Comparison of Monte Carlo methods efficiency to solve radiative energy transfer in high-fidelity unsteady 3D simulations

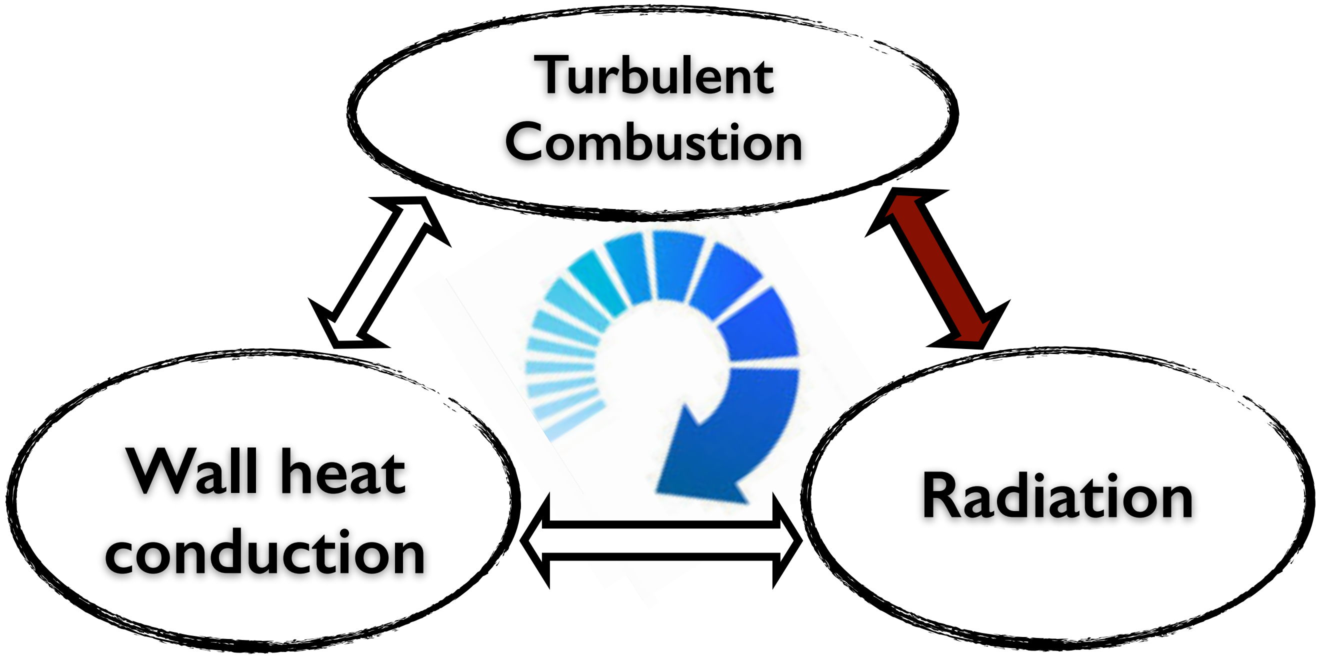
Lorella Palluotto, Nicolas Dumont, Pedro Rodrigues, Chaï Koren,
Ronan Vicquelin, Olivier Gicquel

22nd November 2017

Context: High-fidelity multi physics simulations(1/3)

Multiphysics: Combustion, conduction and radiation

Accurate prediction of wall heat transfer coupling turbulent reactive flows with radiation and conduction heat transfer.



Turbulent Combustion

Wall heat conduction

Radiation

Radiation

Turbulent combustion

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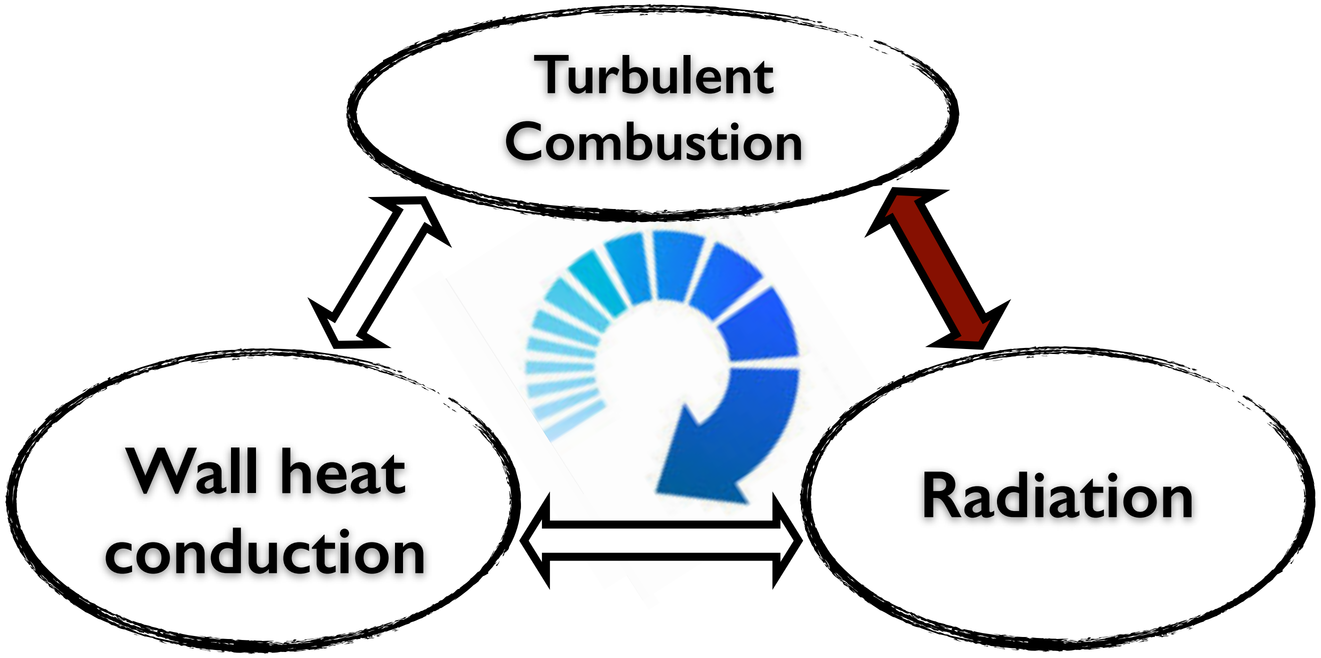

Radiation

- Ray tracing
- Monte Carlo
- DOM
- P1/Optically Thin

Turbulent combustion

- DNS
- LES
- RANS

Accuracy ↑ CPU cost

Combustion-radiation simulations:

time ↓

RANS + DOM:
Coelho et al. Combustion and Flame 2003

RANS + MC:
Tessé et al. Intl. J. Heat Mass Transfer 2004
Whang et al. JQSRT 2008
Mehta et al. Computational Thermal Sciences 2009

LES/DNS + DOM:
Amaya et al. JQSRT 2010
Poitou et al. Combustion an flame 2012
Berger et al. Applied Thermal Engineering 2016

LES/DNS + MC:
Zhang et al. Journal of Fluid Mechanics 2014
Koren et al. ASME TurboExpo 2017
Rodrigues et al. ICNC 2017

Context: High-fidelity multi physics simulations(2/3)

Possible approaches for coupled combustion-radiation simulations

Radiation ↔ **Turbulent Combustion**

For as accurate as possible coupled simulations:

Accuracy ↑ CPU cost

Ray tracing

Monte Carlo

DOM

P1/Optically Thin

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Unaffordable for industrial configurations

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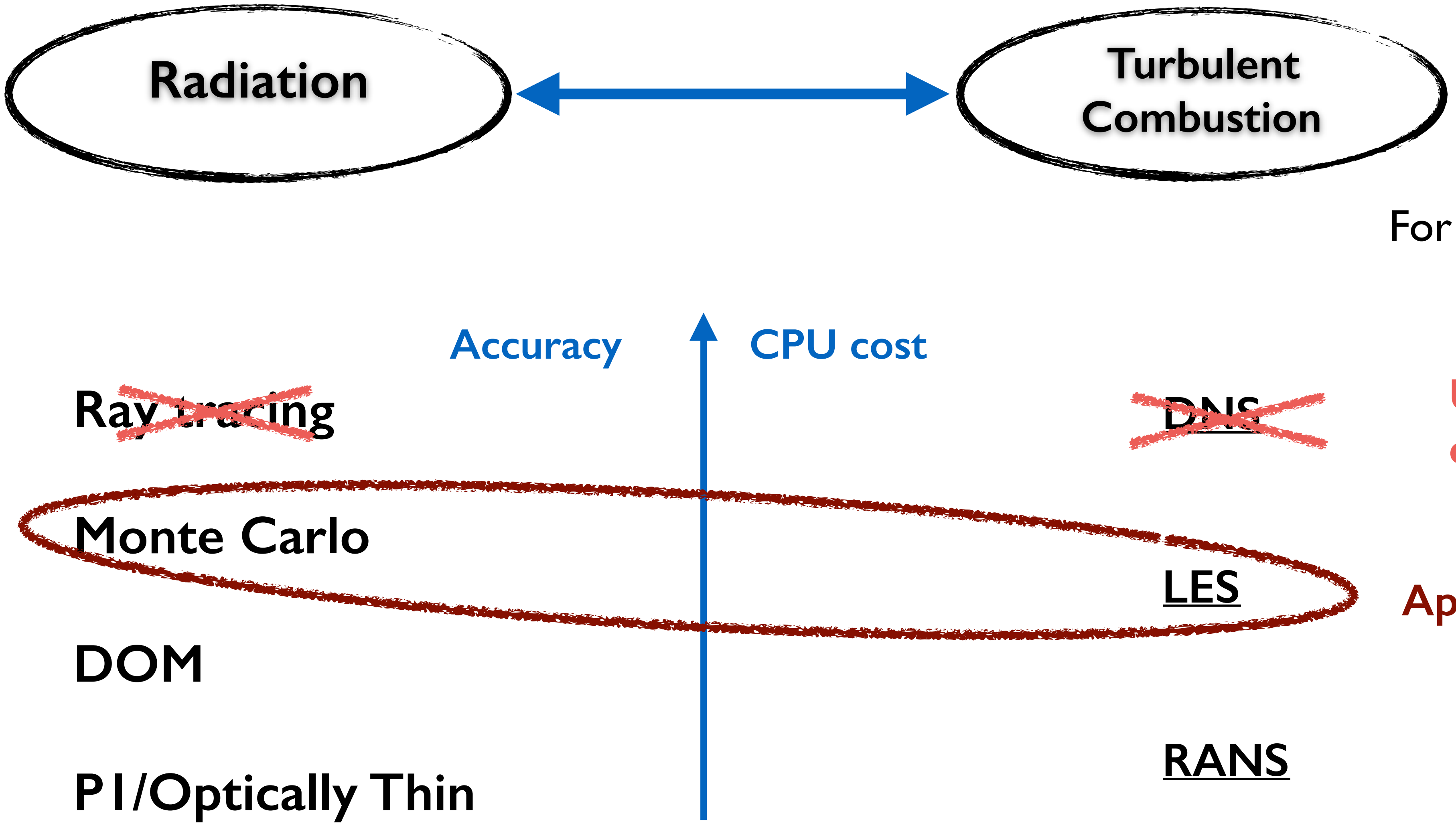

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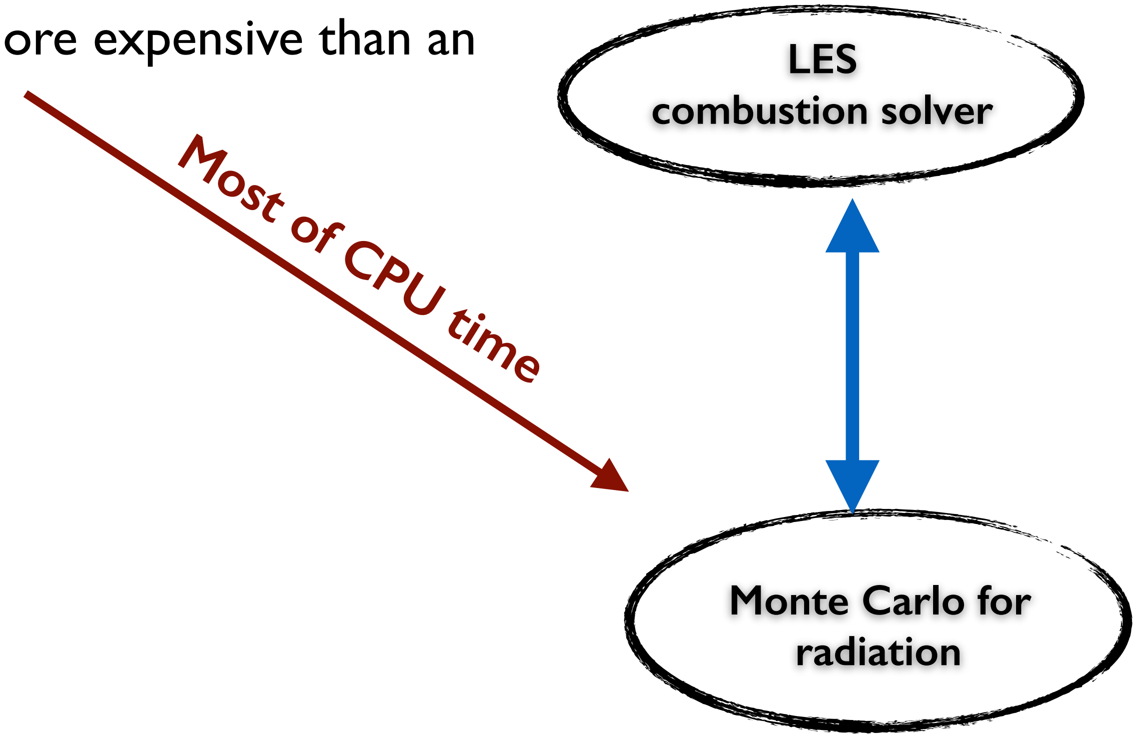
Approaches used in this study

Context: High-fidelity multi physics simulations(3/3)

High-fidelity multi-physics simulations: challenge

High computational cost:

Coupled radiation-combustion simulation **10 times** more expensive than an only-combustion simulation



LES combustion solver

Most of CPU time

Monte Carlo for radiation

Context: High-fidelity multi physics simulations(3/3)

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Orders of magnitude

Coupled simulation of an industrial combustion chamber

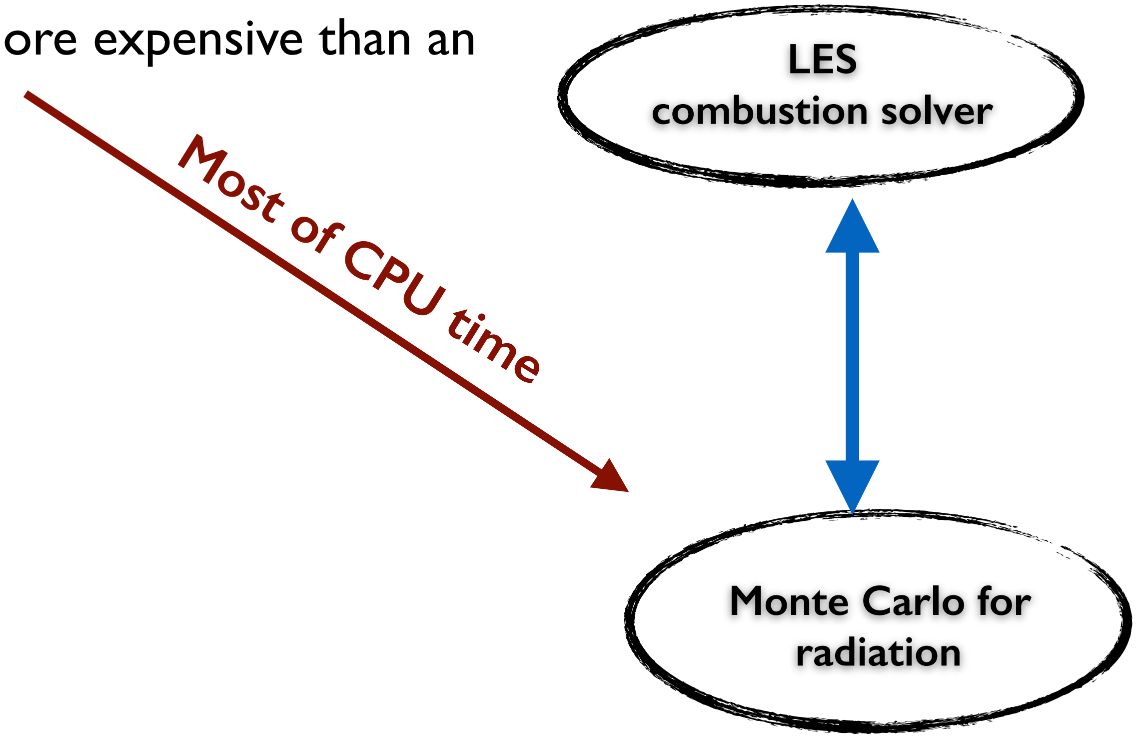
1x10^6 CPUh

Time

- *Serial computation :* 100 years
- *Parallel computation :* 4 days with 10000 cores

Money

Cost : 30000 - 40000 €



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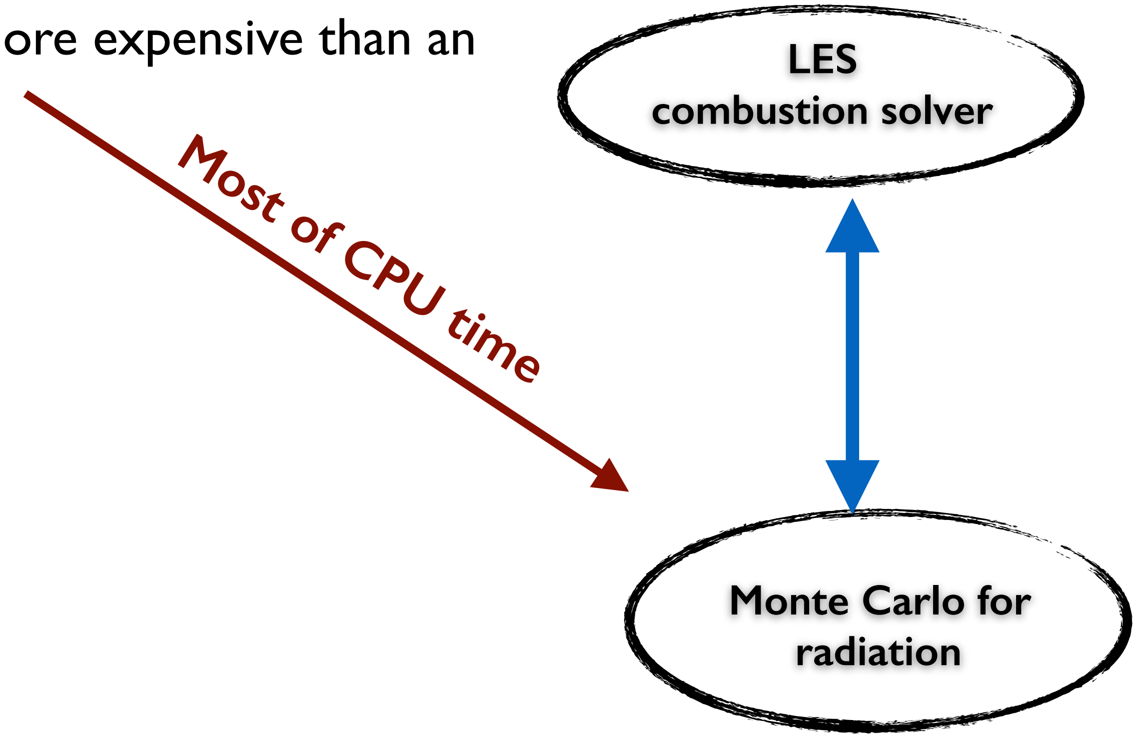
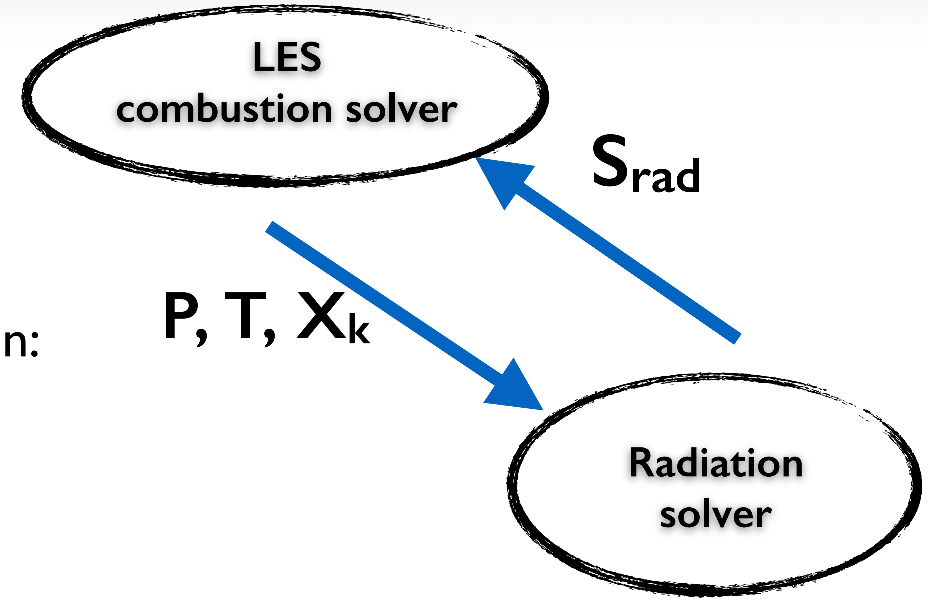


Importance of CPU time reduction! → **Derive more efficient MC methods**

Radiative heat transfer simulations

Set-up

Rainier (code developed at EM2C laboratory)



Data exchanged by the solvers

- Parallel Monte Carlo radiation code to solve the Radiative Transfer Equation:

$$\frac{\partial I_\nu(\mathbf{u}(s),s)}{\partial s} + \kappa_\nu I_\nu(\mathbf{u}(s),s) = \kappa_\nu I_\nu^o(T)$$

Numerical Set-up

- Non-scattering medium
- Radiative properties model: C-K model for gas[1][2] → Narrow band models

Accuracy ↑ CPU cost

Line by Line calculations

Narrow band models

Global models

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[1] R. Goody, R. West, L. Chen, D. Crisp, *J. Quant. Spectrosc. Radiat. Transfer* 42 (1989)

[2] A.Soufiani, J. Taine. *International journal of heat and mass transfer 40.4* (1997)

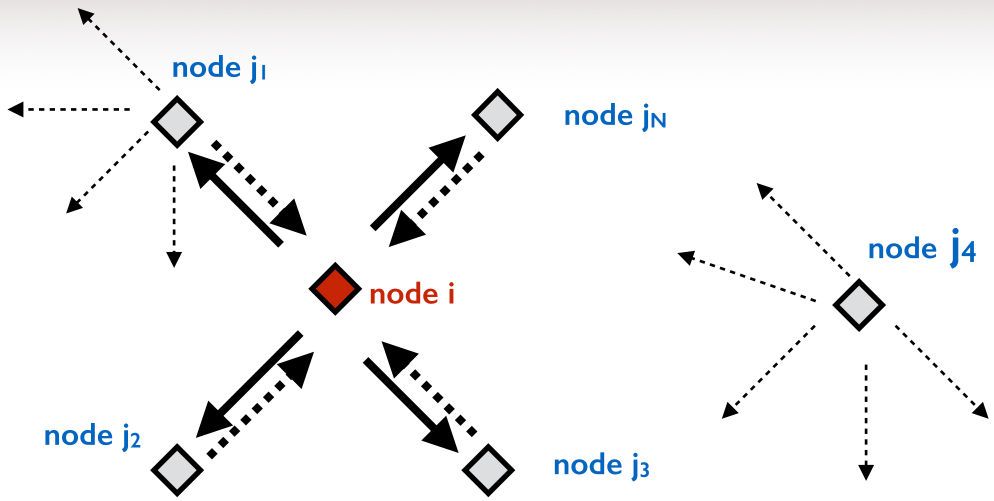
Outline

- Two strategies are investigated in order to reduce the MC error:
  - Importance sampling
  - Quasi-Monte Carlo methods

Existing Monte Carlo method for radiation

Optimized[1] Emission-based Reciprocity Method[2] (OERM)

- Rays followed in a **reverse** direction: from detector to source



Scheme of photons bundles departing from the nodes of the domain

- Reciprocity principle respected for every path

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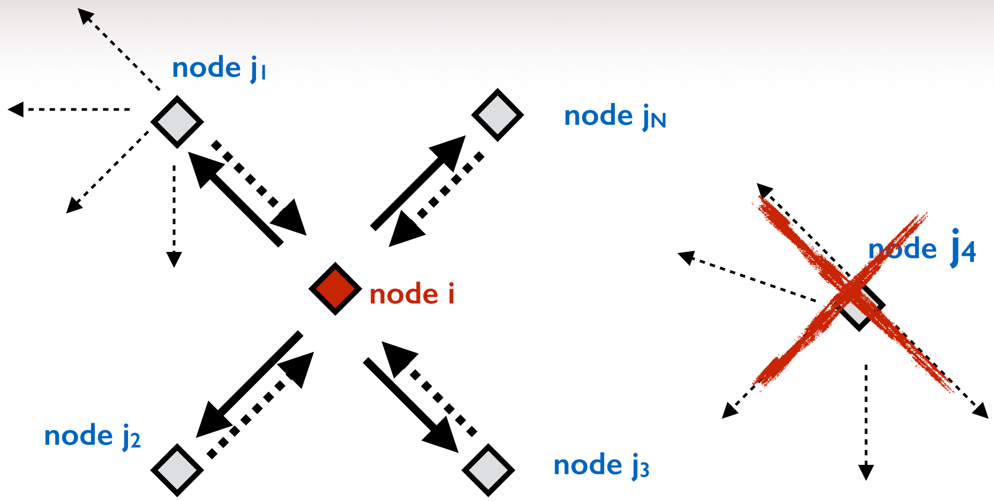

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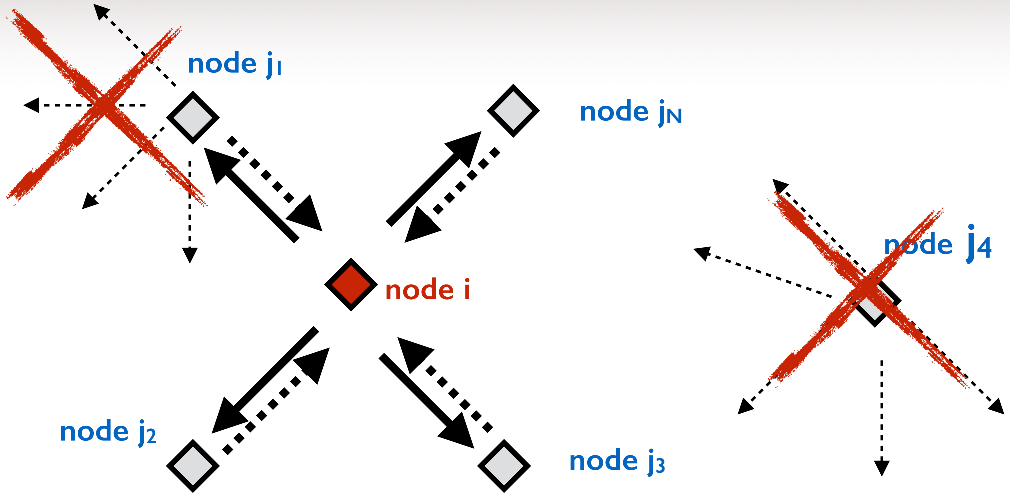

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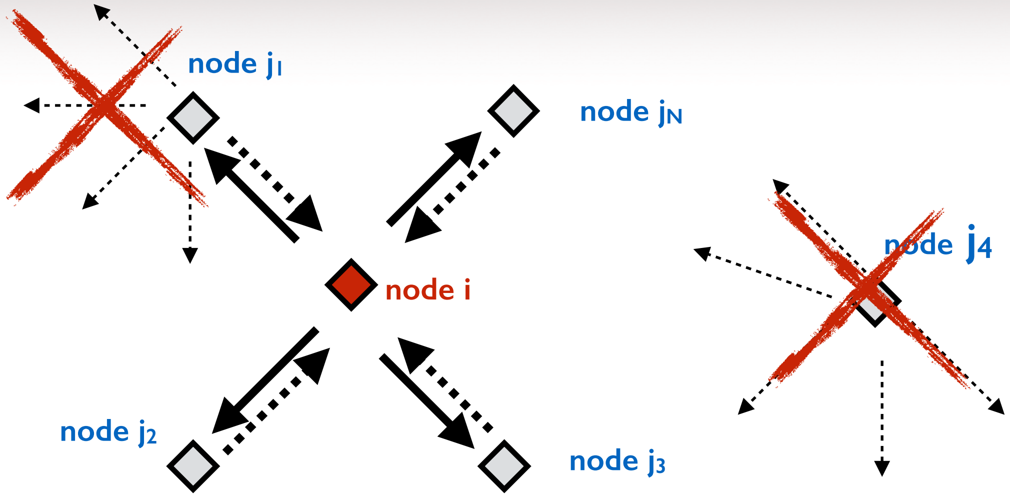

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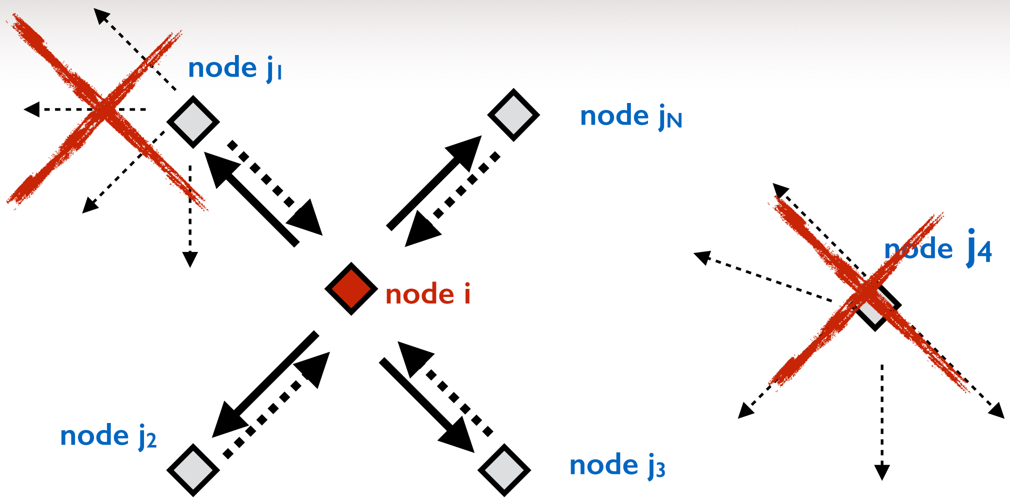
Possibility to control the local convergence

High scalability



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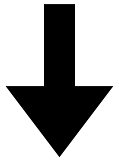

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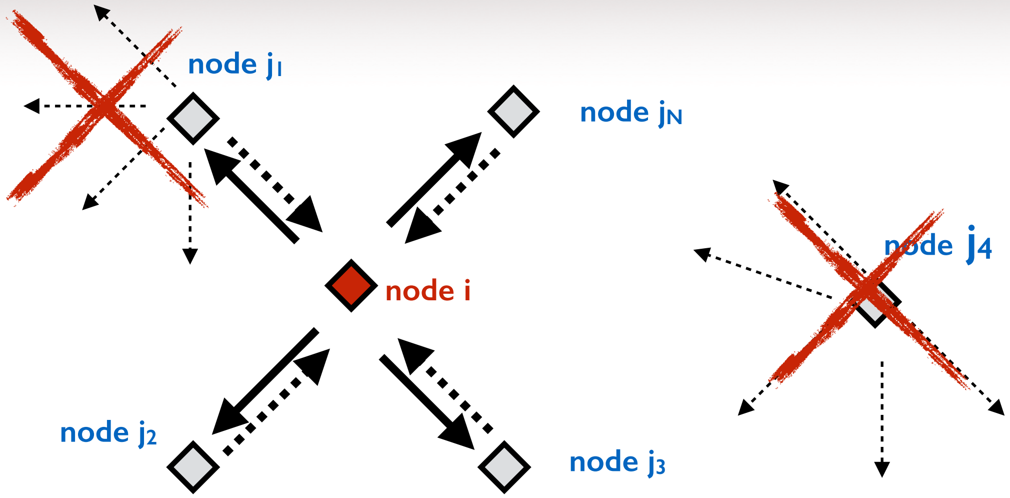

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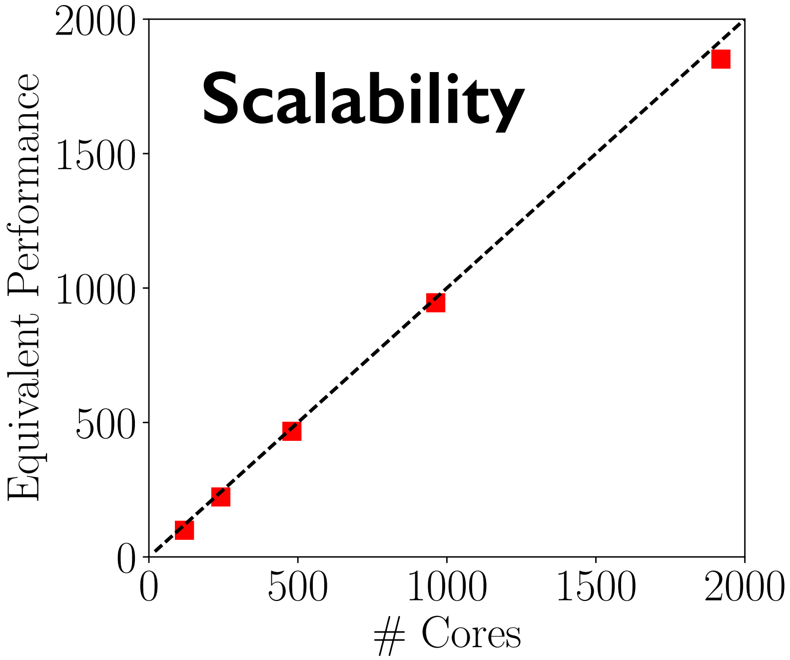

Scalability test performed on 8 millions cells

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Importance sampling

Monte Carlo OERM

IMPORTANCE SAMPLING: One of variance reduction methods to accelerate MC convergence

Monte Carlo error $\epsilon \approx \frac{\sigma}{\sqrt{N}}$

One way to reduce the MC error: reduce σ

How? Sampling in the most important regions of the integration domain

Widely studied topic [1,2,3]

[1] Feldick, A. M., Modest M.F. 2011. AIAA

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Frequency distribution function based on emission at the maximum temperature of the system

$$f_\nu(\nu, T_{max}) = \frac{\kappa_\nu(T_{max}) I^\circ_\nu(T_{max})}{\int_0^{+\infty} \kappa_\nu(T_{max}) I^\circ_\nu(T_{max}) d\nu}$$

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ERM:
frequency distribution function
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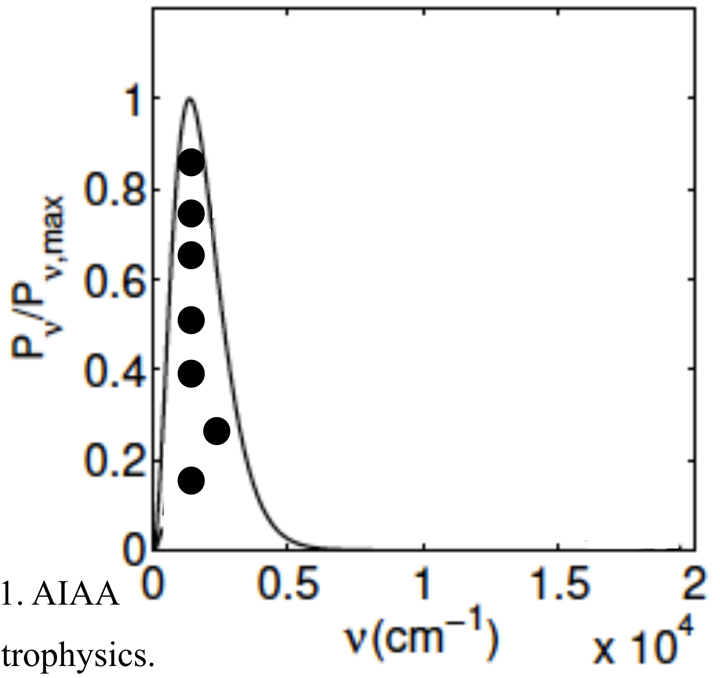

Normalized spectral emitted (—) and absorbed (- - -) power for a cell of 900 K [4]

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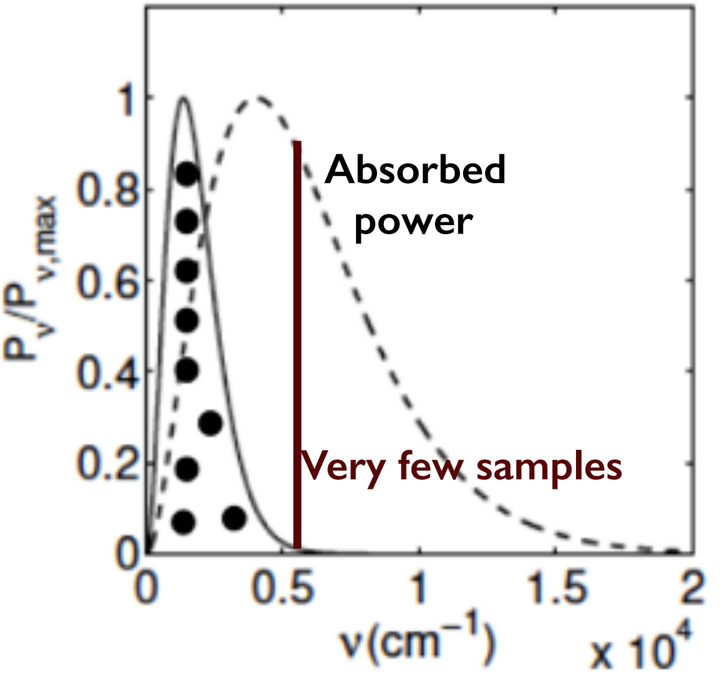

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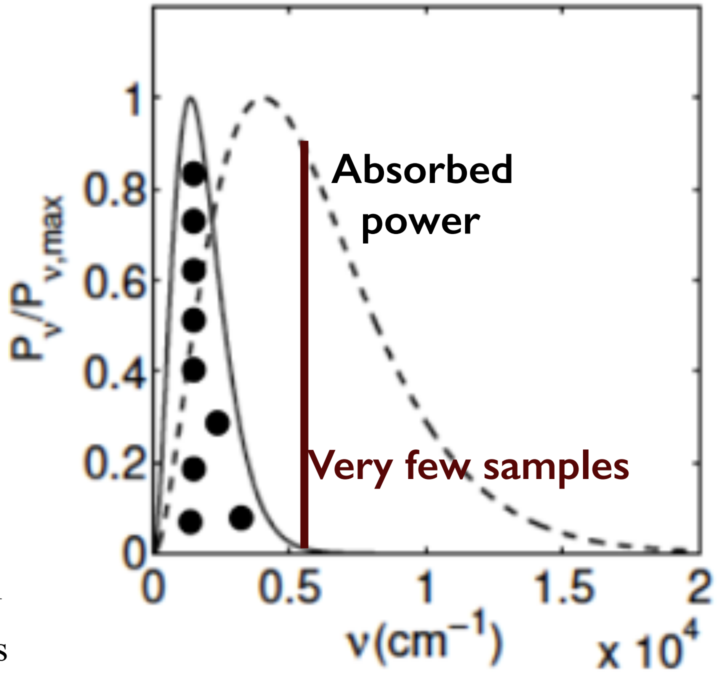
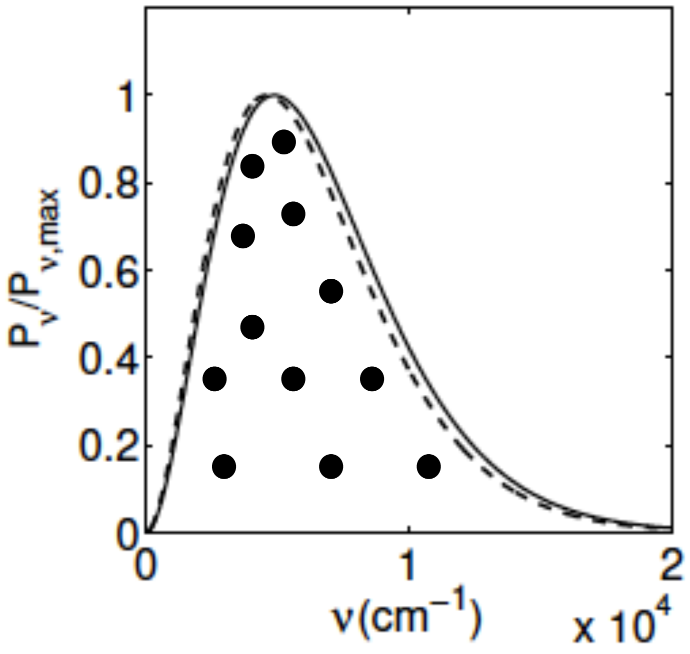


Absorbed power

Very few samples



OERM:
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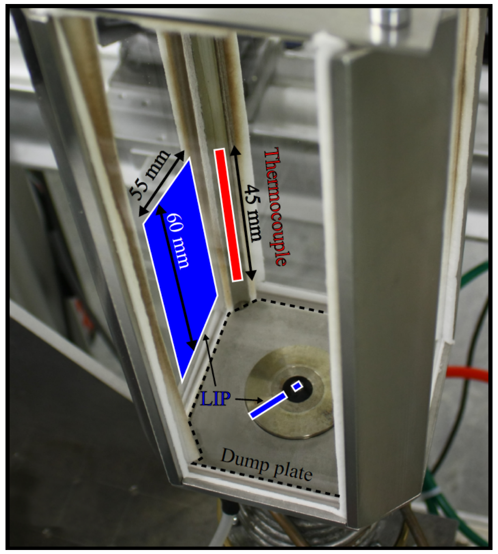
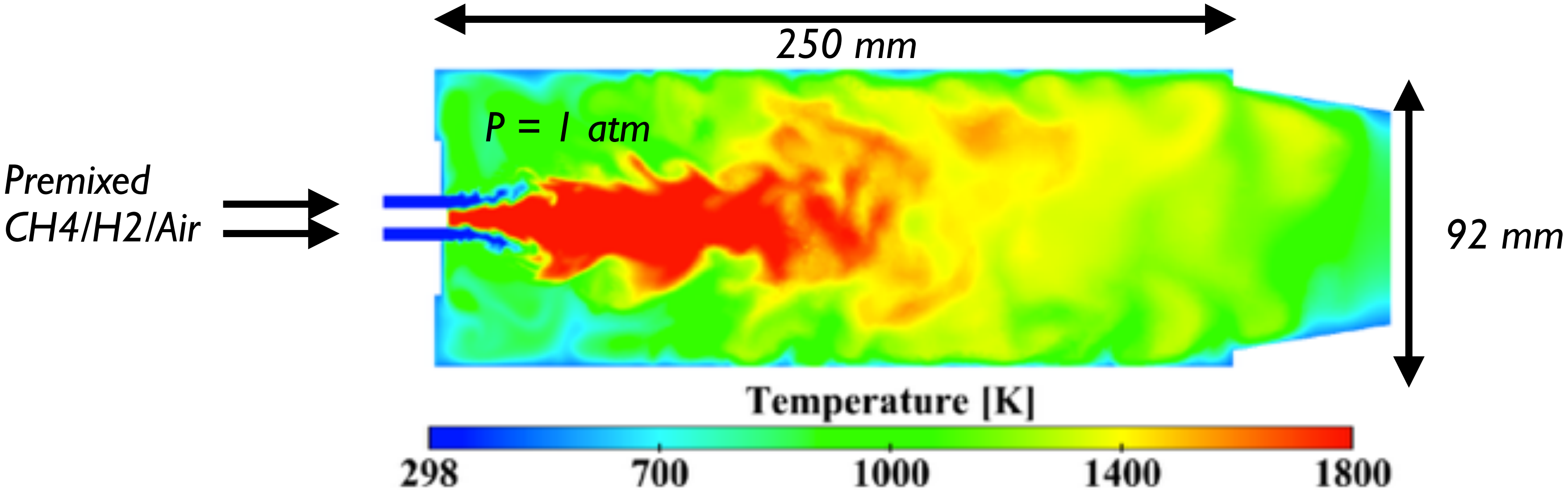
Application: combustion chamber

Premixed swirled flame of CH4 H2 and air

Semi-industrial burner[1]





Instantaneous snapshots of unsteady 3D LES [2]

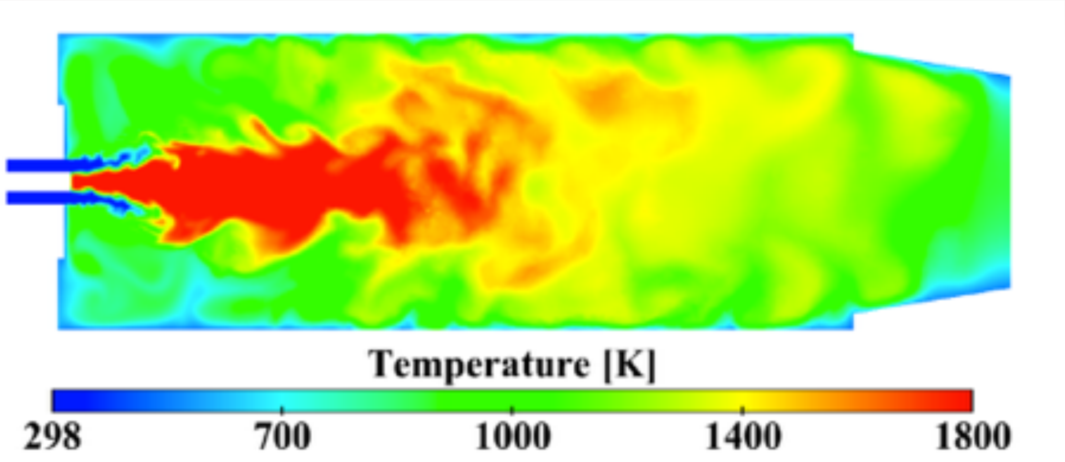
Combustion → **Radiation**

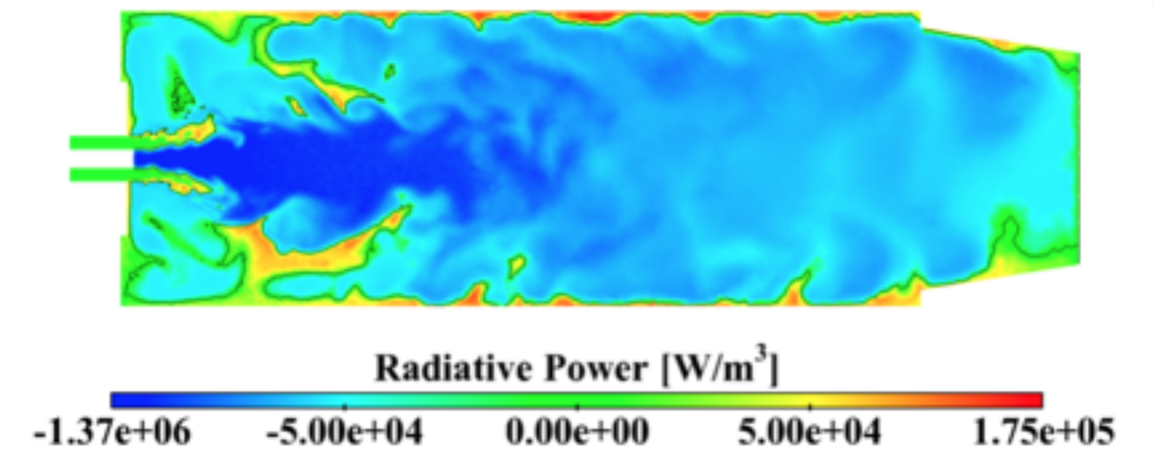
[1] Guiberti, T. (2015, February). Analysis of the topology of premixed swirl-stabilized confined flames. Theses, Ecole Centrale Paris.

[2] Koren, C., Vicquelin, R., and Gicquel, O., 2017. “Highfidelity multiphysics simulation of a confined premixed swirling flame combining large-eddy simulation, wall heat conduction and radiative energy transfer”. ASME Turbo EXPO 2017.

Application: combustion chamber

Radiative heat transfer simulations

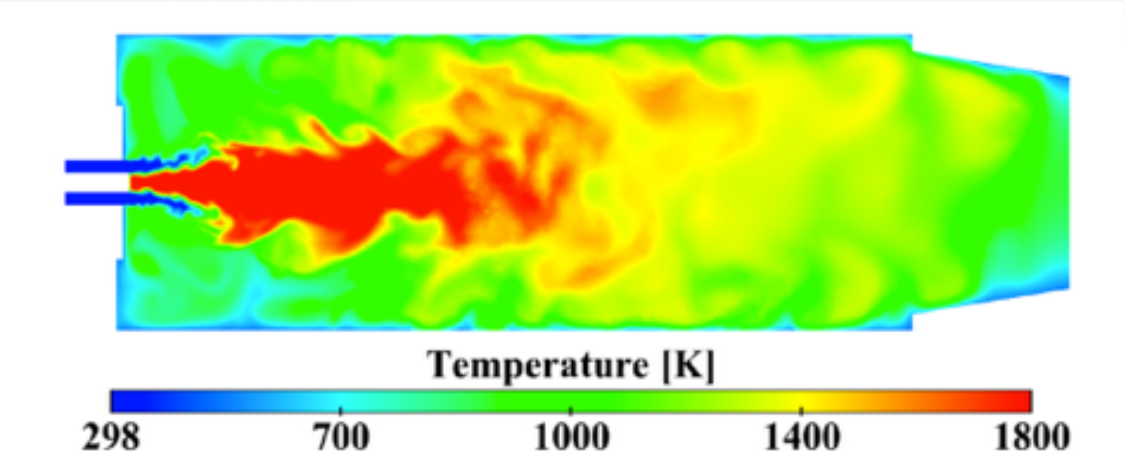


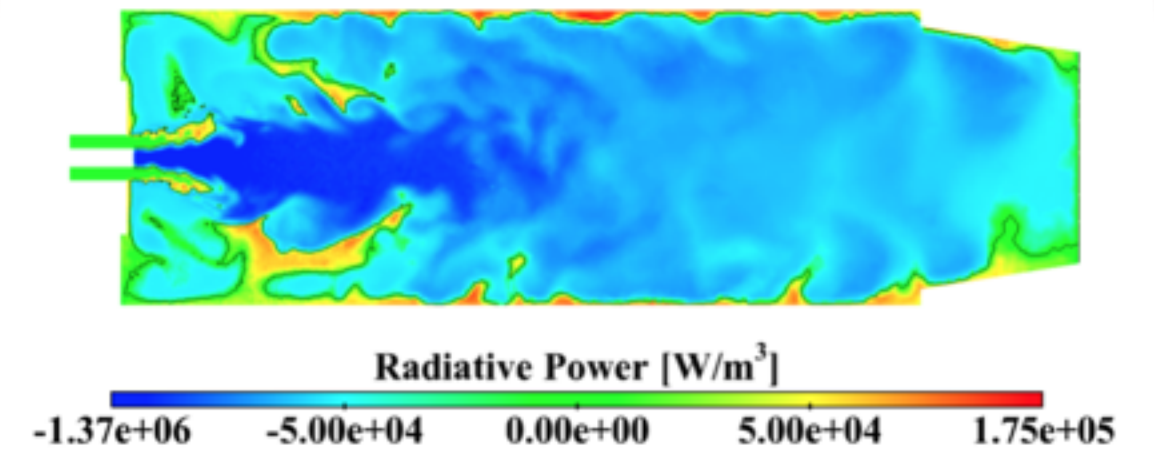


Instantaneous field of radiative power. Black line is the iso-contour for radiative power = 0.

Application: combustion chamber

Radiative heat transfer simulations

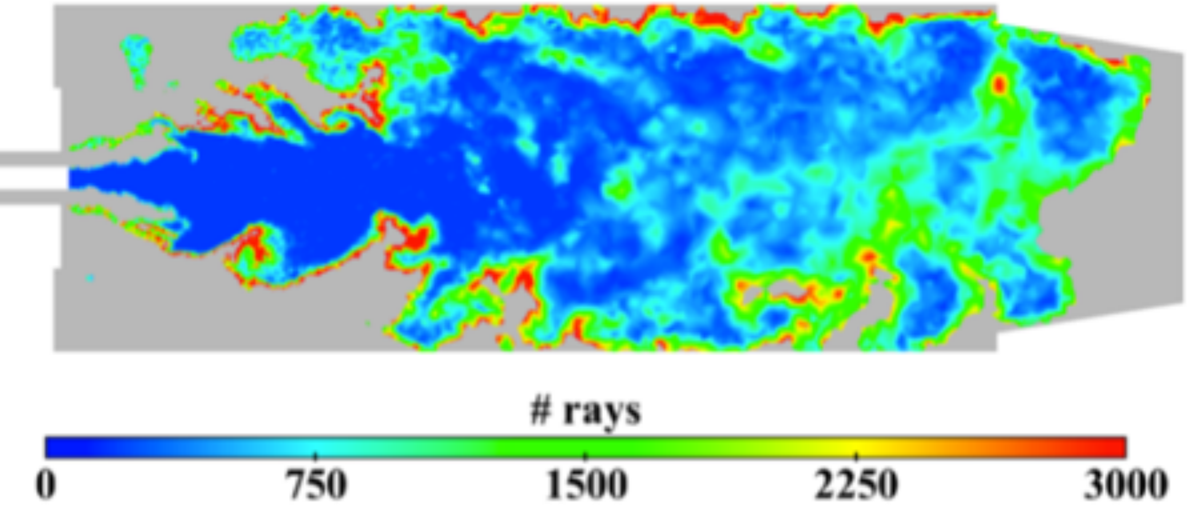




Instantaneous field of radiative power. Black line is the iso-contour for radiative power = 0.

Imposed convergence criteria:

- Relative error = 3%
- Absolute error = 3% of Pmax



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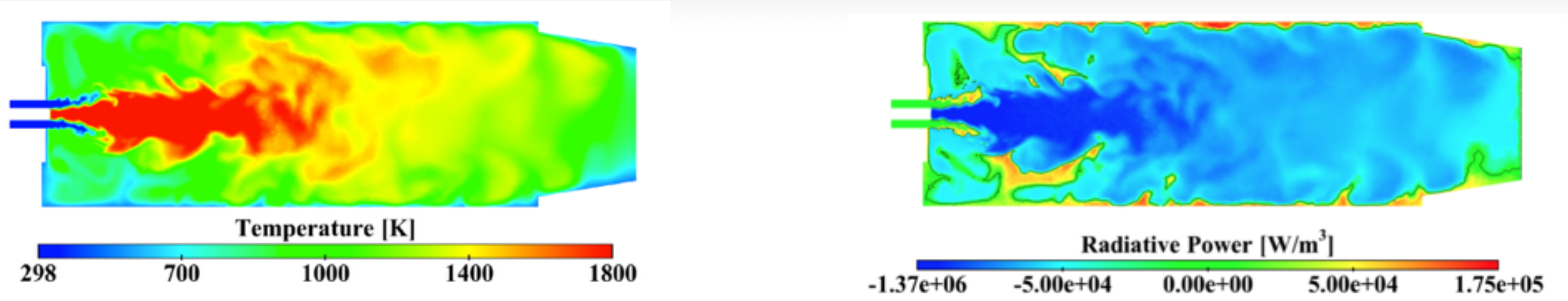

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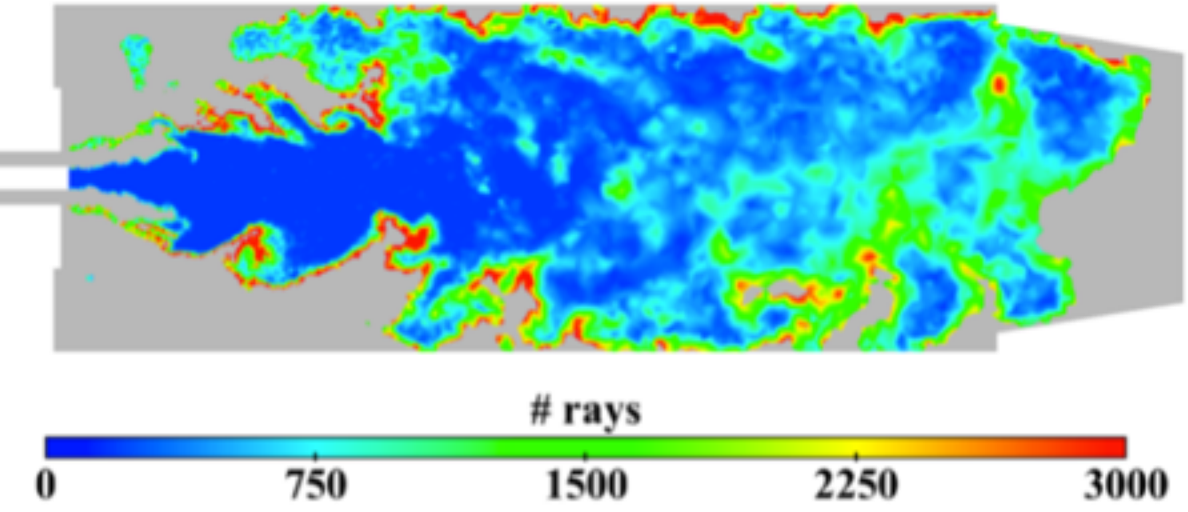
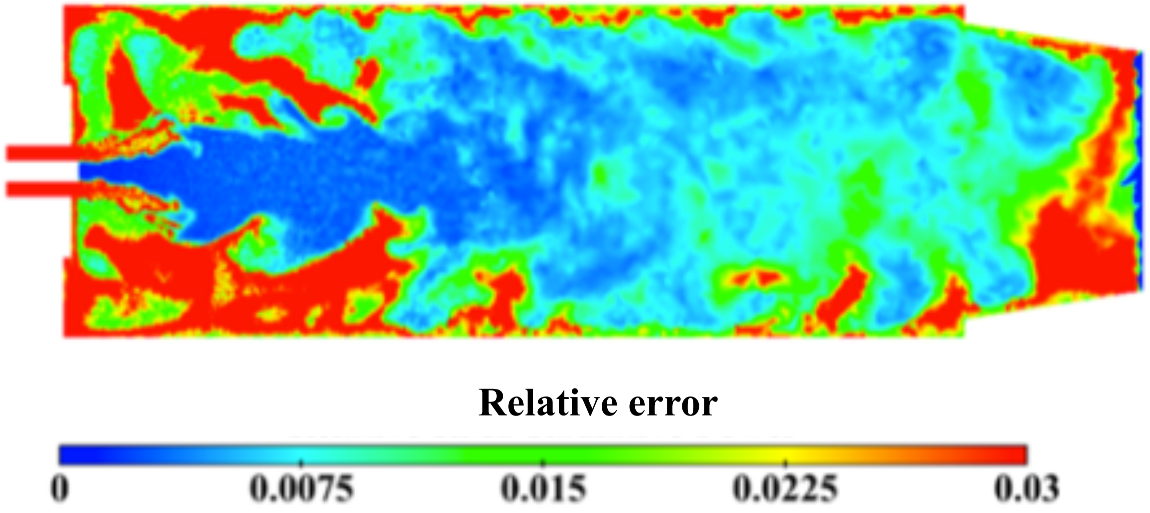


Computations with a fixed rays number

Rays number : 10 000



Outline

- **Two strategies are investigated in order to reduce the MC error:**
  - Importance sampling
  - **Quasi-Monte Carlo methods**

Quasi Monte Carlo methods

To reduce the MC error:

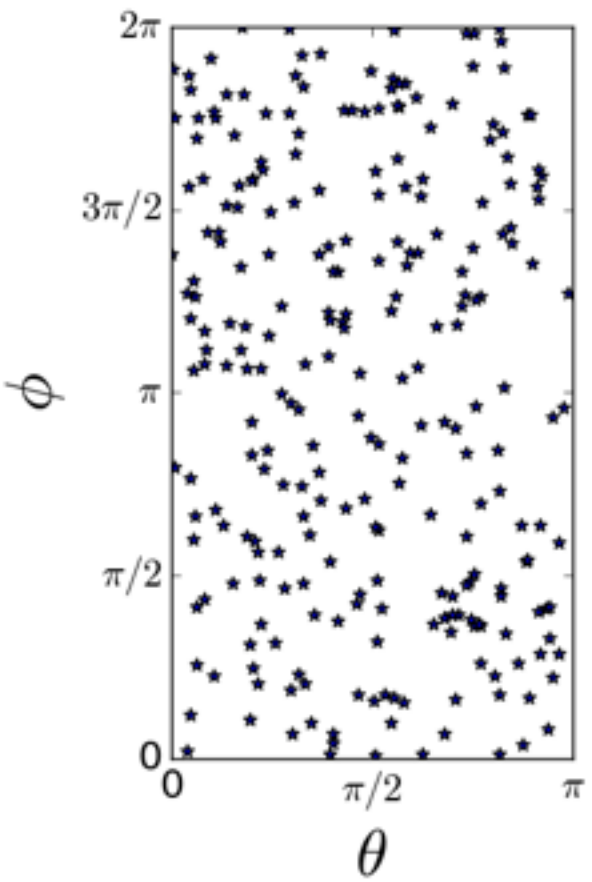
Alternative sampling method

[1] Joe, S., and Kuo, F. Y., 2008. “Constructing Sobol sequences with better two-dimensional projections”. SIAM Journal on Scientific Computing

Quasi Monte Carlo methods

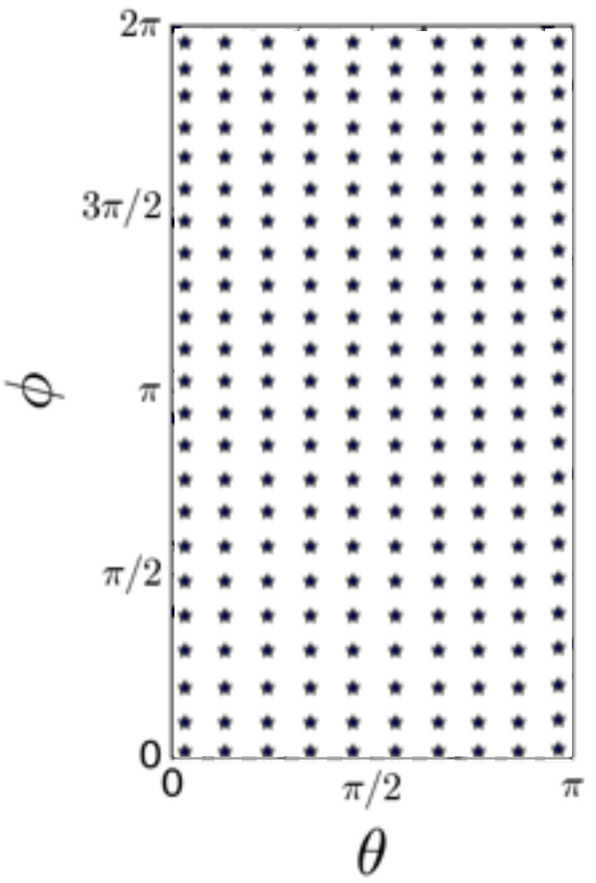
To reduce the MC error:

Alternative sampling method



Random sampling

MC



Deterministic discretization

(Unfeasible in high-D)

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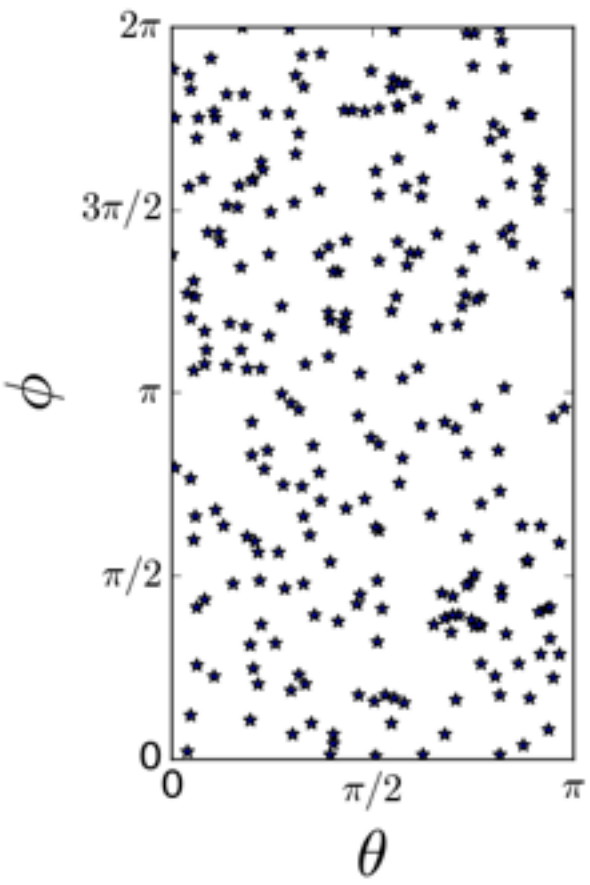

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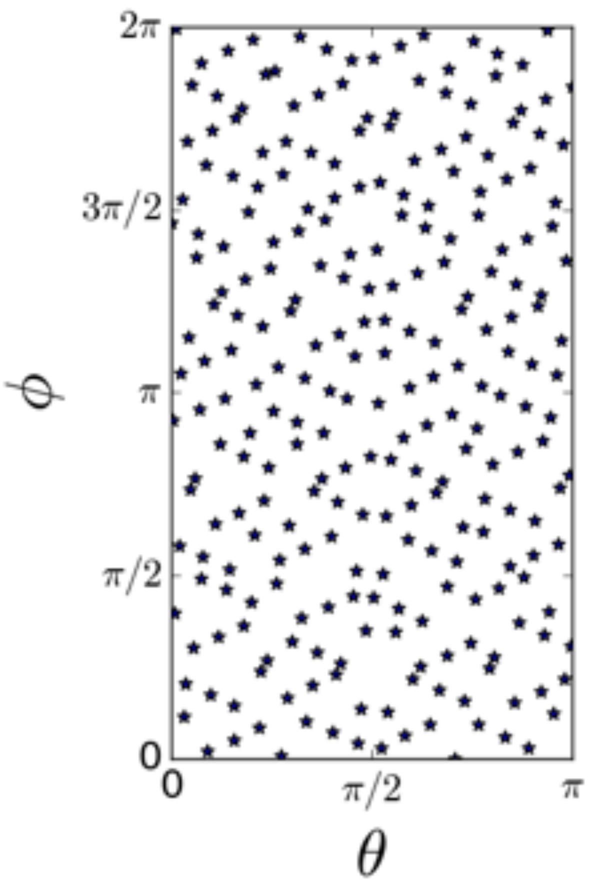

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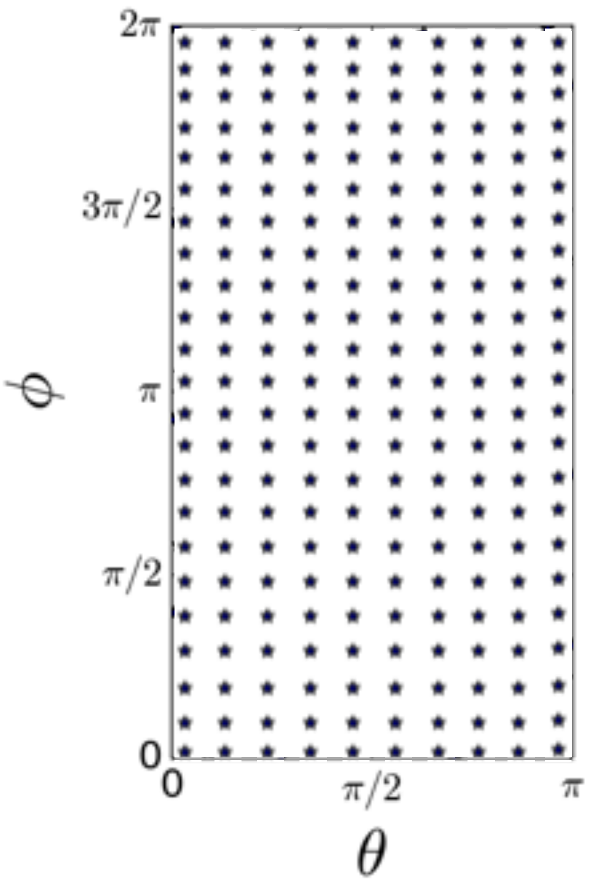

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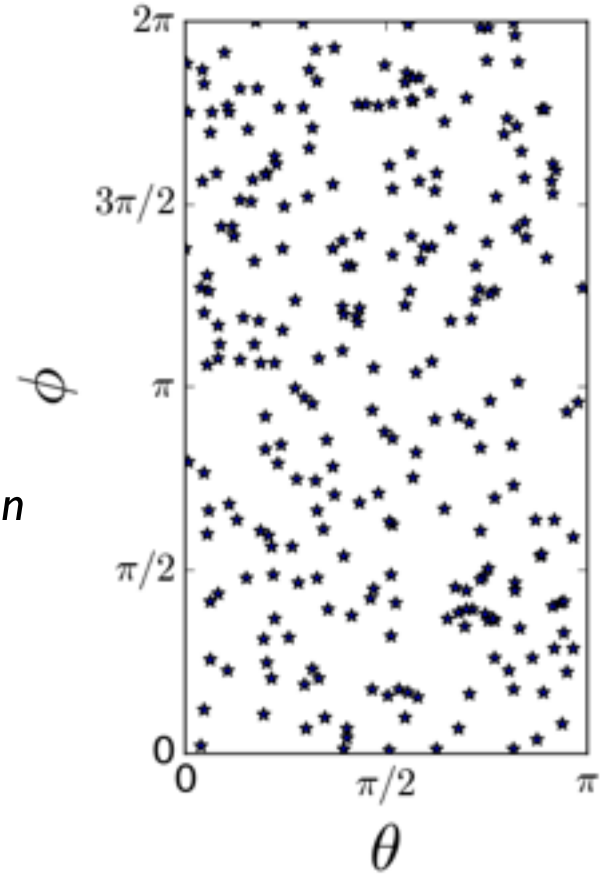

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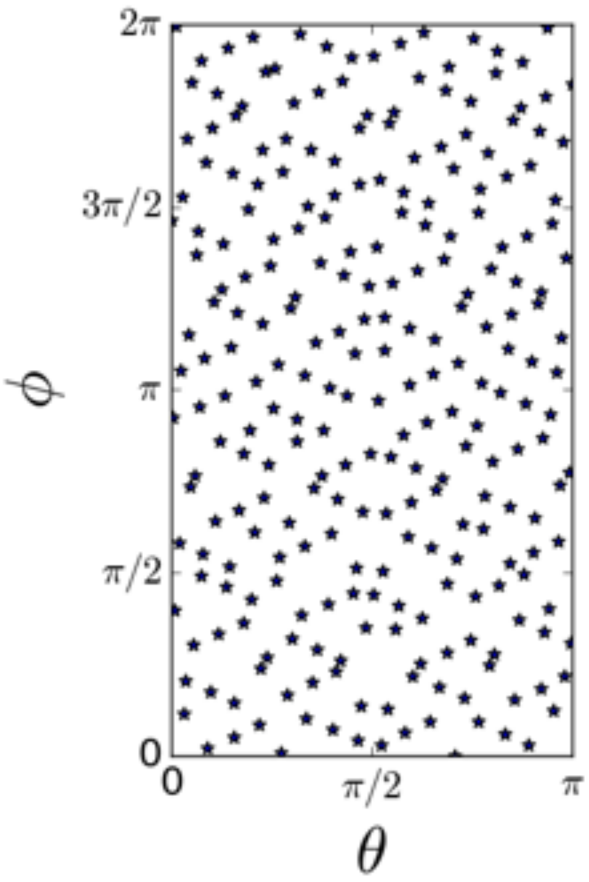

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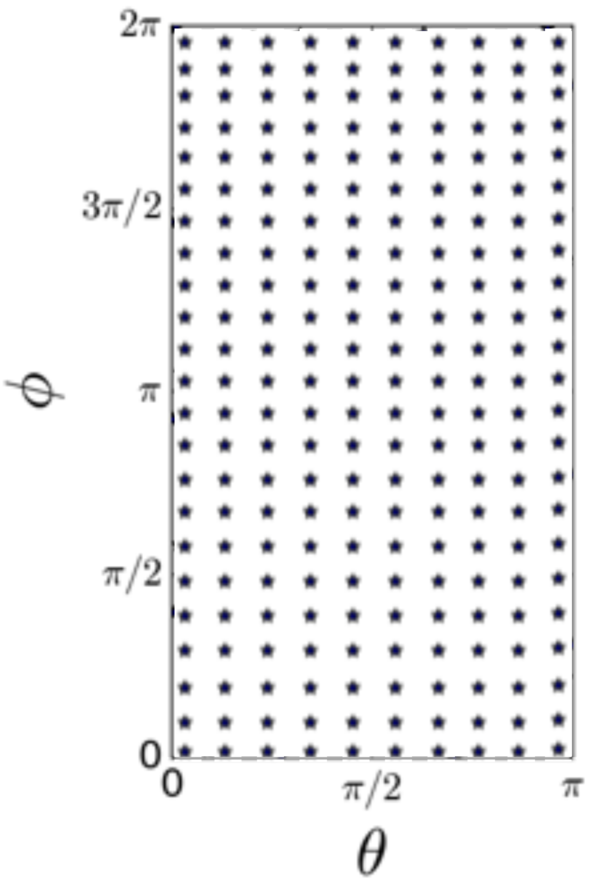

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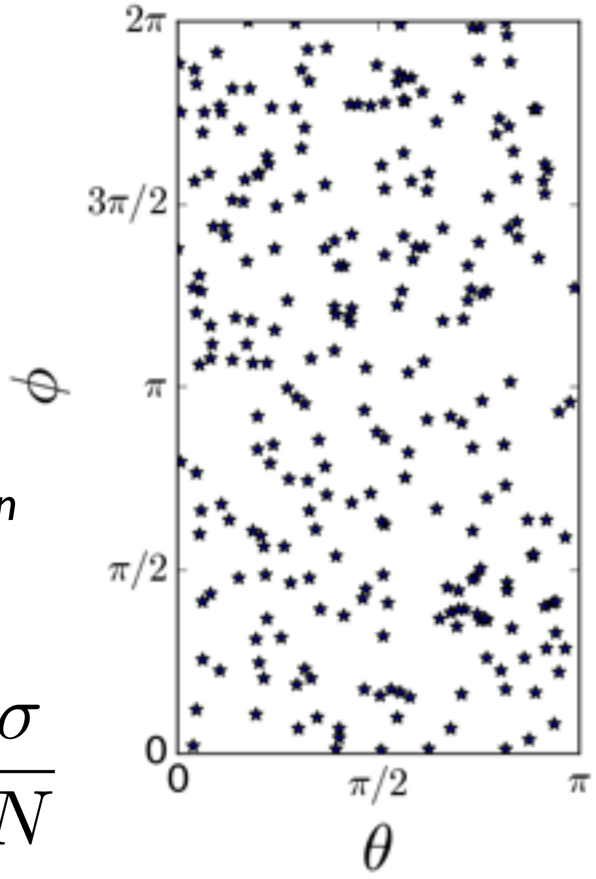

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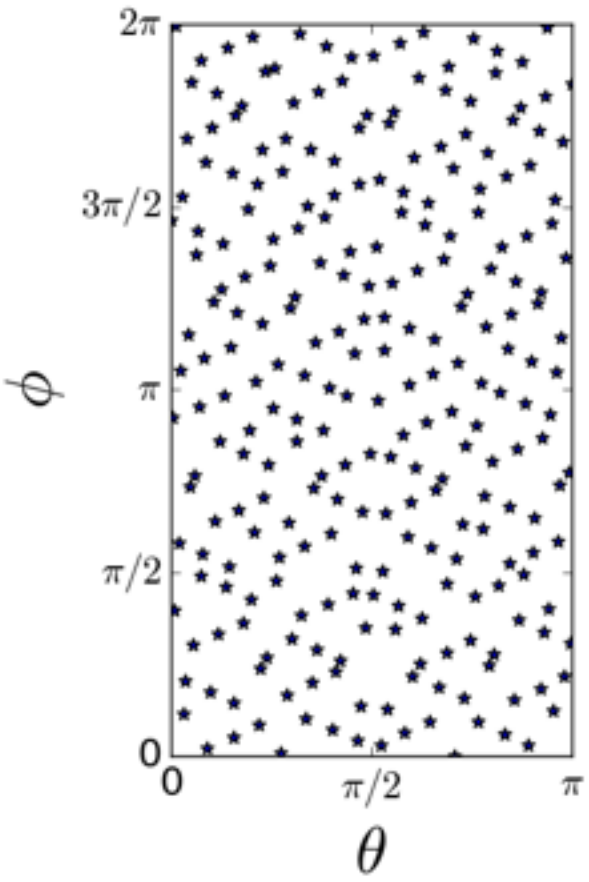

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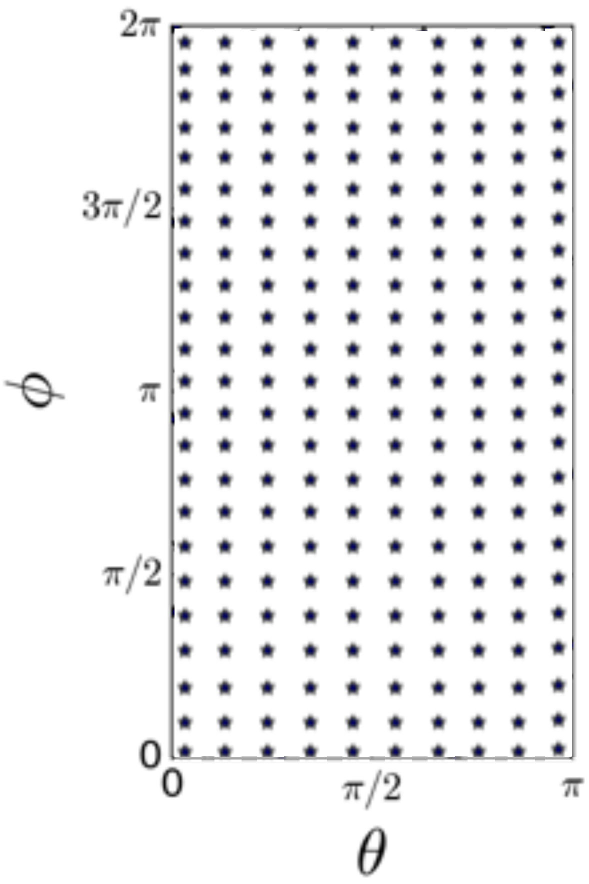

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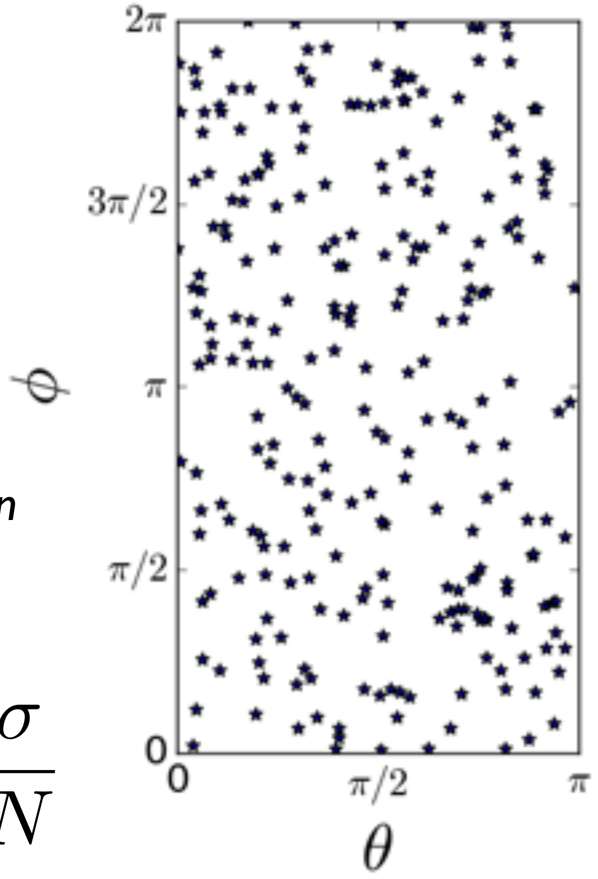

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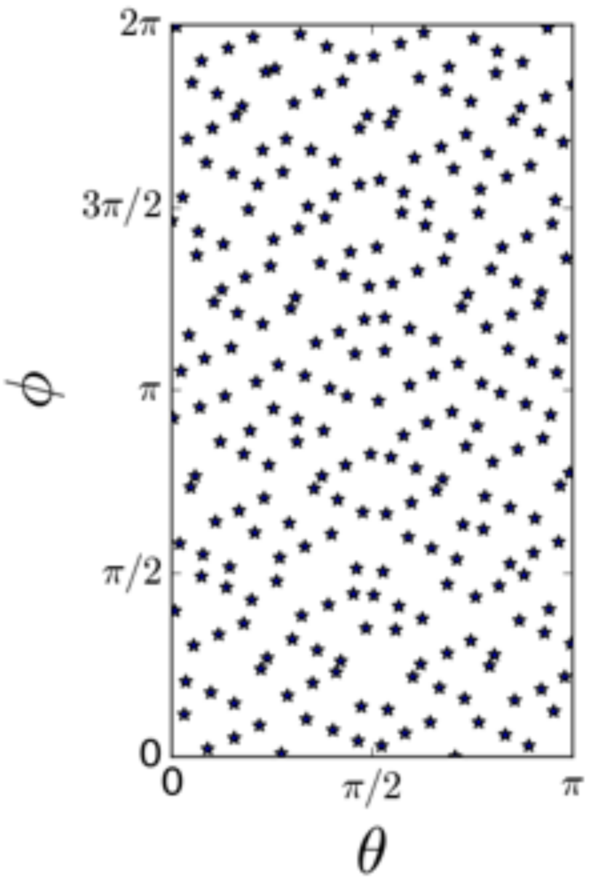

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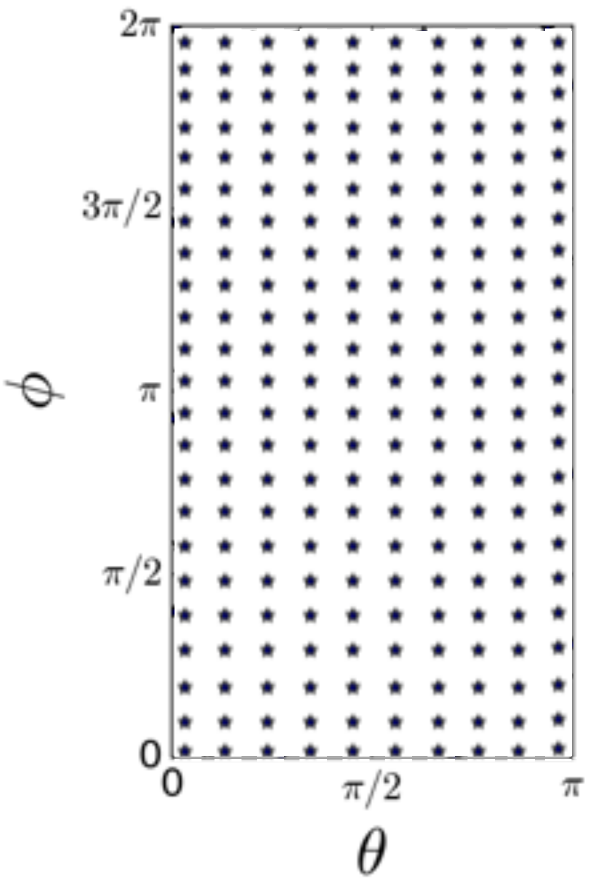

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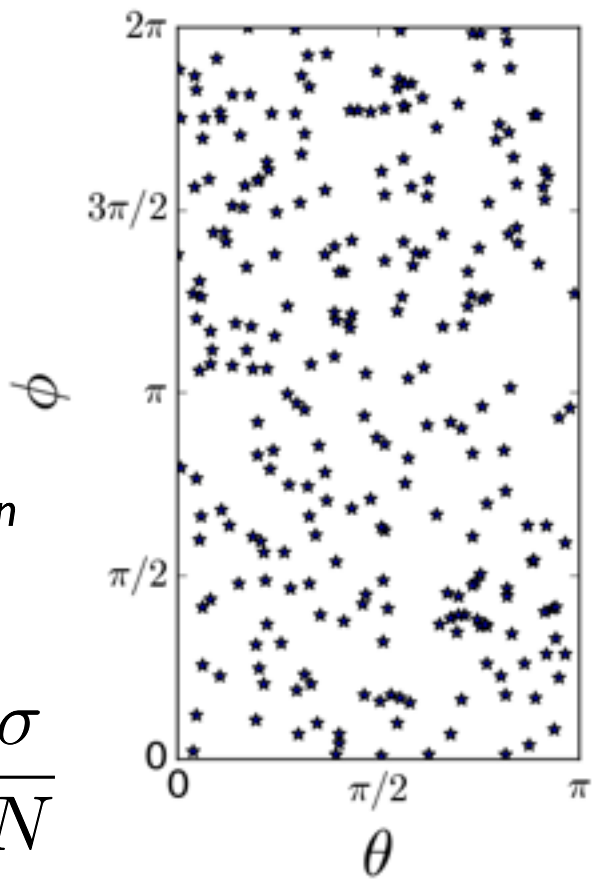
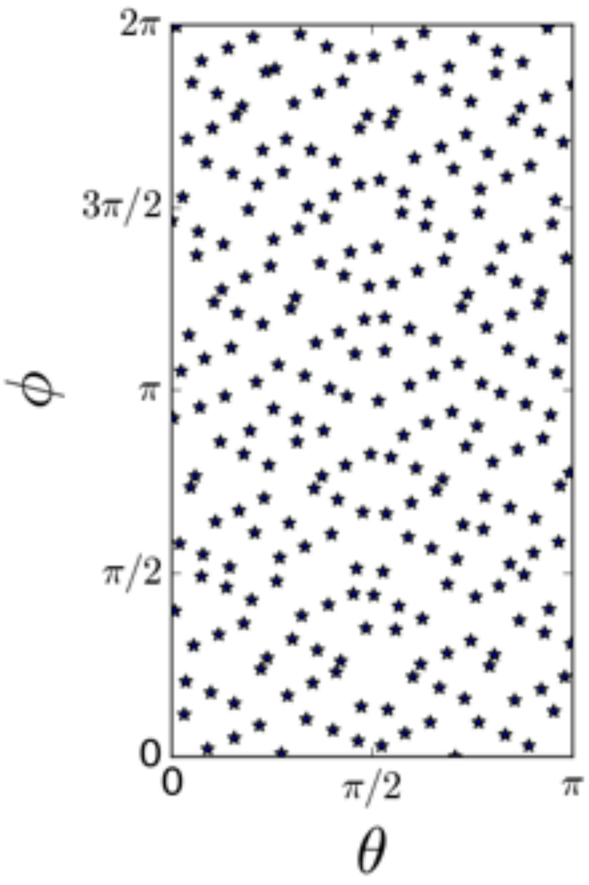


Random sampling

MC



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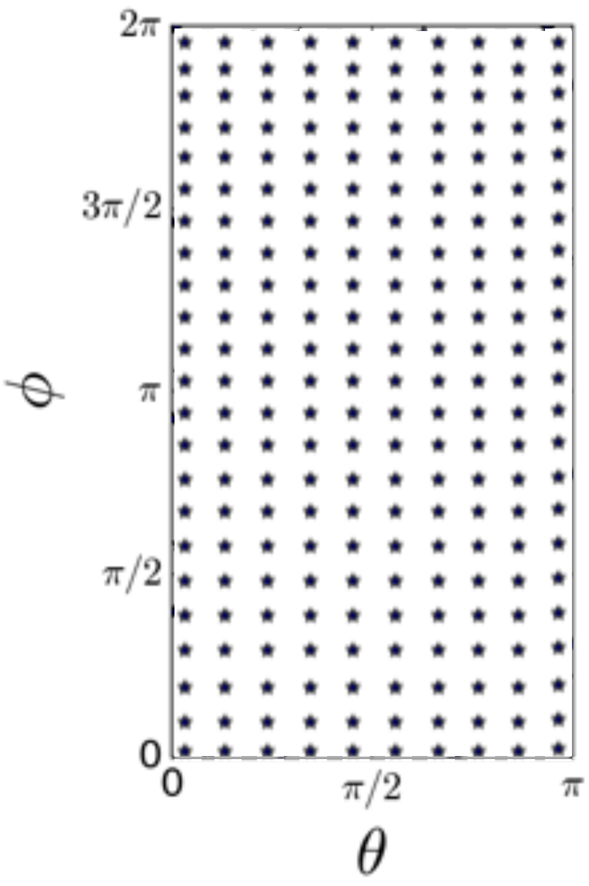

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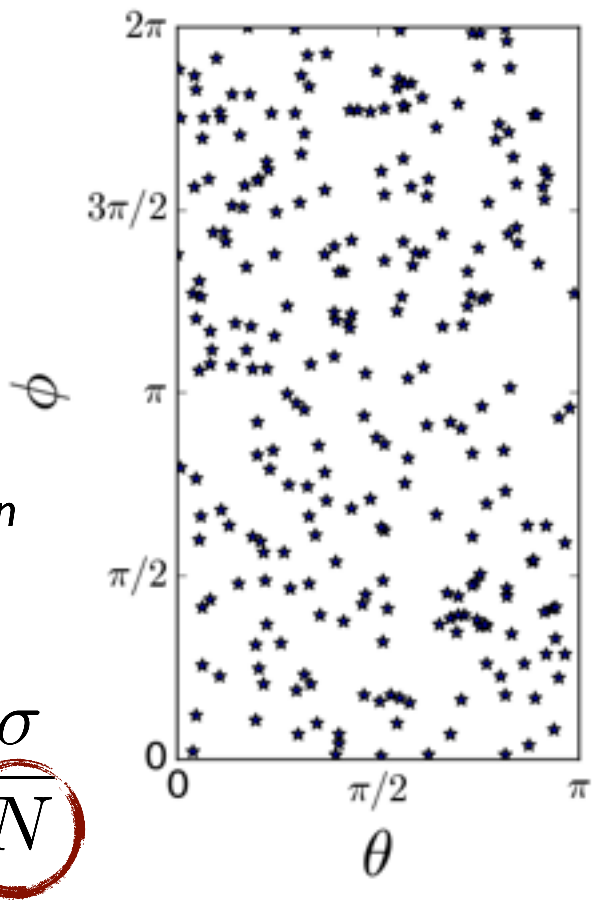

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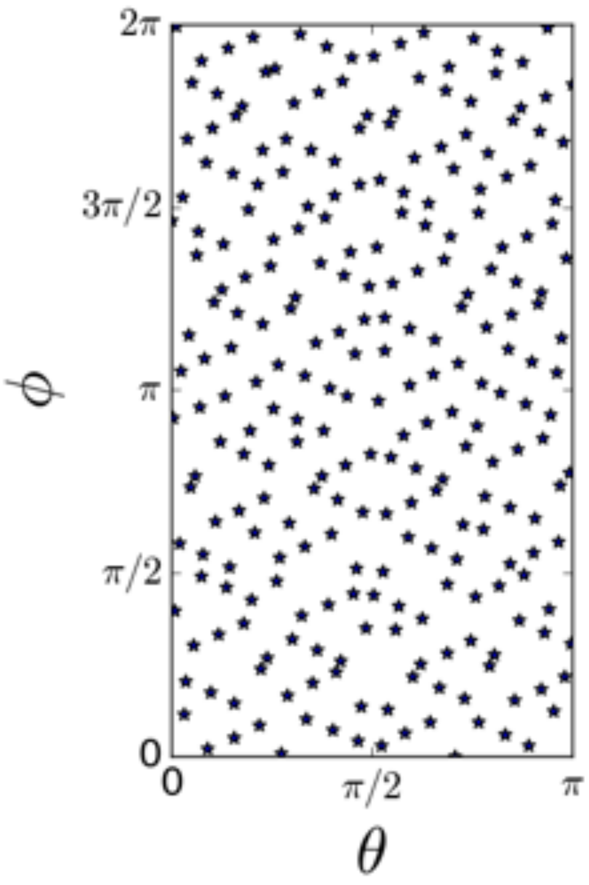

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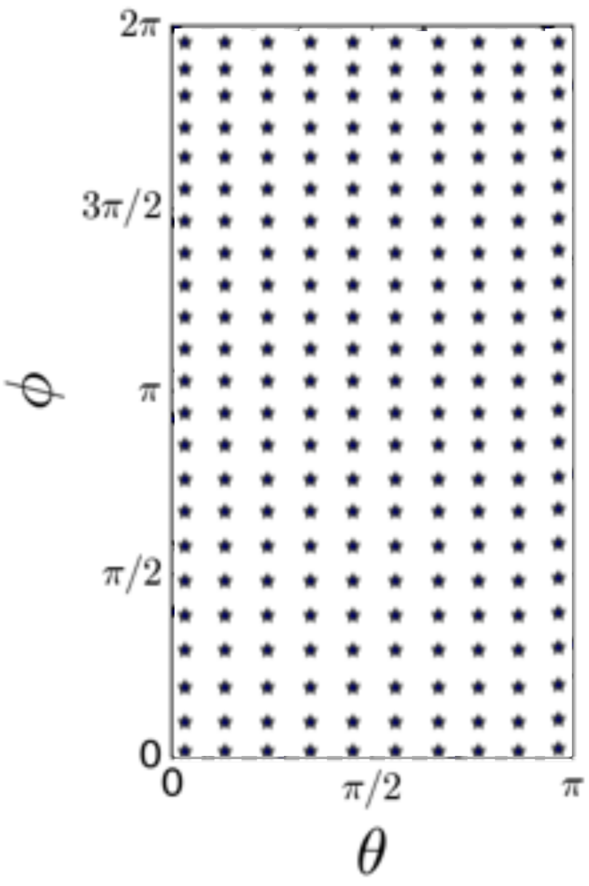

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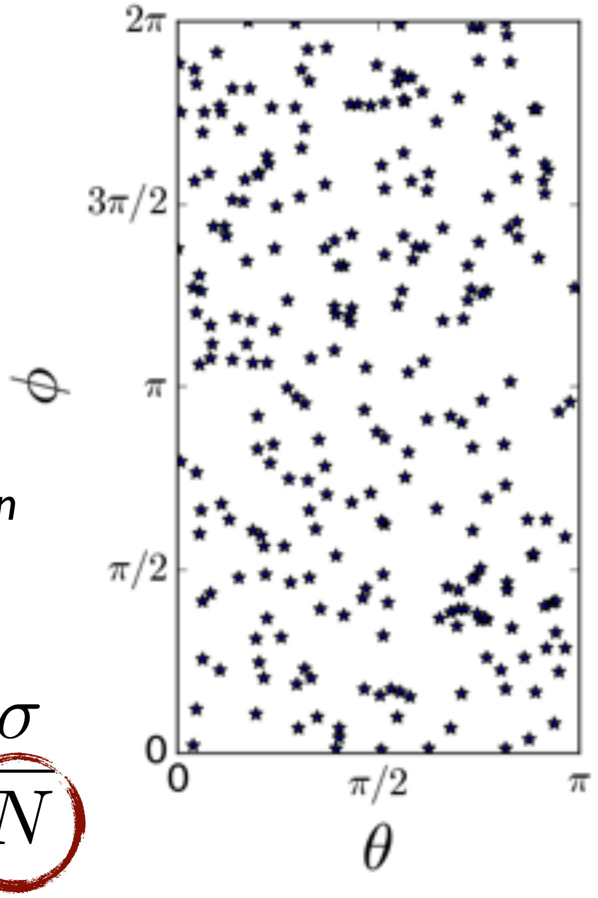

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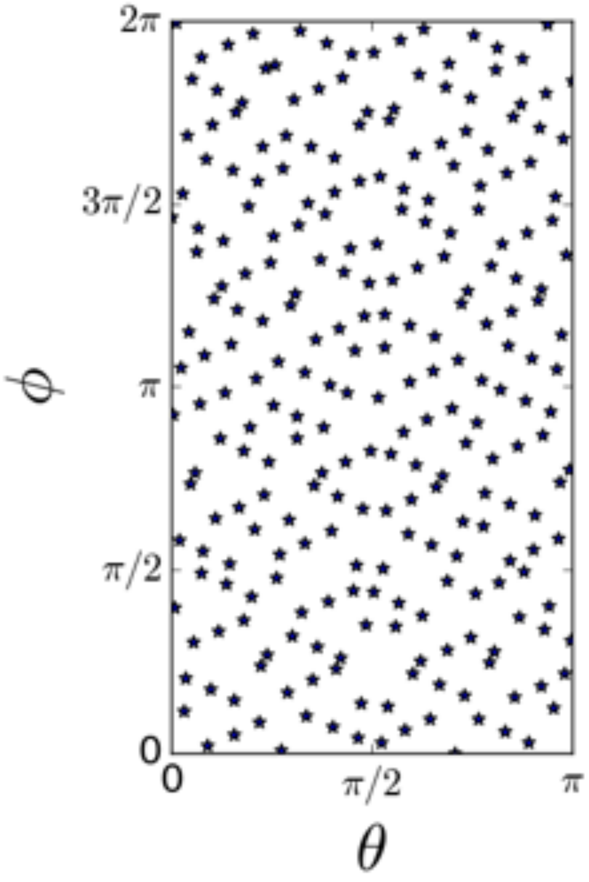

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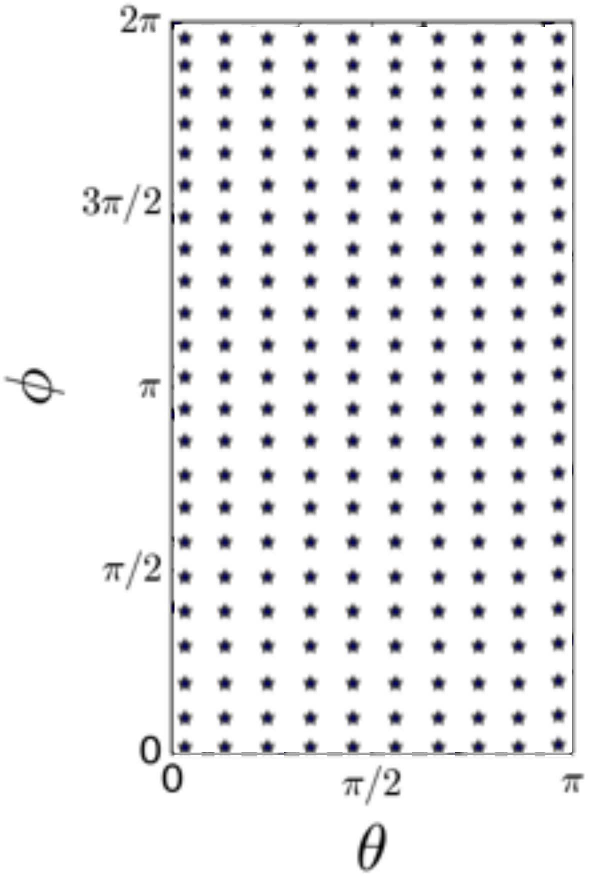

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QMC in radiative heat transfer

Simple 2-D configurations

➡ *O'Brien, D. M. 1992 "Accelerated quasi Monte Carlo integration of the radiative transfer equation".*

➡ *Kersch, A., Morokoff, W., and Schuster, A., 1994. "Radiative heat transfer with quasi-monte carlo methods"*

NEW

First time applied in a real 3-D application

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OERM: Monte Carlo vs Quasi-Monte Carlo

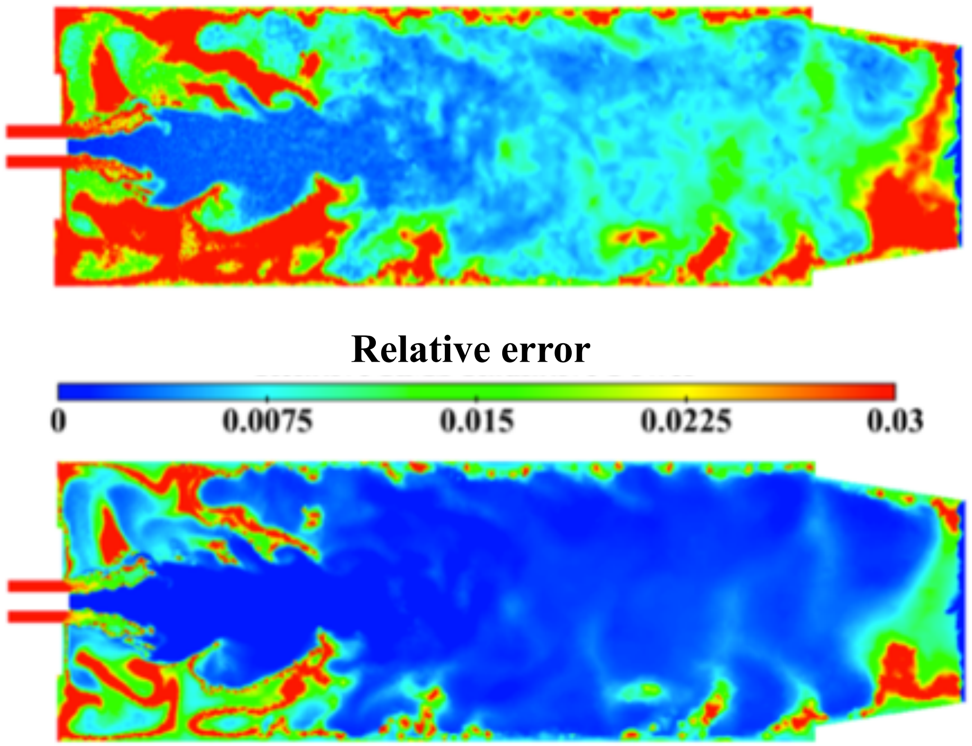
Quasi-Monte Carlo can be combined with any method

Here: QMC-OERM compared to Monte Carlo-OERM

Computations with a fixed rays number

Rays number : 10 000

Monte Carlo:



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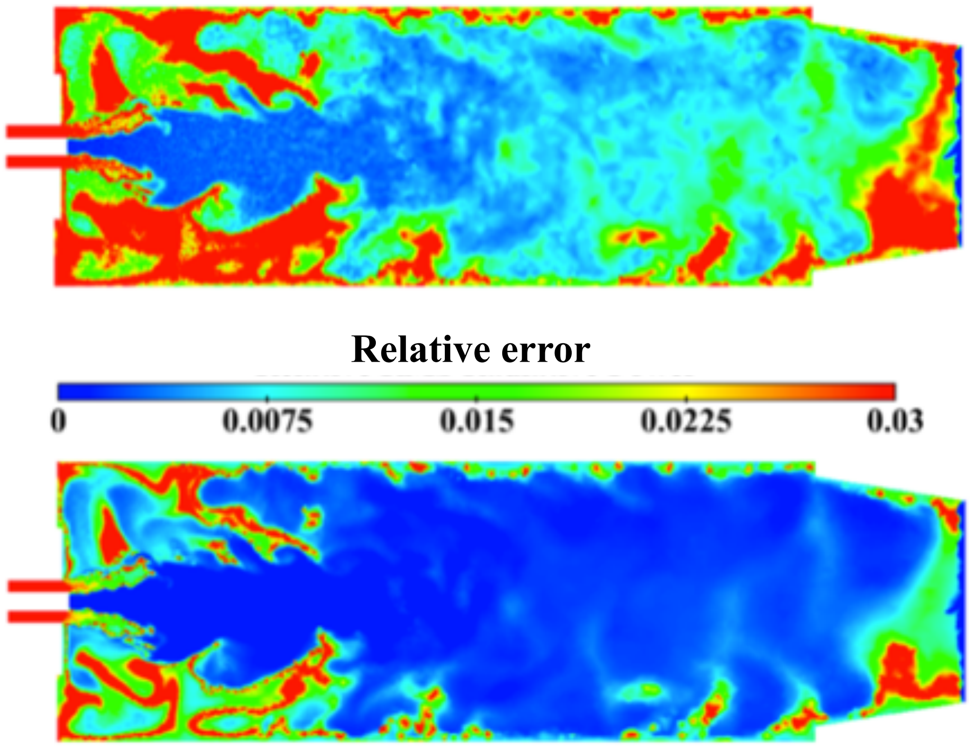
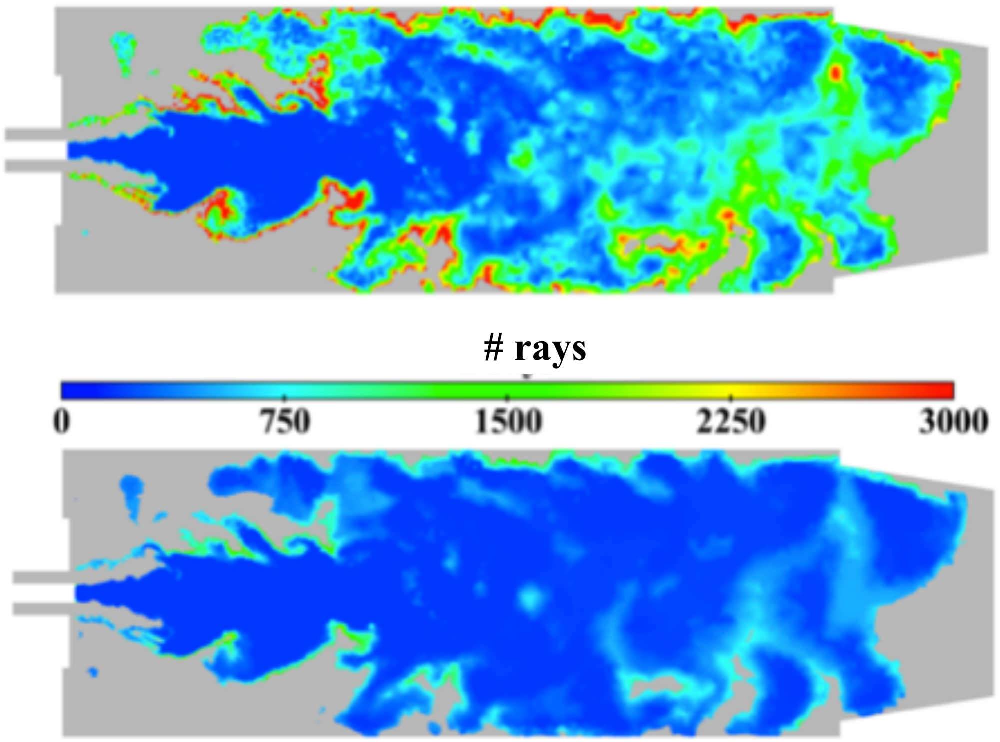


Computations with controlled convergence

Relative error : 5%

Absolute error : 10% (of Pmax)



CPU efficiency of MC and QMC methods

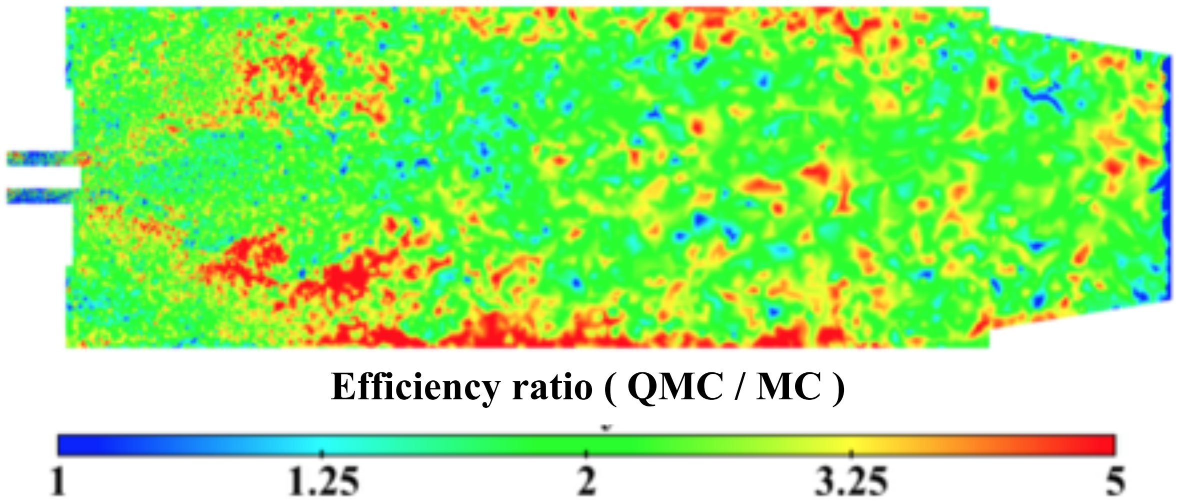
- ***Local efficiency of methods***[1]:

$$\eta_i = \frac{1}{\sigma_i^2 \; T_{CPU,i}}$$

σ_i^2 = Local variance

T_{CPU} = computational time

$$\frac{\eta_{QMC}}{\eta_{MC}}$$



Ratio bigger than 1 in almost the whole domain

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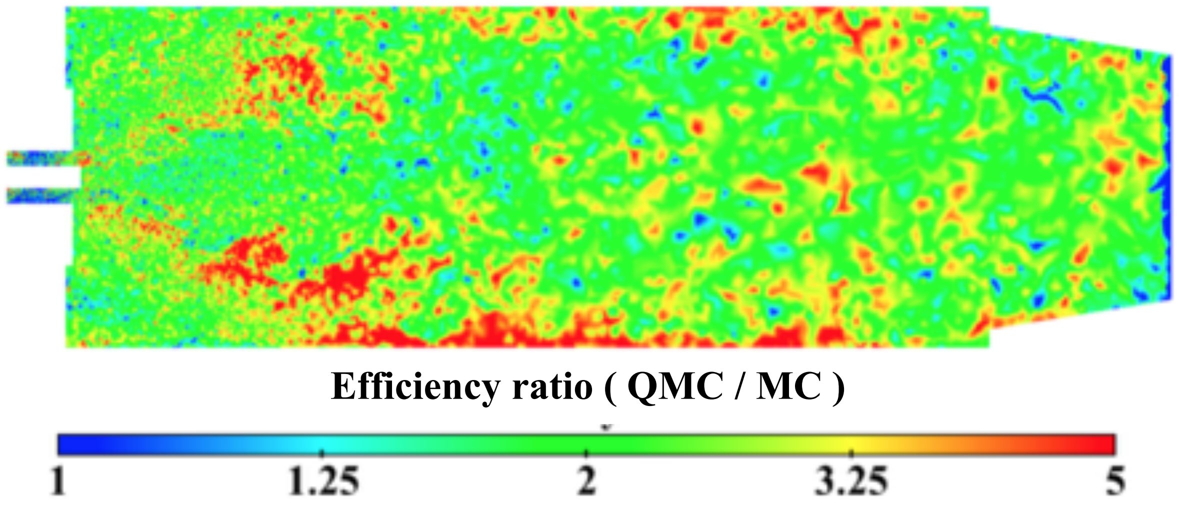

Ratio bigger than 1 in almost the whole domain

Ratio of CPU time

- **MC and QMC computational time**:

- $$\frac{T_{CPU,MC}}{T_{CPU,QMC}} = 2.7$$ ➡ QMC 3 times faster than MC!

Such an improvement makes coupled simulations more affordable

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Conclusions and perspectives

Monte Carlo methods: accurate but computationally expensive

➞ *Need to reduce CPU time to afford coupled 3D simulations of reactive flows*

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→ *Need to reduce CPU time to afford coupled 3D simulations of reactive flows*

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  - OERM applied to industrial configuration

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- **Scalable Monte Carlo method**
  - High scalability up to 2000 cores
  - Control of local convergence
- **Importance sampling: one way for error reduction**
  - OERM applied to industrial configuration
- **Quasi-Monte Carlo methods: second way for error reduction**
  - **3 times** more efficient than Monte Carlo
  - Next step: Towards coupled multi-physics simulations

CLEAN GAS

Thank you for your attention!

This project has received funding from the European Unions Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 643134. It was also granted access to the HPC resources of CINES under the allocation 2016-020164 made by GENCI.

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Quasi-Monte Carlo convergence

- The approximation error of the quasi-Monte Carlo method is:

$$\varepsilon \approx \frac{(logN)^s}{N}$$

- where s is the number of dimension

Computational time

Table of computational time of radiative heat transfer simulations for the retained configurations

- Controlled convergence computations criteria:

  Relative error : 3%

  Absolute error : 3 % (of P_{max})

- Number of cores: 168

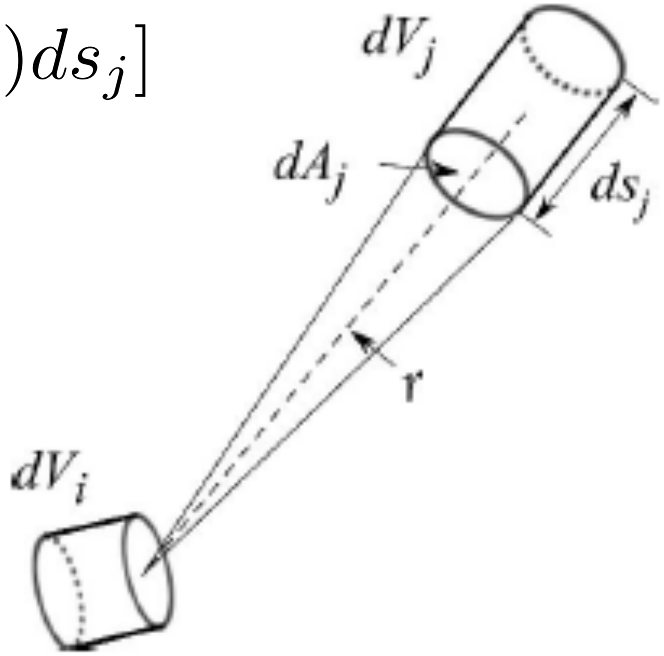
- Optimized-ERM

	Quasi-Monte Carlo
Combustion chamber	190

Reciprocity principle

- The energy emitted by the differential volume element dV_i and absorbed by dV_j (= dA_j x ds_j) is:

$$dP^{ea}_{\nu,ij} = [4\pi\kappa_\nu(T_i)I^0_\nu(T_i)dV_i] \times \left(\frac{dA_j}{4\pi r^2}\right) \times \tau_{\nu,r} \times \kappa_\nu(T_j)ds_j]$$



Radiative exchange between two differential volume elements

- The equation can be recast as:

$$\frac{dP^{ea}_{\nu,ij}}{I^0_\nu(T_i)} = \tau_{\nu,r}\kappa_\nu(T_i)\kappa_\nu(T_j)\frac{dV_idV_j}{r^2}$$

- Similarly, in terms of the energy emitted by i and absorbed by j:

$$\frac{dP^{ea}_{\nu,ji}}{I^0_\nu(T_j)} = \tau_{\nu,r}\kappa_\nu(T_i)\kappa_\nu(T_j)\frac{dV_idV_j}{r^2}$$

$$\frac{dP^{ea}_{\nu,ij}}{I^0_\nu(T_i)} = \frac{dP^{ea}_{\nu,ji}}{I^0_\nu(T_j)}$$

- **Reciprocity principle**: the ratio between dPeaij and dPeaji is equal to the corresponding equilibrium spectral intensity ratio