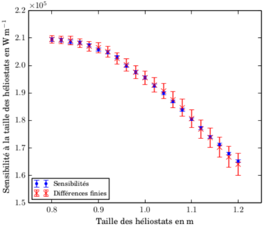
- convergence rates is independent of the number of nested integrals
  → *phenomenological complexity*
- computer graphics tools for orthogonal handling of the geometric data
  → *fast path-tracing insensitive to geometric complexity*
  → *inverse design*

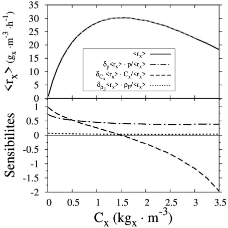
Monte Carlo method

Numerical simulations benefit from path-integral formulations:

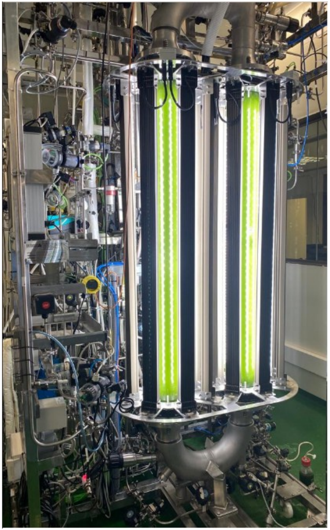
- convergence rates is independent of the number of nested integrals
  → *phenomenological complexity*
- computer graphics tools for orthogonal handling of the geometric data
  → *fast path-tracing insensitive to geometric complexity*
  → *inverse design*
- sensitivity analysis
  → *guides optimization*



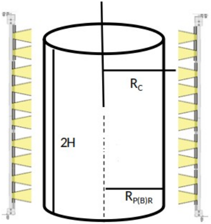


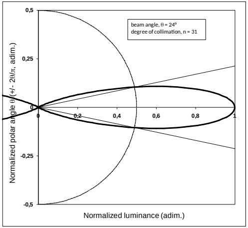


UAB photobioreactor configuration

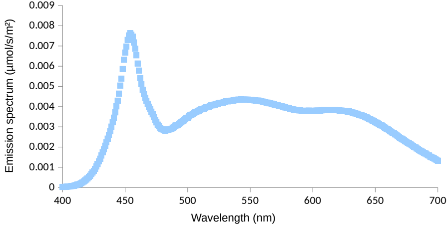


Cylindrical photobioreactor





Radial illumination by 8 panels made of 80 white LEDs + optics θ = 24°

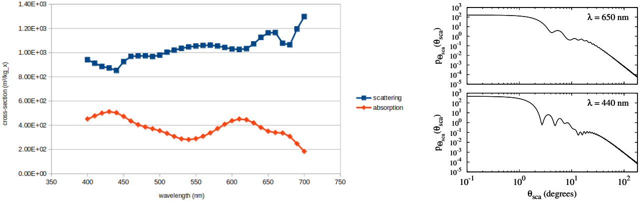


A focus on radiative transfer and thermokinetic coupling

- Radiative transfer equation

$$\boldsymbol{\omega}\cdot\mathrm{grad}_x L_\lambda(x,\boldsymbol{\omega}) = -C_x\,(\sigma_{a,\lambda}+\sigma_{s,\lambda})L_\nu(x,\boldsymbol{\omega}) + C_x\,\sigma_{s,\lambda}\int_{4\pi} L_\lambda(x,\boldsymbol{\omega}')\,p_{\Omega,\lambda}(\boldsymbol{\omega}|\boldsymbol{\omega}')d\omega'$$

- Radiative properties (schiff: www.meso-star.com/projects/schiff/schiff.html)



Arthrospira platensis: cross-sections $\sigma_{a,\lambda}$ *and* $\sigma_{s,\lambda}$

phase function $p_{\Omega,\lambda}(\boldsymbol{\omega}|\boldsymbol{\omega}')$

Hybrid model and experimental results from Vincent Rochatte, PhD at Institut Pascal

- Thermokinetic coupling law at each point x

$$r_{\mathrm{O}_2}(x) = Cx\,\Phi\,\rho_m\,\frac{K}{K+\mathcal{A}(x)}\mathcal{A}(x) \quad ; \quad \mathcal{A}(x) = \sigma_{a,\lambda}\int_{4\pi} L_\lambda(x,\boldsymbol{\omega})d\omega$$

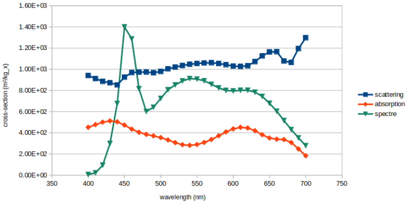
- Volume averages: $<\mathcal{A}>$ and $<r_{\mathrm{O}_2}>$

Two-flux approximation for radiative transfer

- Grey approximation

$$\bar{\sigma}_i = \int_{\lambda_{min}}^{\lambda_{max}} f_{source}(\lambda)\,\sigma_{i,\lambda}\,d\lambda$$

$$\bar{p}_\Omega = \int_{\lambda_{min}}^{\lambda_{max}} \frac{f_{source}(\lambda)\,\sigma_{s,\lambda}}{\bar{\sigma}_s}\,p_{\Omega,\lambda}\,d\lambda$$



- Two-flux approximation for 1d cylindrical systems

$$\mathcal{A}(x) = 2\bar{\sigma}_a\,q_0\,\frac{\mathcal{I}_0(\delta\,r)}{\mathcal{I}_0(\delta\,R) + \alpha\,\mathcal{I}_1(\delta\,R)}$$

with $\mathcal{I}$ the Bessel functions, q_0 the incident flux density,
$\delta = C_x\sqrt{\bar{\sigma}_a(\bar{\sigma}_a + 2b\bar{\sigma}_s)}$, $\alpha = \sqrt{\frac{\bar{\sigma}_a}{\bar{\sigma}_a + 2b\bar{\sigma}_s}}$, $b = \int_{2\pi^-} p_{\Omega,\lambda}(\boldsymbol{\omega}|\boldsymbol{\omega}')d\boldsymbol{\omega}$

Can be implemented in spreadsheets and programmable logic controllers

Results

$Cx = 0.05\,g/l$	Ref. (1% err.)	2-flux	diff.	max
$<\mathcal{A}>$ $(\mu mol/s/m^3)$	43550	34944	20%	46667
$<r_{O_2}>$ $(mol/l/h)$	$4.39\cdot 10^{-4}$	$4.35\cdot 10^{-4}$	1%	$19\cdot 10^{-4}$

$Cx = 0.10\,g/l$	Ref. (1% err.)	2-flux	diff.	max
$<\mathcal{A}>$ $(\mu mol/s/m^3)$	46200	42522	8%	46667
$<r_{O_2}>$ $(mol/l/h)$	$8.45\cdot 10^{-4}$	$8.30\cdot 10^{-4}$	2%	$19\cdot 10^{-4}$

$Cx = 0.20\,g/l$	Ref. (1% err.)	2-flux	diff.	max
$<\mathcal{A}>$ $(\mu mol/s/m^3)$	46450	42630	8%	46667
$<r_{O_2}>$ $(mol/l/h)$	$13.9\cdot 10^{-4}$	$13.6\cdot 10^{-4}$	2%	$19\cdot 10^{-4}$

Results

$Cx = 0.05\, g/l$	Ref. (1% err.)	2-flux	diff.	max
$< \mathcal{A} > (\mu mol/s/m^3)$	43550	34944	20%	46667
$< r_{\mathrm{O}_2} > (mol/l/h)$	$4.39 \cdot 10^{-4}$	$4.35 \cdot 10^{-4}$	1%	$19 \cdot 10^{-4}$

$Cx = 0.10\, g/l$	Ref. (1% err.)	2-flux	diff.	max
$< \mathcal{A} > (\mu mol/s/m^3)$	46200	42522	8%	46667
$< r_{\mathrm{O}_2} > (mol/l/h)$	$8.45 \cdot 10^{-4}$	$8.30 \cdot 10^{-4}$	2%	$19 \cdot 10^{-4}$

$Cx = 0.20\, g/l$	Ref. (1% err.)	2-flux	diff.	max
$< \mathcal{A} > (\mu mol/s/m^3)$	46450	42630	8%	46667
$< r_{\mathrm{O}_2} > (mol/l/h)$	$13.9 \cdot 10^{-4}$	$13.6 \cdot 10^{-4}$	2%	$19 \cdot 10^{-4}$

Results

$Cx = 0.05\, g/l$	Ref. (1% err.)	2-flux	diff.	max
$< \mathcal{A} > (\mu mol/s/m^3)$	43550	34944	20%	46667
$< r_{O_2} > (mol/l/h)$	$4.39 \cdot 10^{-4}$	$4.35 \cdot 10^{-4}$	1%	$19 \cdot 10^{-4}$

$Cx = 0.10\, g/l$	Ref. (1% err.)	2-flux	diff.	max
$< \mathcal{A} > (\mu mol/s/m^3)$	46200	42522	8%	46667
$< r_{O_2} > (mol/l/h)$	$8.45 \cdot 10^{-4}$	$8.30 \cdot 10^{-4}$	2%	$19 \cdot 10^{-4}$

$Cx = 0.20\, g/l$	Ref. (1% err.)	2-flux	diff.	max
$< \mathcal{A} > (\mu mol/s/m^3)$	46450	42630	8%	46667
$< r_{O_2} > (mol/l/h)$	$13.9 \cdot 10^{-4}$	$13.6 \cdot 10^{-4}$	2%	$19 \cdot 10^{-4}$

Results

With radiative properties for *Arthrospira platensis* in different culture conditions
(reference model solved with Monte Carlo; 1% err.)

$Cx = 0.05\, g/l$	C1 (Rochatte)	C2 (Dauchet)	diff.	max
$<\mathcal{A}>$ ($\mu mol/s/m^3$)	43550	18136	58%	46667
$<r_{\mathrm{O}_2}>$ ($mol/l/h$)	$4.39{\cdot}10^{-4}$	$4.25{\cdot}10^{-4}$	3%	$19{\cdot}10^{-4}$

$Cx = 0.10\, g/l$	C1 (Rochatte)	C2 (Dauchet)	diff.	max
$<\mathcal{A}>$ ($\mu mol/s/m^3$)	46200	38100	18%	46667
$<r_{\mathrm{O}_2}>$ ($mol/l/h$)	$8.45{\cdot}10^{-4}$	$8.27{\cdot}10^{-4}$	1%	$19{\cdot}10^{-4}$

Conclusions & Perspectives

- **Radiative properties are variable**
  - illumination → pigment content
  - mixing → size and shape of the micro-organisms
- **The grey approximation accuracy depends on radiative properties**
  - cyanobacteria have "almost grey" spectral properties
  - use caution if spectral variations are sharp
    - eukaryotes (*e.g.chlamydomonas reinhardtii*)
    - photosensitizers for artificial photosynthesis (100% error)
- **Simplification of the system geometry is not always possible**
  - high energetic performance requires internal illumination (NPGC ESA project) leading to complex geometries
- **Two-flux approximation**, in our test case
  - can lead to 50% error on radiative transfer
  - but 2% error on $< r_{O_2} >$ for cyanobacteria (no respiration)

Thank you for your attention

PAVIN platform: a 3,5 m^2 heliostat reflects sunilght into concentration/dilution structures within a 50 m^2 lab housing prototypes (TRL 3-5). Daily experimentation outside on smaller prototypes.