Combustion for Low Emission Application of Natural Gas

Modelling, accuracy and impact of radiative heat transfer in the coupled simulation of an atmospheric premixed flame confined by semi-transparent viewing windows.

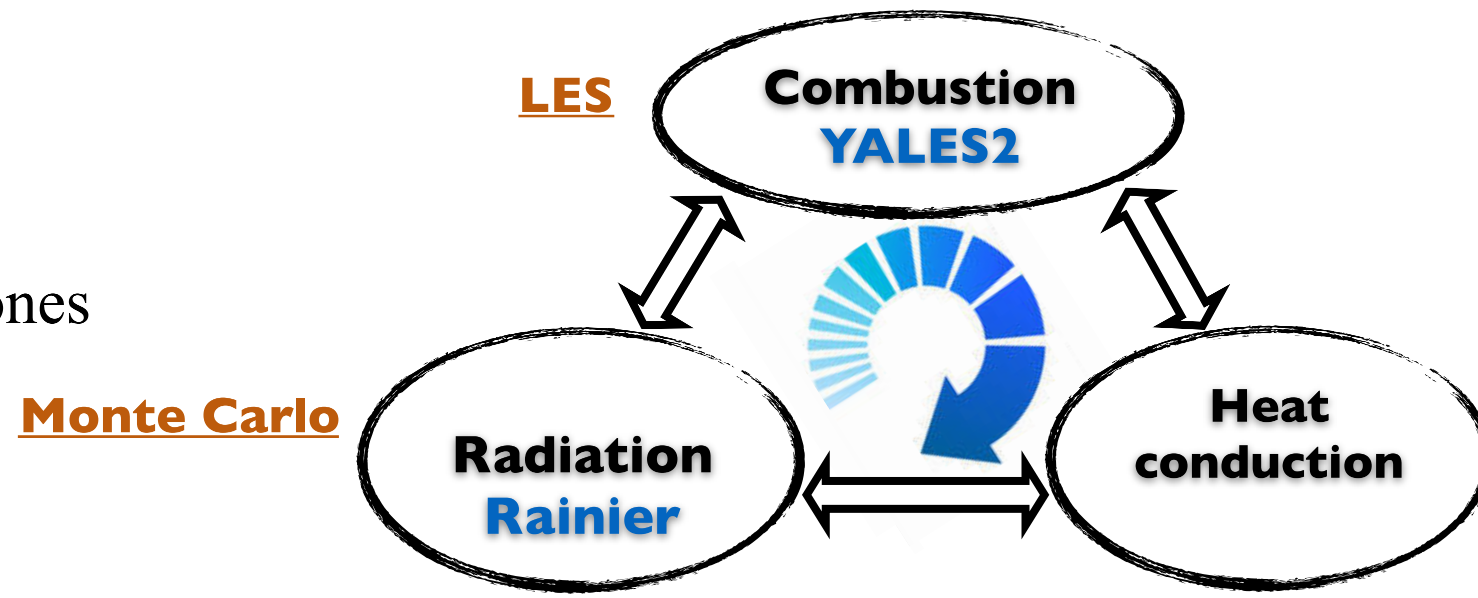
Lorella Palluotto, Ronan Vicquelin, Olivier Gicquel

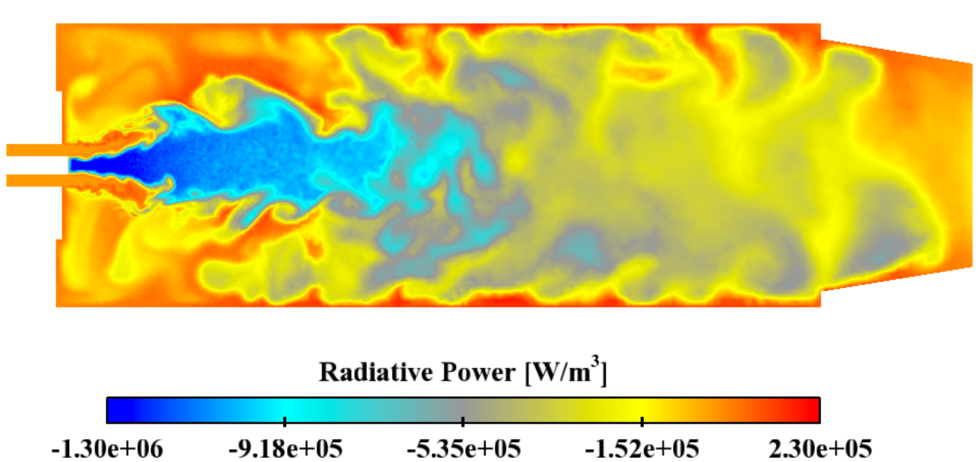
Context

Importance of radiative heat transfer in combustion applications

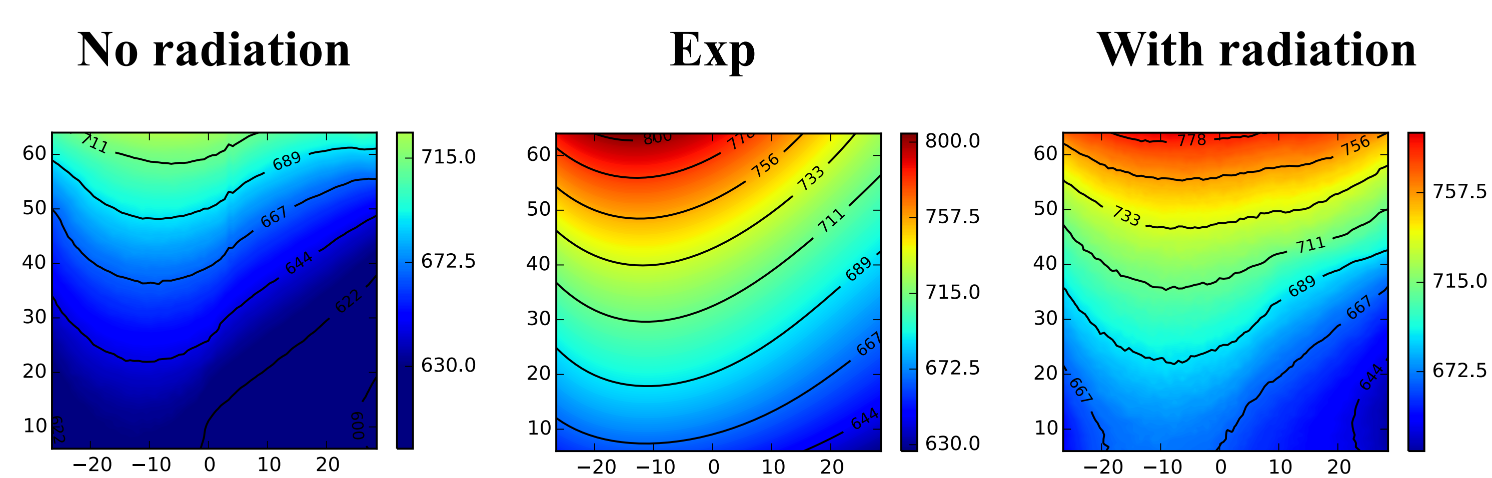
Semi-industrial burner

- Fully coupled methodology
- Radiative fluxes same order than convective ones
- Wall temperature prediction





Wall temperature



[1] Koren, Chai, Ronan Vicquelin, and Olivier Gicquel. *Flow, Turbulence and Combustion* 101.1 (2018): 77-102.

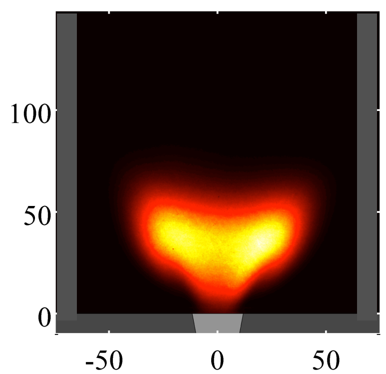
Context

Importance of radiative heat transfer in combustion applications

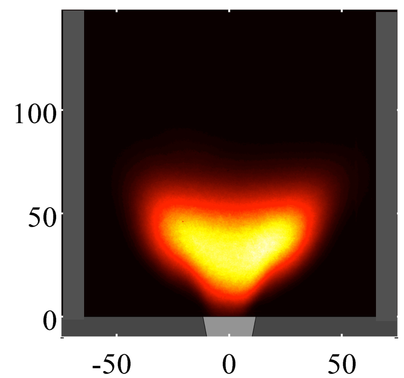
Oxy-combustion:

- Highly CO2-concentrated exhaust gases
- Facilitate the CO2 capture process
- No Nox

OXYtec chamber[1] at EM2C lab



Flame A
CH4/Air

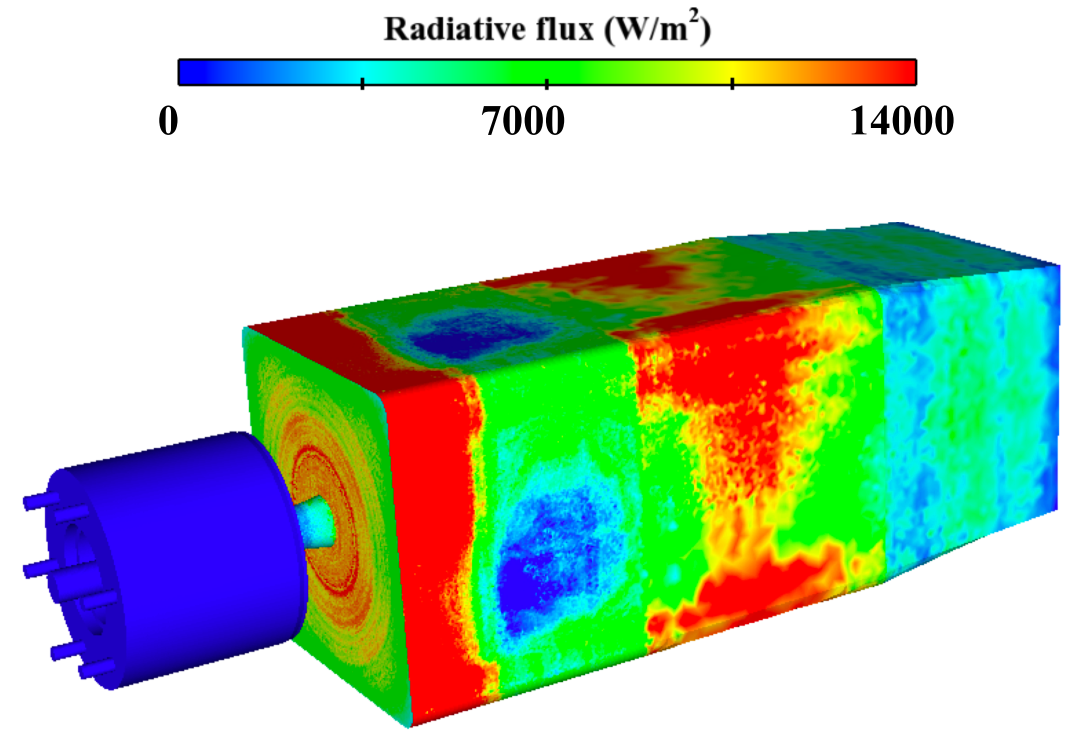


Flame B
CH4-O2-CO2

High CO_2 concentration

➡ Radiation is significative

Burnt gases	CO2	H2O
A	0.14	0.12
C	0.83	0.12



CH4-Air

Radiative Fluxes = 20% of Pth

CH4-O2-CO2

Radiative flux may be higher

Simulations in progress…

[1] .P. Jourdaine, C. Mirat, J. Caudal, T. Schuller. Stabilization mechanisms of swirling premixed flames with an axial-plus-tangential swirler. *ASME 2017*

Coupled simulations: state of the art

Commonly used approaches for radiation and combustion

Accuracy ↑

Fluid solver	Radiation solver	Gas radiative properties
DNS	MC	LBL
LES	DOM	Narrow band
RANS	P1	Global models

CPU cost ↑

Coupled simulations: state of the art

References	Fluid solver	Radiation solver	Gas rad properties	Application
Adams and Smith 1995	RANS	DOM	Gray Gas	Confined turbulent sooting flame
Coelho et al. 2003 *Habibi et al. 2007* *Wang et al. 2008*	RANS	DOM	Global	Turbulent jet flame Steam cracking furnace Turbulent jet flame
Snegirev et al. 2004 *Mehta et al. 2009*	RANS	MC	Global	Turbulent flames Turbulent sooting flames
Tessé et al. 2004	RANS	MC	CK	Turbulent sooting flame
Zhao et al. 2013	RANS	MC	LBL	Oxy-combutsion
Poitou et al. 2012 *Berger et al. 2016*	LES	DOM	Global	Confined turbulent flame Helicopter combustion chamber
Jones and Paul et al. 2005	LES	DOM	Gray Gas	Gas turbine combustor
Gupta et al. 2013	LES	MC	LBL	Turbulent jet flame (1M cells)
Koren et al. 2018 *Rodrigues et al. 2018*	LES	MC	CK	Laboratory-scale combustor
Dos Santos et al. 2008	LES	Ray tracing	CK	2D burner
Wu et al. 2005	DNS	MC	Gray Gas	1D turbulent flame
El Hafi et al. 2002 *Zhang et al. 2013*	DNS	MC	CK	1D flame Turbulent channel flow

Coupled simulations: state of the art

References	Fluid solver	Radiation solver	Gas rad properties	Application
Adams and Smith 1995	RANS	DOM	Gray Gas	Confined turbulent sooting flame
Coelho et al. 2003 *Habibi et al. 2007* *Wang et al. 2008*	RANS	DOM	Global	Turbulent jet flame Steam cracking furnace Turbulent jet flame
Snegirev et al. 2004 *Mehta et al. 2009*	RANS	MC	Global	Turbulent flames Turbulent sooting flames
Tessé et al. 2004	RANS	MC	CK	Turbulent sooting flame
Zhao et al. 2013	RANS	MC	LBL	Oxy-combutsion
Poitou et al. 2012 *Berger et al. 2016*	LES	DOM	Global	Confined turbulent flame Helicopter combustion chamber
Jones and Paul et al. 2005	LES	DOM	Gray Gas	Gas turbine combustor
Gupta et al. 2013	LES	MC	LBL	Turbulent jet flame (1M cells)
Koren et al. 2018 *Rodrigues et al. 2018*	LES	MC	CK	Laboratory-scale combustor
Dos Santos et al. 2008	LES	Ray tracing	CK	2D burner
Wu et al. 2005	DNS	MC	Gray Gas	1D turbulent flame
El Hafi et al. 2002 *Zhang et al. 2013*	DNS	MC	CK	1D flame Turbulent channel flow

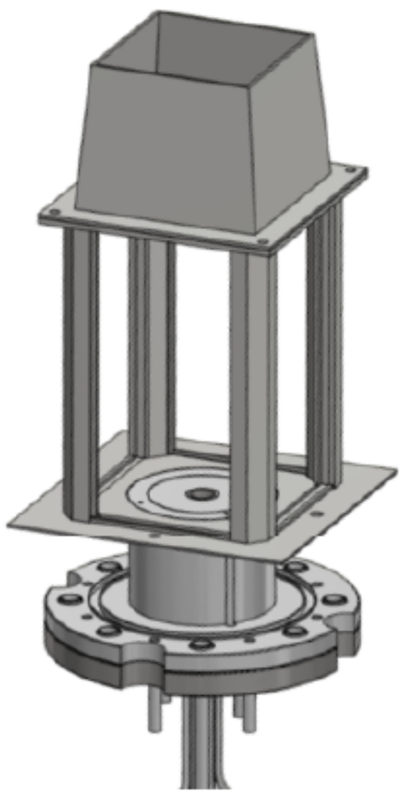
Coupled simulations: state of the art

References	Fluid solver	Radiation solver	Gas rad properties	Application
Adams and Smith 1995	RANS	DOM	Gray Gas	Confined turbulent sooting flame
Coelho et al. 2003 *Habibi et al. 2007* *Wang et al. 2008*	RANS	DOM	Global	Turbulent jet flame Steam cracking furnace Turbulent jet flame
Snegirev et al. 2004 *Mehta et al. 2009*	RANS	MC	Global	Turbulent flames Turbulent sooting flames
Tessé et al. 2004	RANS	MC	CK	Turbulent sooting flame
Zhao et al. 2013	RANS	MC	LBL	Oxy-combutsion
Poitou et al. 2012 *Berger et al. 2016*	LES	DOM	Global	Confined turbulent flame Helicopter combustion chamber
Jones and Paul et al. 2005	LES	DOM	Gray Gas	Gas turbine combustor
Gupta et al. 2013	LES	MC	LBL	Turbulent jet flame (1M cells)
Koren et al. 2018 *Rodrigues et al. 2018*	LES	MC	CK	Laboratory-scale combustor
Dos Santos et al. 2008	LES	Ray tracing	CK	2D burner
Wu et al. 2005	DNS	MC	Gray Gas	1D turbulent flame
El Hafi et al. 2002 *Zhang et al. 2013*	DNS	MC	CK	1D flame Turbulent channel flow

Objectives

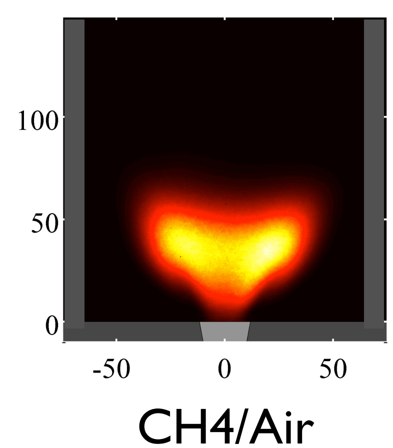
Quantification of thermal effects in air-methane and oxy-methane flames

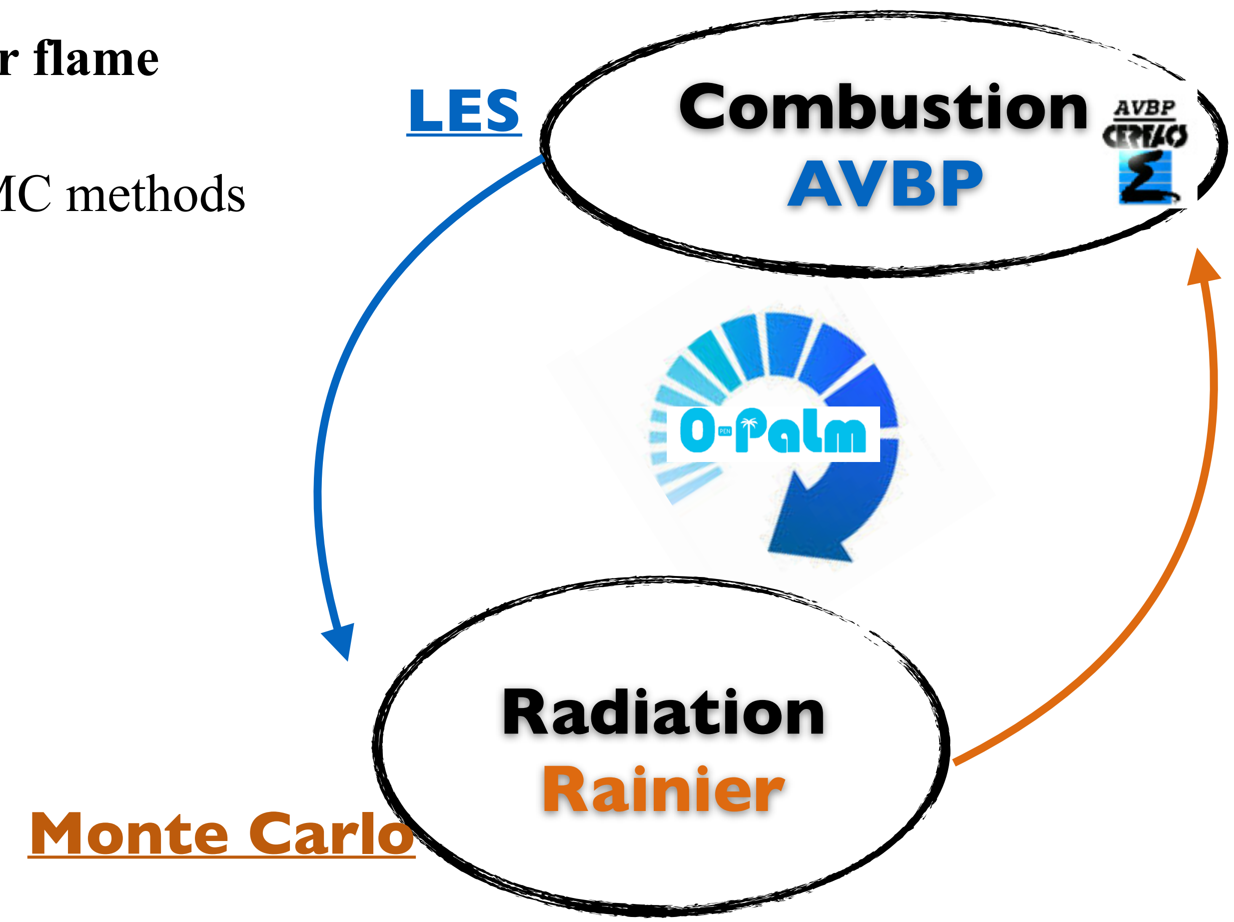
Complex target application



Coupled simulations of a CH4-Air flame

LES of turbulent reactive flows + MC methods





Fluid solver	Radiation solver	Gas radiative properties
LES	MC	Narrow band

Outline

LES of a premixed swirled flame

- *Presentation of Oxytec chamber*
- *LES results*

Coupled simulations: numerical set-up

- *Monte Carlo solver*
- *CPU cost-accuracy trade off*

First results of coupled simulations

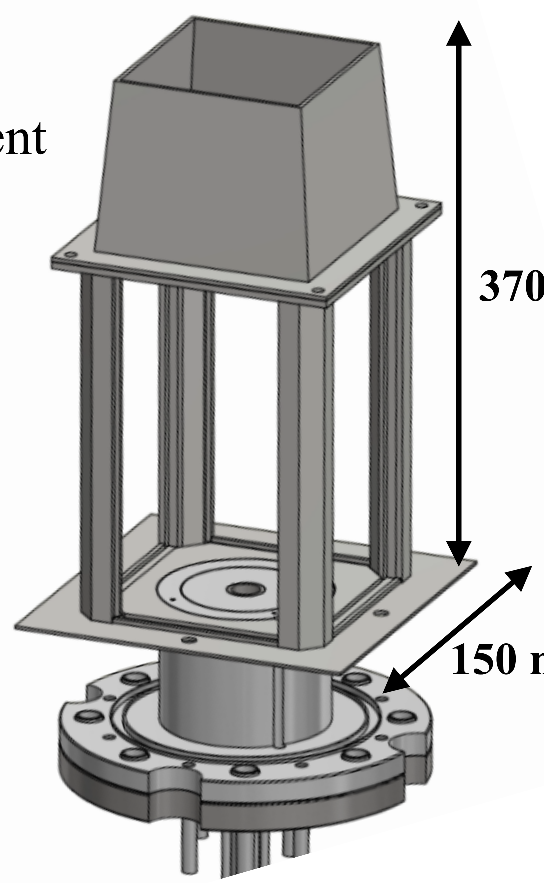
- *Impact of spectral properties of quartz*
- *Radiative heat transfer in a methane air flame*

AIR LIQUIDE/ANR Oxytec chamber

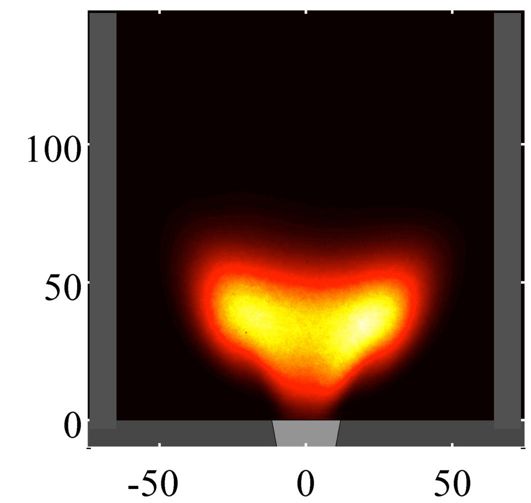
Experimental rig at EM2C

Target application: OxyTec chamber

- Experimental rig.[1,2,3,4] located at EM2C lab
- Premixed swirled CH4-Air flame



OH-chemiluminescence images[2]



Flame A

CH4/Air

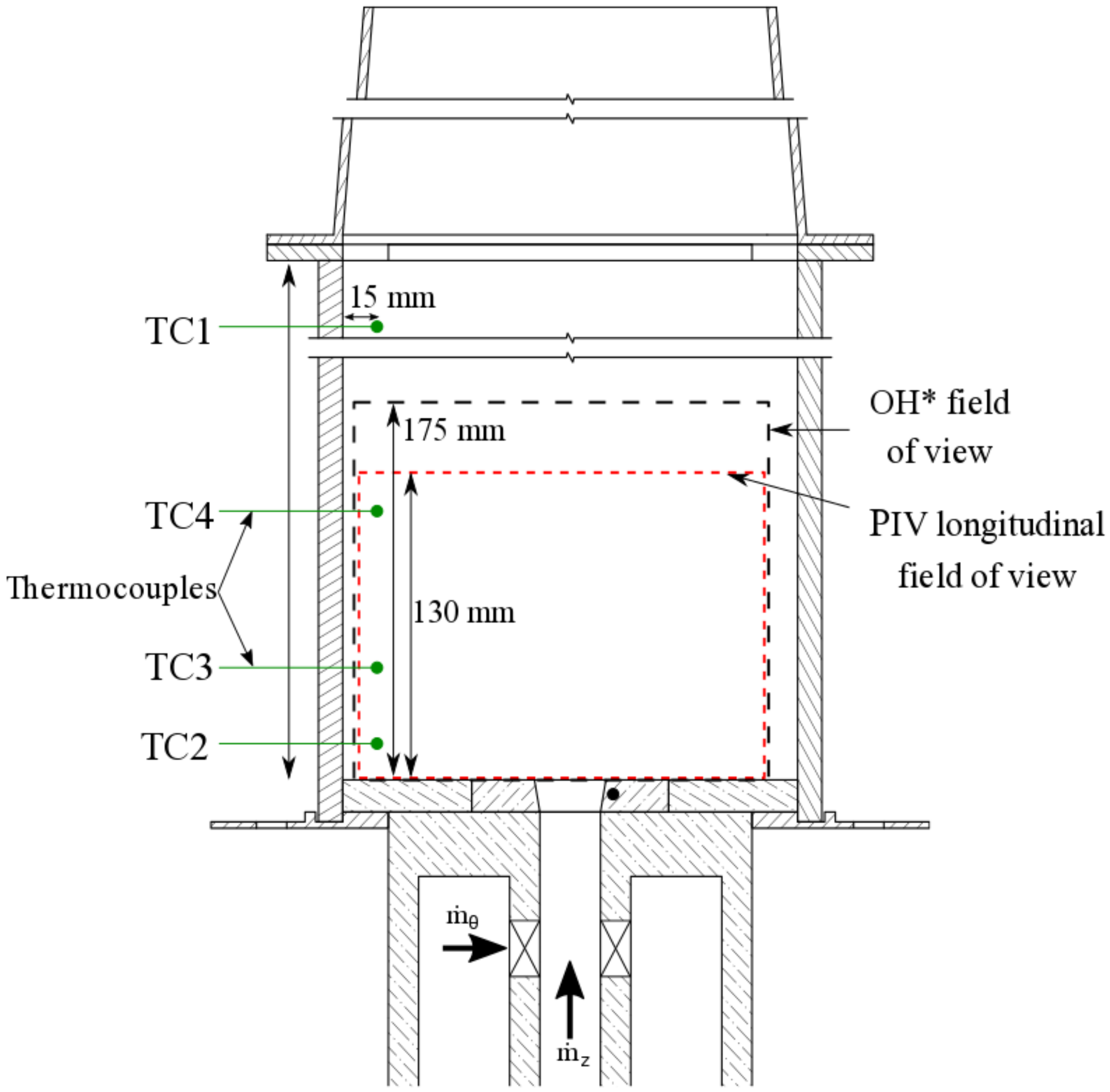
Y_{CH4}	Y_{O2}	Y_{N2}	S_L (m/s)	Tad (K)	P (kW)	Eq.Ratio	Swirl number
0.05	0.22	0.73	0.36	2186	14	0.95	0.85

1 Jourdaine, P., Mirat, C., Beaunier, J., Caudal, J., Joumani, Y., & Schuller, T. (2016, June). ASME Turbo Expo 2016
2 P. Jourdaine, C. Mirat, J. Caudal, T. Schuller. Stabilization mechanisms of swirling premixed flames with an axial-plus-tangential swirler. ASME 2017
3 Jourdaine, P., Mirat, C., Caudal, J., & Schuller, T. (2018). Journal of Engineering for Gas Turbines and Power, 140(8), 081502.
4 : A. Degenève, P. Jourdaine, C. Mirat, J. Caudal, R. Vicquelin, and T. Schuller. 2nd International Workshop on Oxy-Fuel Combustion, Bochum, Germany, (2018)

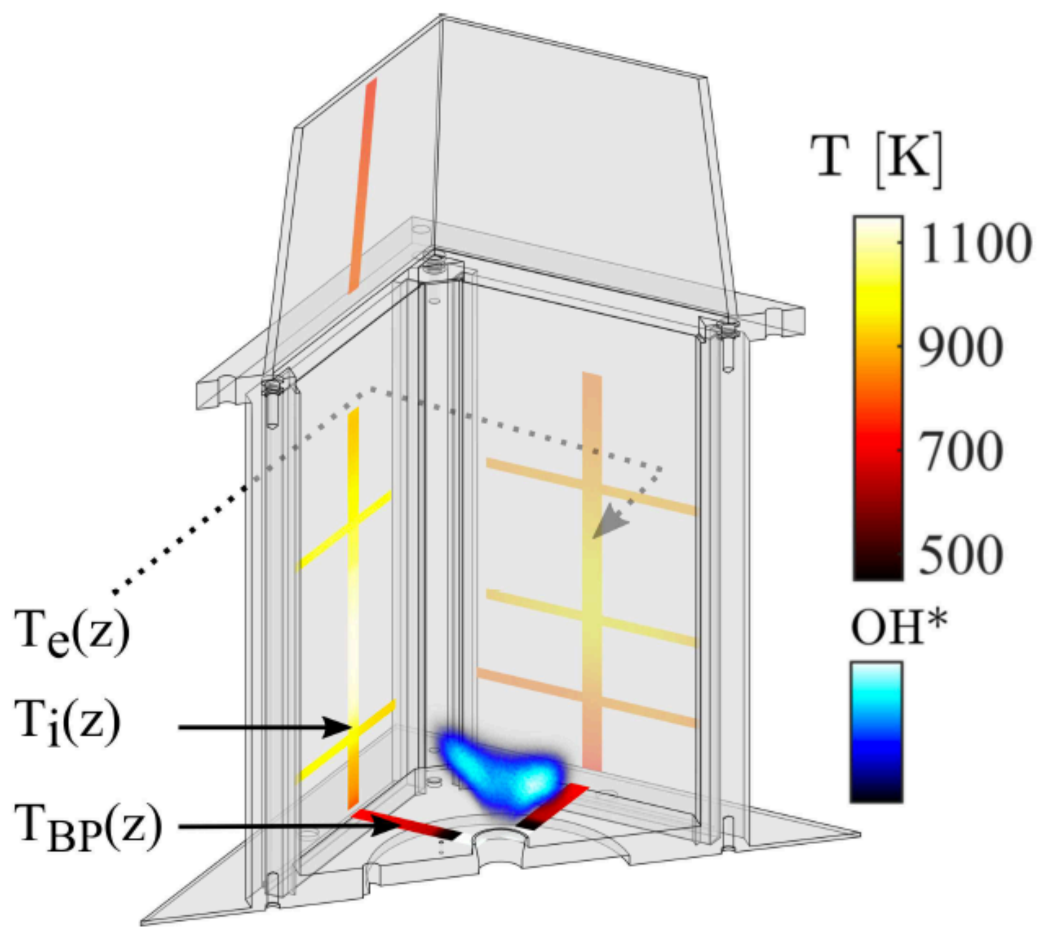
AIR LIQUIDE/ANR Oxytec chamber

Measurements

- ***Velocity***: *PIV, LDV*
- ***Temperature***: *thermocouples, LIP*
- ***Flame***: *OH-chemiluminescence, OH-PLIF*



LIP measurements from A. Degenève[1]



1 : .Degenève, A., Jourdaine, P., Mirat, C., Caudal, J., Vicquelin, R., & Schuller, T. (2019). Analysis of wall temperature and heat flux distributions in a swirled combustor powered by a methane-air and a CO2-diluted oxyflame. Fuel, 236, 1540-1547.

Large Eddy Simulations

AVBP (CFD code developed by CERFACS and IFPEN)

- 3-D compressible Navier-Stokes
- Unstructured and hybrid grids
- Massively parallel

Case Set-up

- Computational grid:
  - 50 millions cells

- Numerical scheme:
  TTGC (Two-Step Taylor Galerkin 'C' - third order accurate in space and time)

- LES subgrid model: Sigma model[11]

- Combustion model: Thickened Flame model for LES[2]

  - 2-step mechanism[3]
  - Dynamic thickening, Charlette efficiency model[4]

1 : Nicoud, F., Toda, H. B., Cabrit, O., Bose, S., and Lee, J "Using singular values to build a subgrid-scale model for large eddy simulations." Physics of Fluids. 2011
2 : O. Colin et al., A Thickened flame model for large eddy simulations of turbulent premixed combustion, Physics of Fluids (2000)
3 : G. Boudier, Methane/air flame with 2-step chemistry: 2s ch4 cm2, Tech. report, CERFACS, 2007
4 : F. Charlette et al., *A power-law flame wrinkling model for LES of premixed turbulent combustion. Combustion and Flame (2002)*
5 : A. Degenève, P. Jourdaine, C. Mirat, J. Caudal, R. Vicquelin, and T. Schuller. 2nd International Workshop on Oxy-Fuel Combustion, Bochum, Germany, (2018)

Large Eddy Simulations

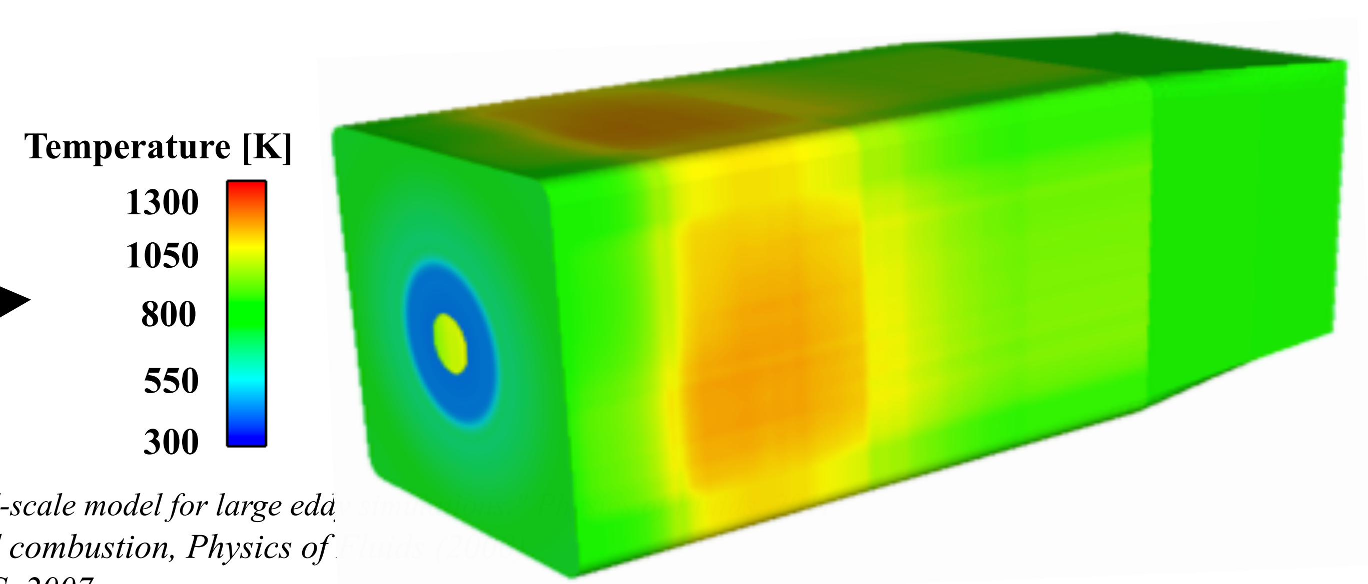
AVBP (CFD code developed by CERFACS and IFPEN)

- 3-D compressible Navier-Stokes
- Unstructured and hybrid grids
- Massively parallel

Case Set-up

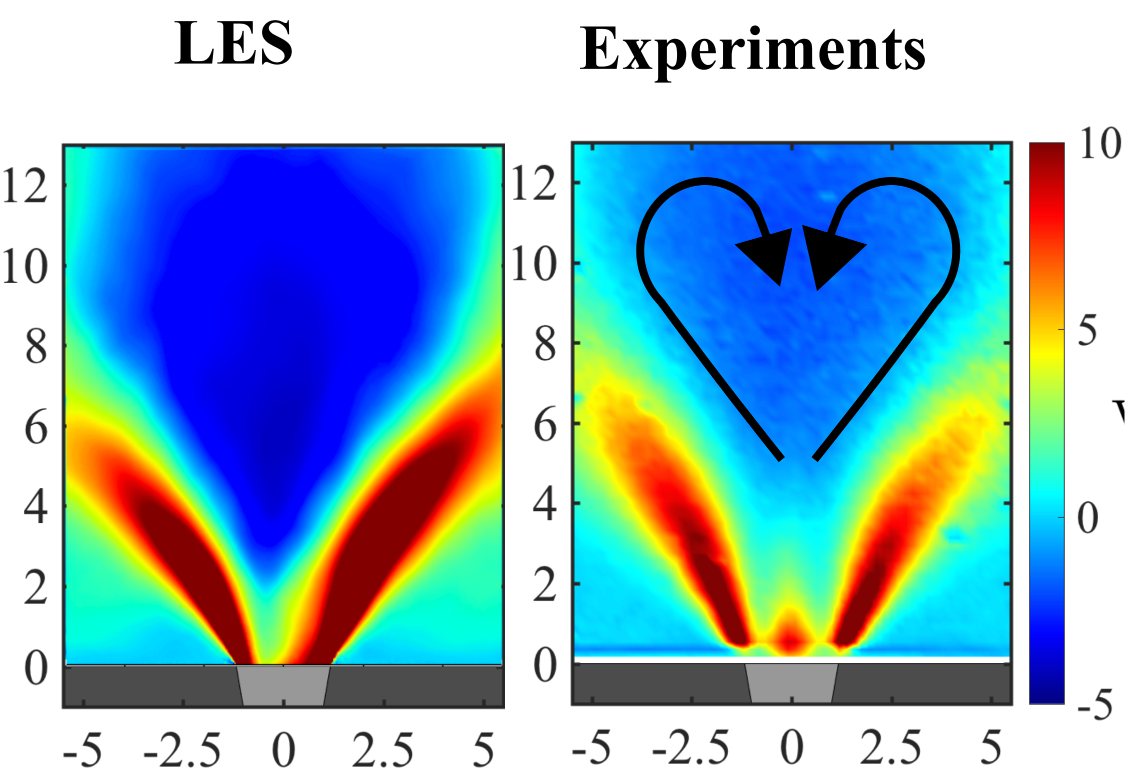
- Computational grid:
    - 50 millions cells
- Numerical scheme:
  TTGC (Two-Step Taylor Galerkin 'C' - third order accurate in space and time)
- LES subgrid model: Sigma model[1]
- Combustion model: Thickened Flame model for LES[2]
    - 2-step mechanism[3]
    - Dynamic thickening, Charlette efficiency model[4]
- Walls:
    - **Imposed temperature**

Laser Induced Phosphorescence (LIP)[5]



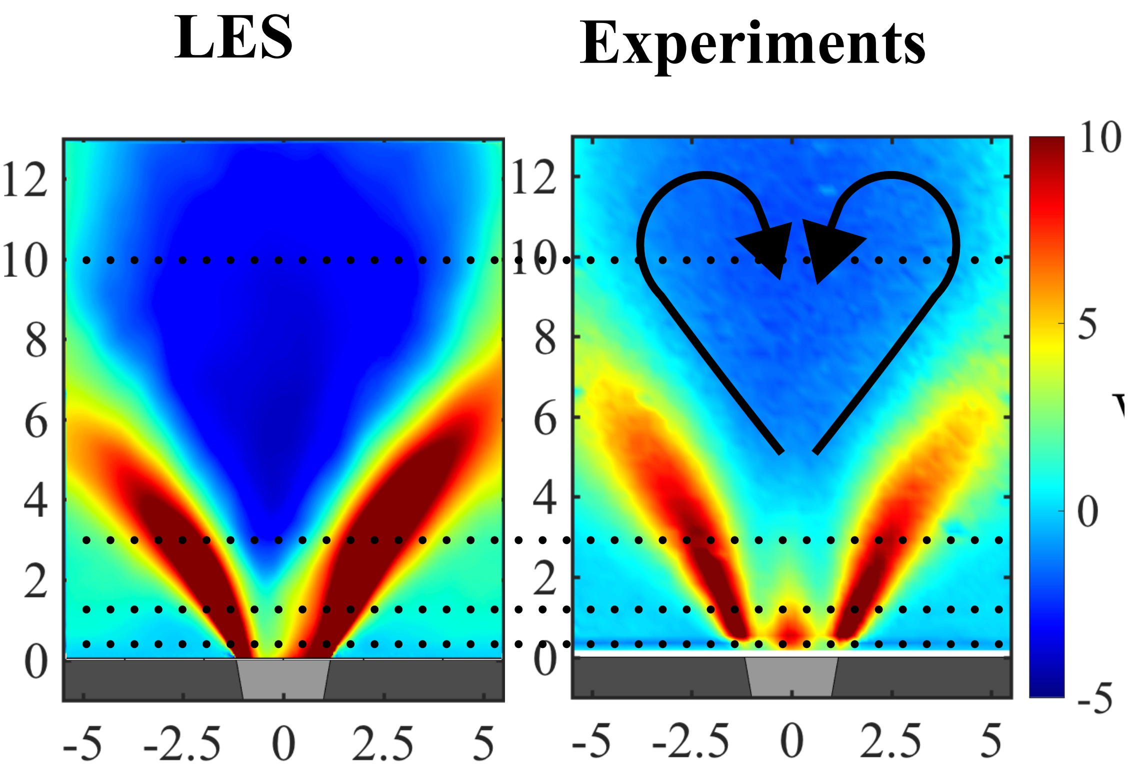
1 : Nicoud, F., Toda, H. B., Cabrit, O., Bose, S., and Lee, J "Using singular values to build a subgrid-scale model for large edd
2 : O. Colin et al., A Thickened flame model for large eddy simulations of turbulent premixed combustion, Physics of
3 : G. Boudier, Methane/air flame with 2-step chemistry: 2s ch4 cm2, Tech. report, CERFACS, 2007
4 : F. Charlette et al., *A power-law flame wrinkling model for LES of premixed turbulent combustion. Combustion and Flame (2002)*
5 : A. Degenève, P. Jourdaine, C. Mirat, J. Caudal, R. Vicquelin, and T. Schuller. 2nd International Workshop on Oxy-Fuel Combustion, Bochum, Germany, (2018)

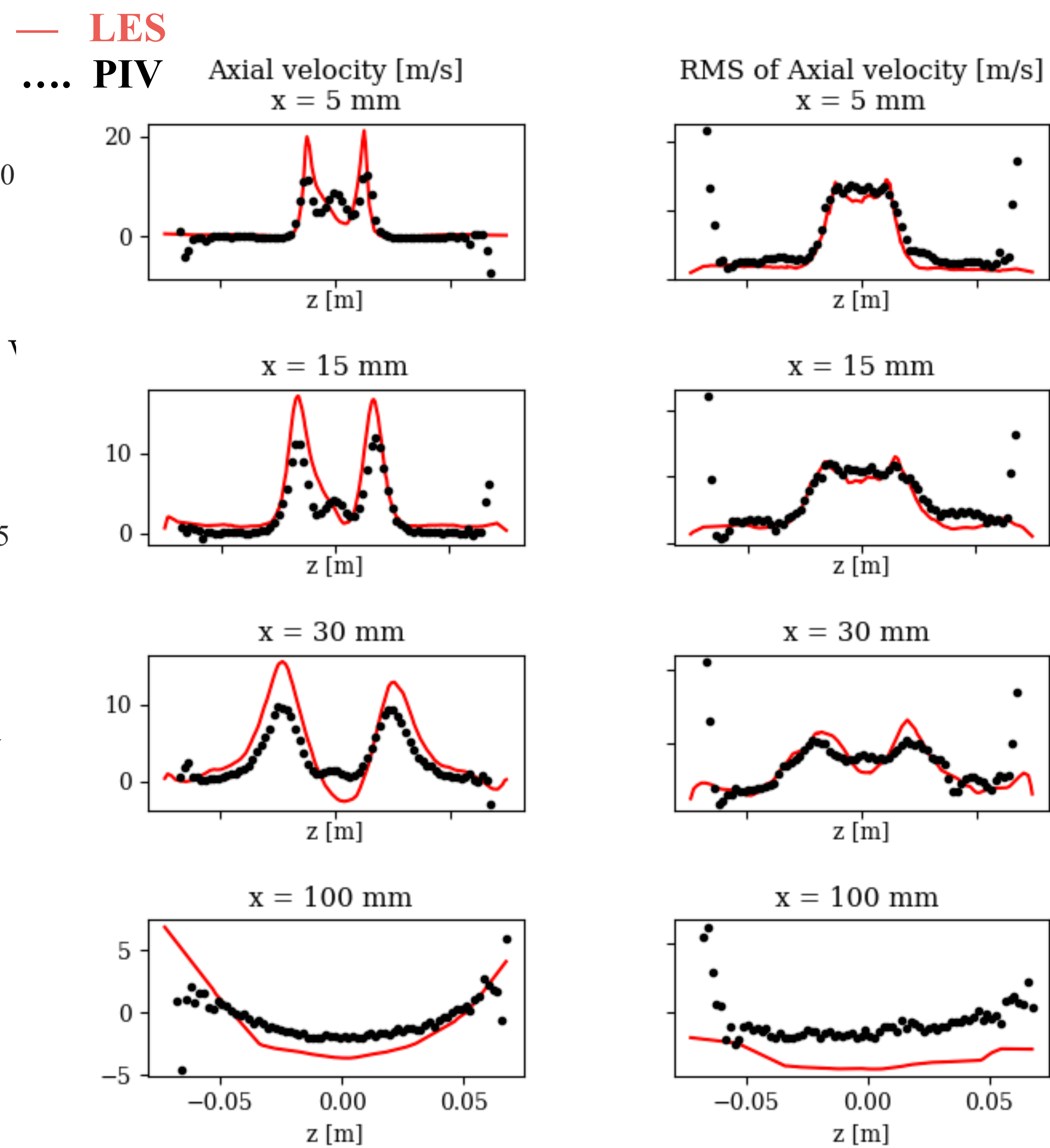
Oxytec chamber: Validation
Axial velocity



Oxytec chamber: Validation

Axial velocity



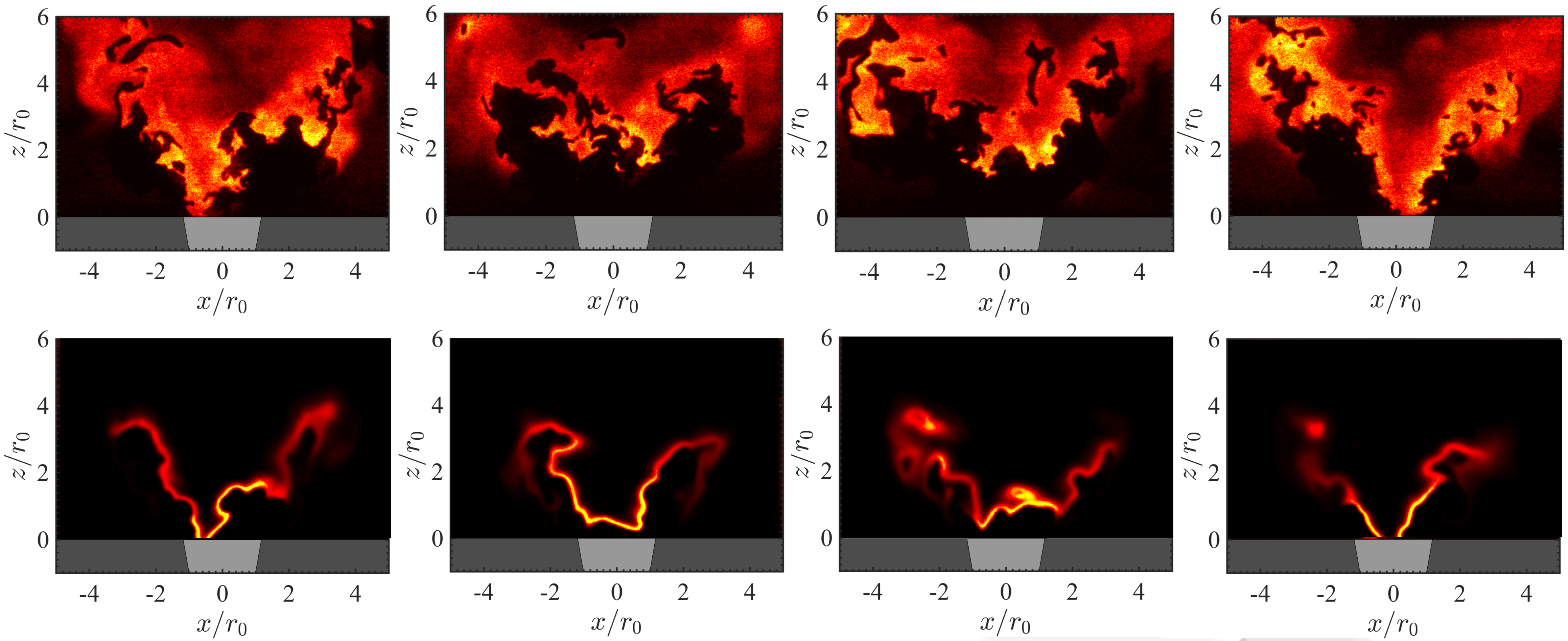


- Position of stagnation point not retrieved
- Central velocity peak not retrieved

Oxytec chamber: flame front

Exp OH-PLIF

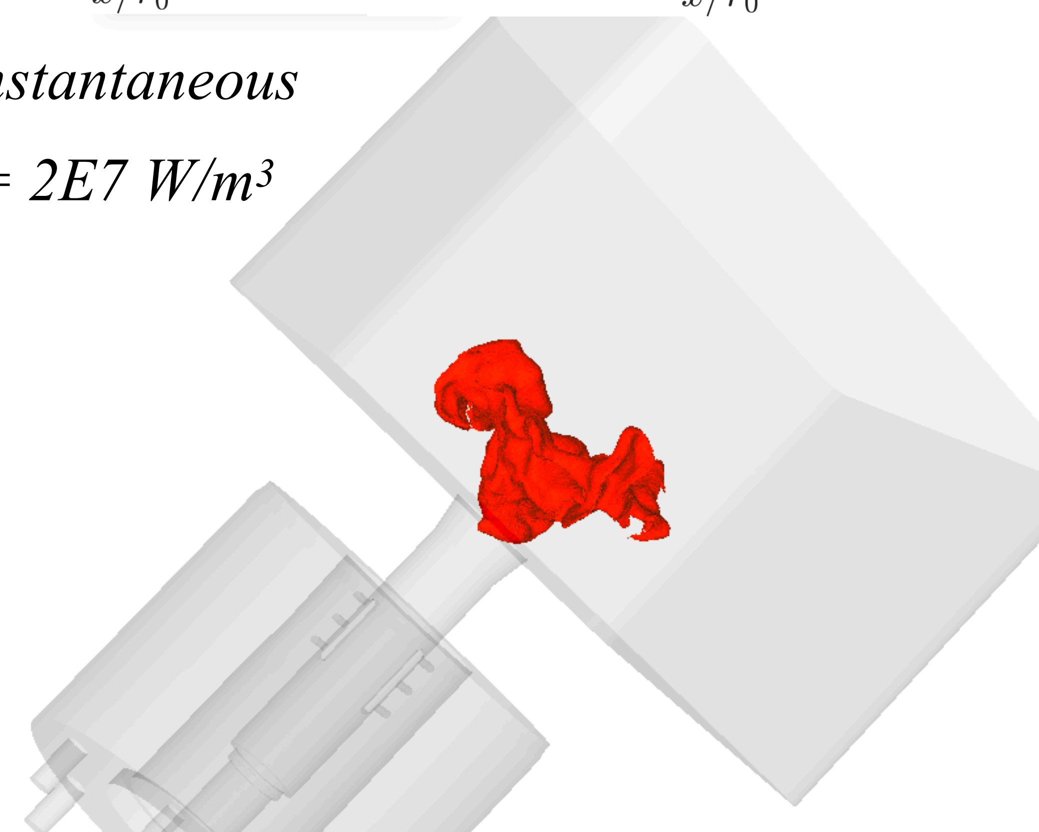
LES



Instantaneous HR-field

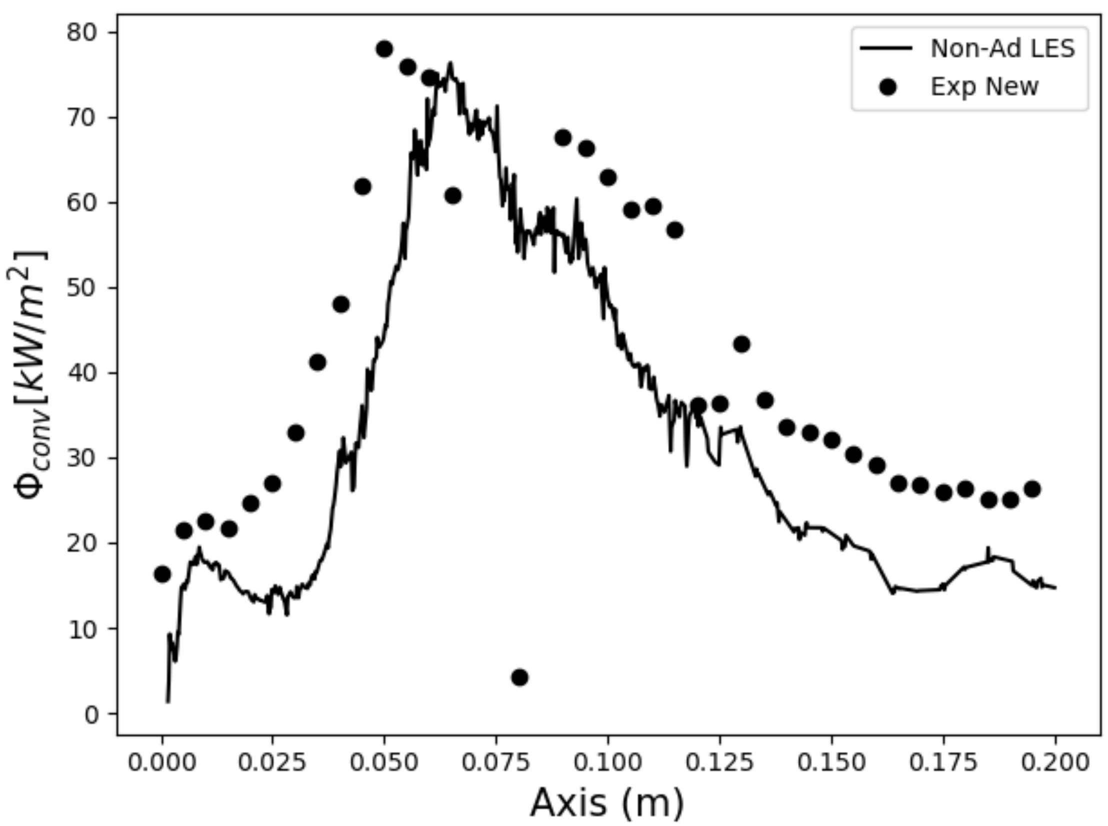
Iso-surface of instantaneous

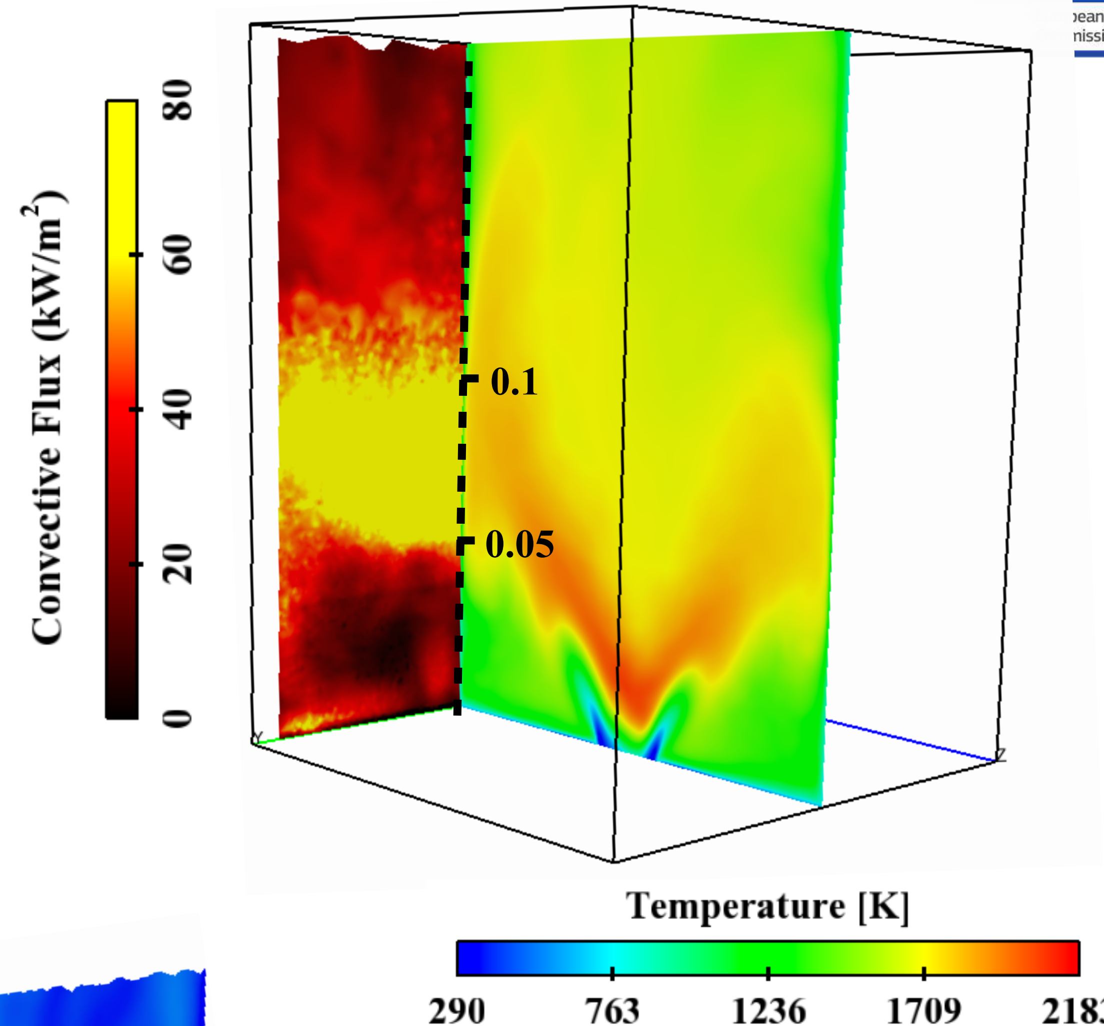
Heat Release = 2E7 W/m³



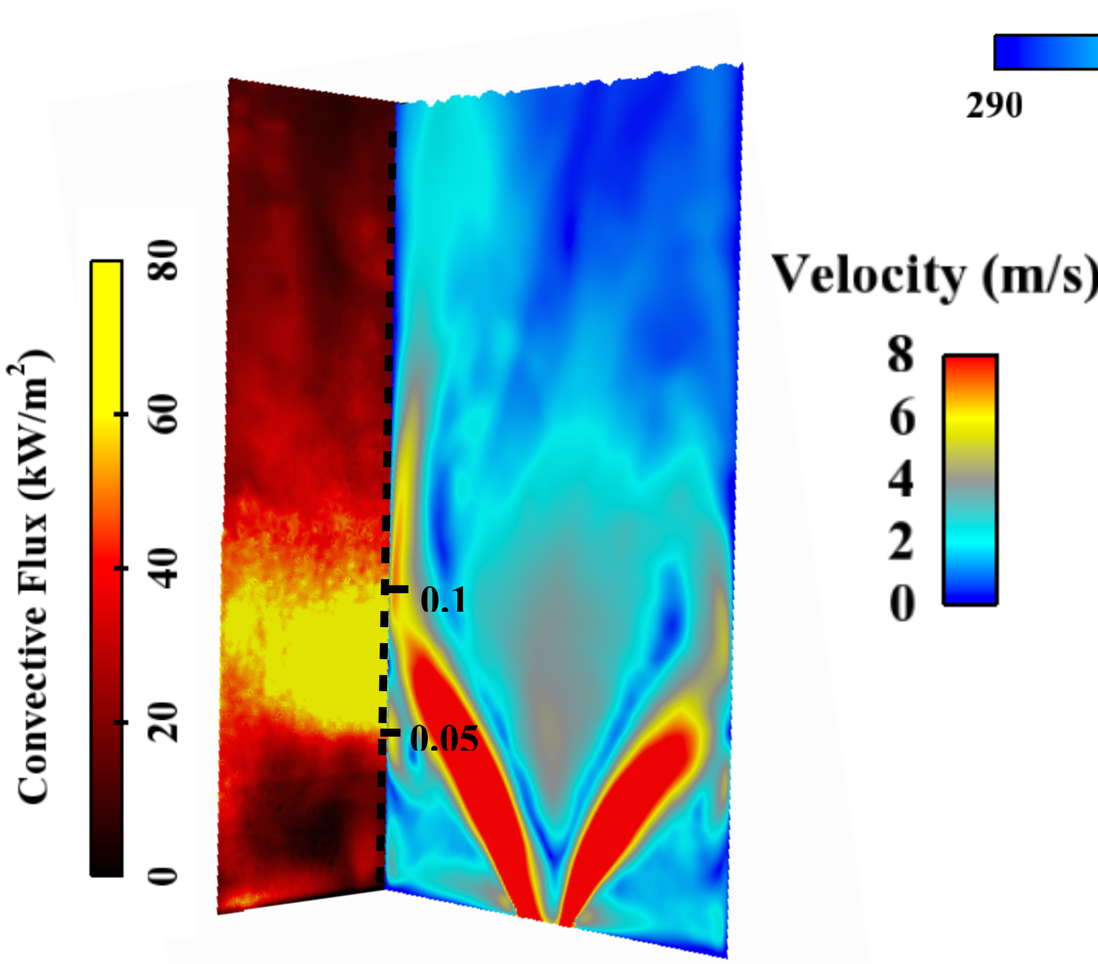
Highly fluctuating flame

Wall heat fluxes





- Good agreement
- Numerical fluxes are underestimated in some regions



Outline

LES of a premixed swirled flame

- *Presentation of Oxytec chamber*
- *LES results*

→

Conclusions

Some discrepancy about:

- *Flow topology*
- *Conductive fluxes*

Coupled simulations: numerical set-up

- *Monte Carlo solver*
- *CPU cost-accuracy trade off*

First results of coupled simulations

- *Impact of spectral properties of quartz*
- *Radiative heat transfer impact on a methane air flame*

Outline

LES of a premixed swirled flame

- *Presentation of Oxytec chamber*
- *LES results*

Coupled simulations: numerical set-up

- *Monte Carlo solver*
- *CPU cost-accuracy trade off*

First results of coupled simulations

- *Impact of spectral properties of quartz*
- *Radiative heat transfer impact on a methane air flame*

Conclusions

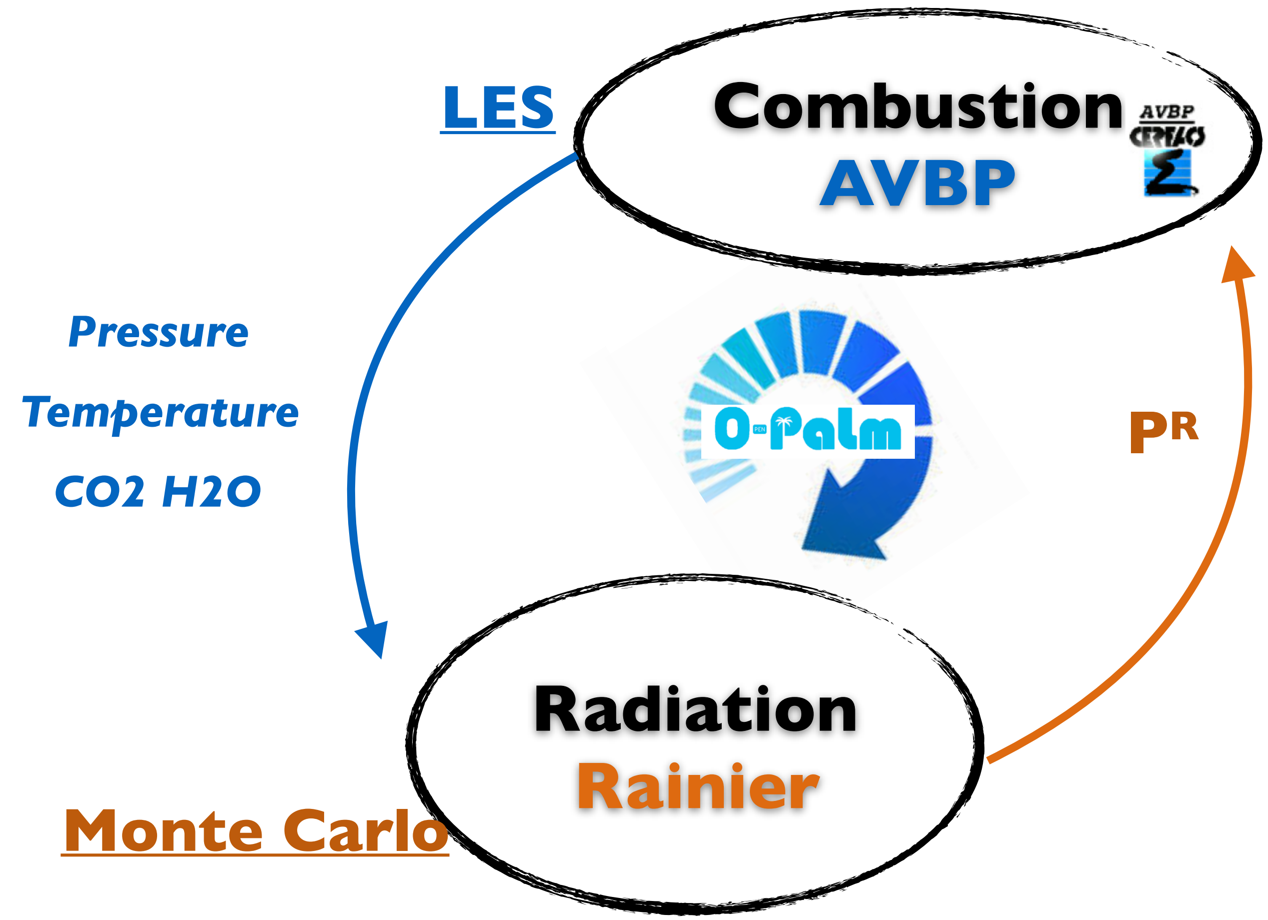
Some discrepancy about:

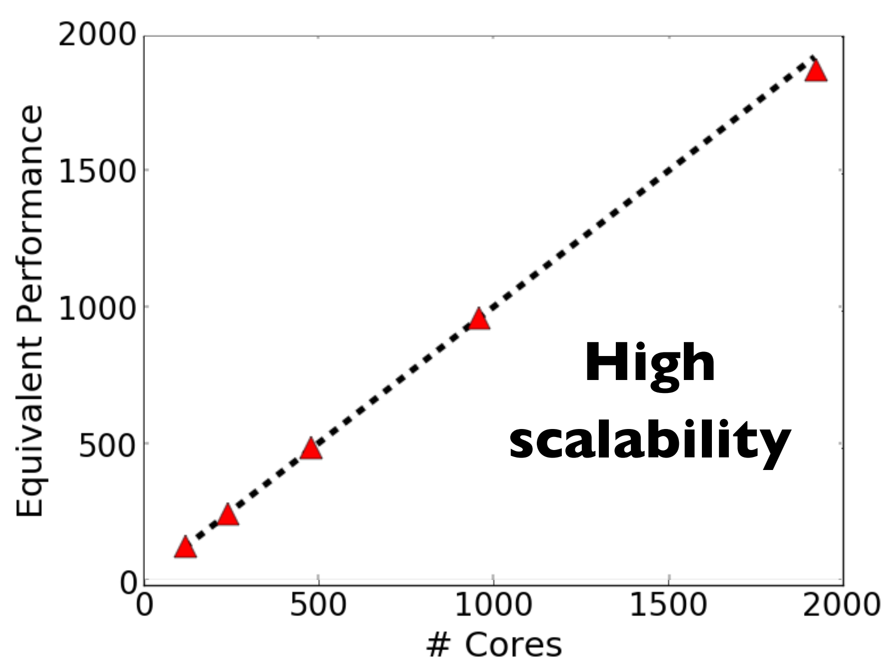
- *Flow topology*
- *Conductive fluxes*

LES coupled with MC radiation solver:

Radiation solver: Rainier

- Parallel code that solves the RTE
- Non-scattering medium
- SGS TRI are not taken into account
- **Quasi-Monte Carlo** method [1]:
  Emission-based Reciprocity Method (**ERM**) [2]
- Accurate model for gas radiative properties:
  correlated c-k distribution[3]





Radiative source term in energy conservation equation: P^R

$$P^R = \underbrace{\int_0^\infty \int_{4\pi} \kappa_\nu I_\nu d\Omega d\nu}_{P_{absorbed}} - \underbrace{4\pi \int_0^\infty \kappa_\nu I_\nu^0(T) d_\nu}_{P_{emitted}}$$

1 : Palluotto, L., Dumont, N., Rodrigues, P., Koren, C., Vicquelin, R., & Gicquel, O. 2017. « Comparison of Monte Carlo Methods Efficiency to Solve Radiative Energy Transfer in High Fidelity Unsteady 3D Simulations. » ASME Turbo Expo 2017

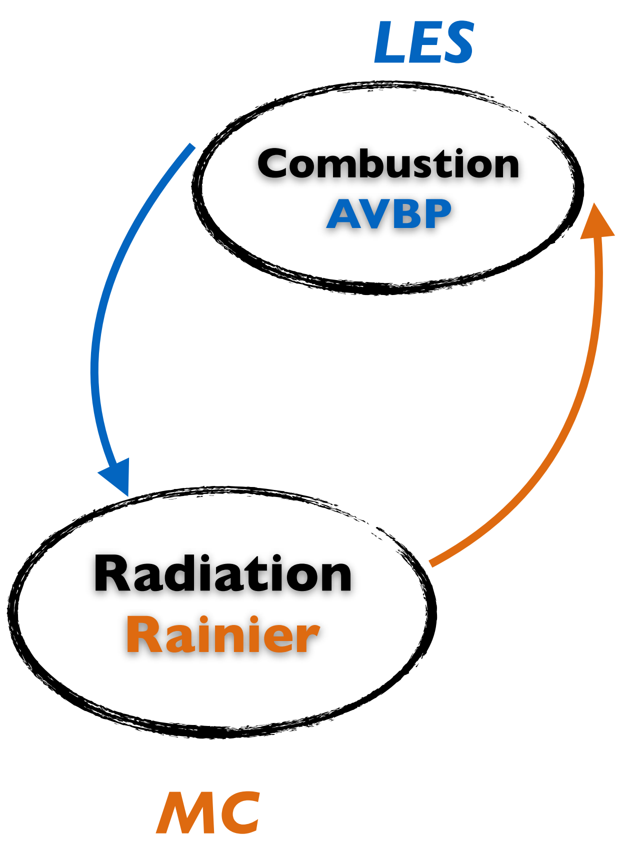
2 : L. Tessé, F. Dupoirieux, B. Zamuner and J. Taine, International Journal of Heat and Mass Transfer

3: Taine, J., and Soufiani, A., 1999. "Gas radiative properties: From spectroscopic data to approximate models". Vol. 33 of Advances in Heat Transfer . Elsevier, pp. 295 – 414.

LES-MC coupling

Questions:

- *Computational **grid** for **radiative** heat transfer simulation?*
    - ***Mesh convergence***



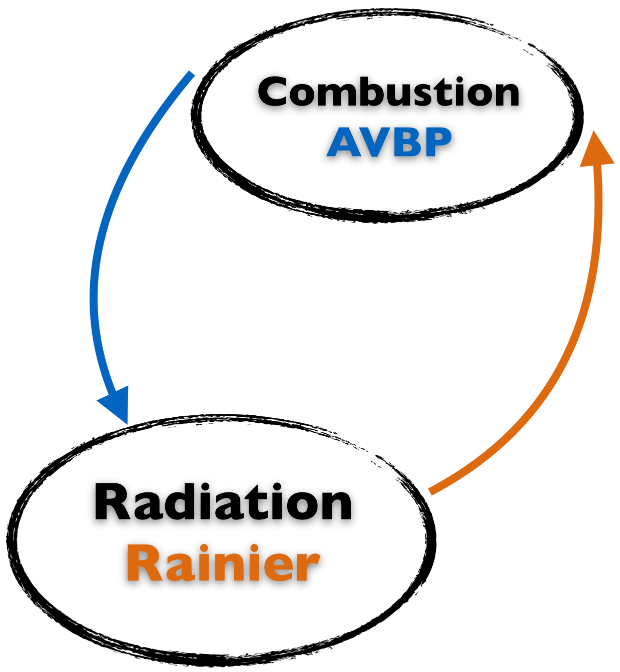
- *How often the solvers exchange data?*
    - ***Coupling error estimation***

CPU cost- accuracy trade off need to be found

Coupled Simulations:

Mesh Convergence

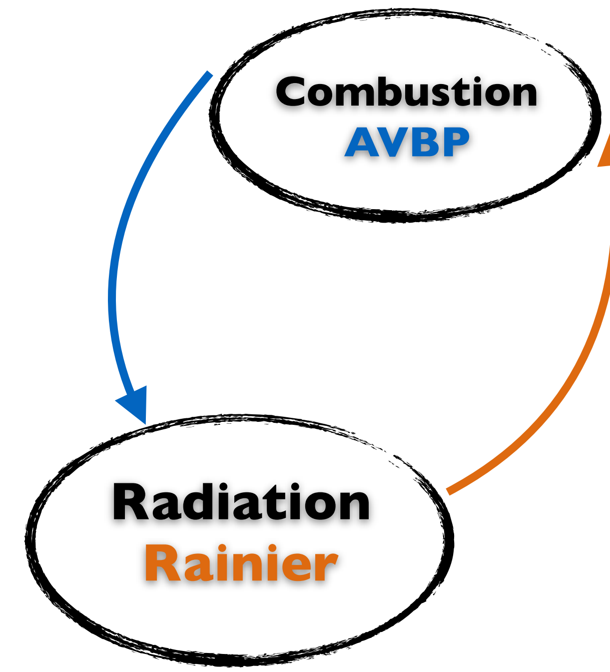
Mesh LES	Mesh nodes (millions)
Mesh 1	9



Coupled Simulations:

Mesh Convergence

Mesh LES	Mesh nodes (millions)
Mesh 1	9



Computational grid for radiative heat transfer simulation?

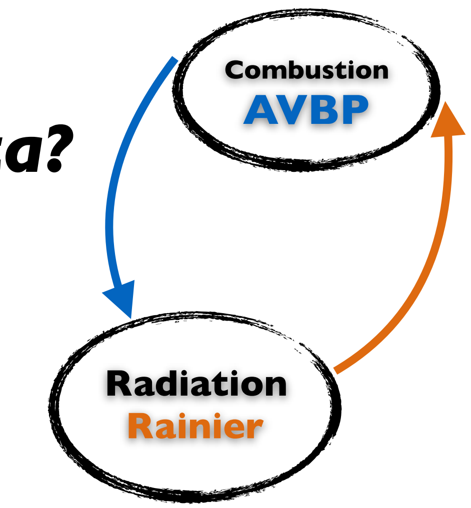
$$e_1 = \frac{\Phi_{rad} - \Phi_{rad,Sc1}}{\Phi_{rad,Sc1}}$$

Mesh Rainier	Mesh nodes (millions)	e_1 (%)	CPU time ratio
Mesh 1	9	-	-
Mesh 2	4	1.7 %	3
Mesh 3	2.7	2.2 %	5.6

Coupled Simulations:

Choice of Coupling Frequency

How often LES and radiation solvers exchange data?



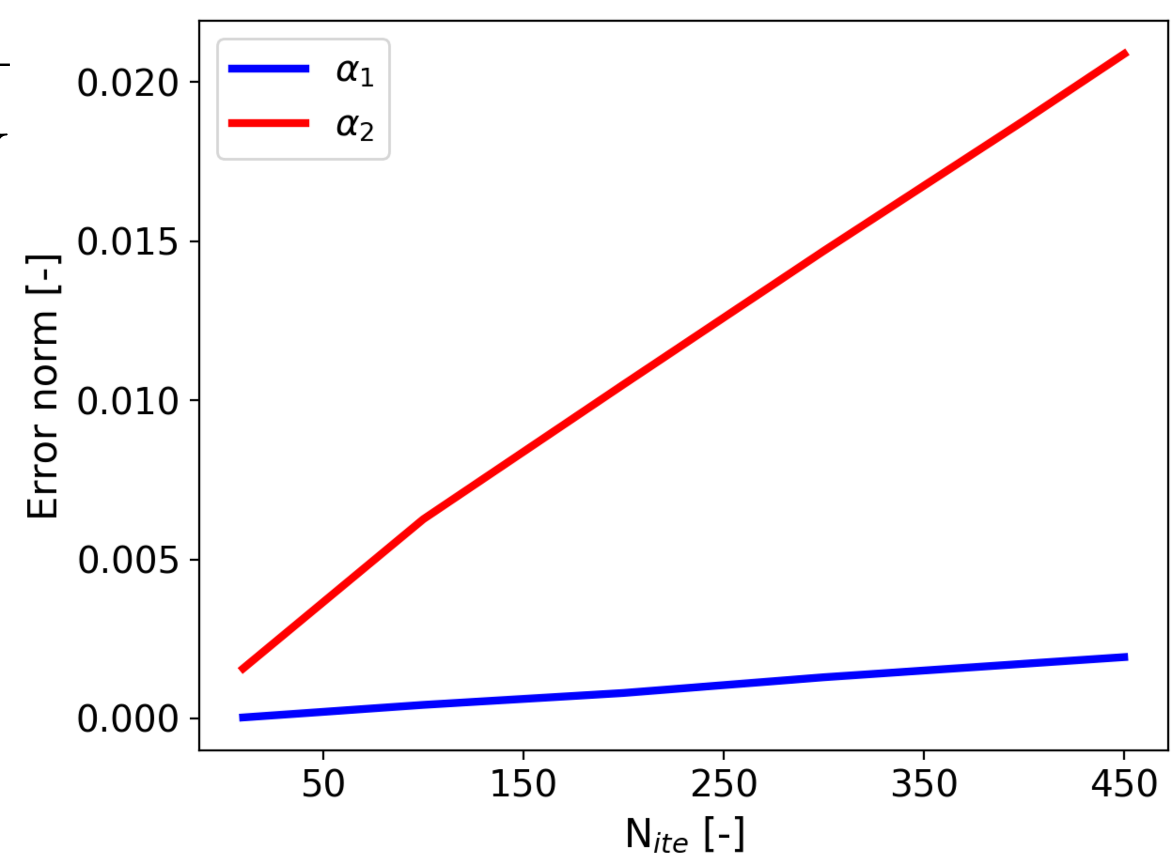
Error evaluated in terms of L2 error norm of temperature and radiative power

$$\alpha_1(N) = \sqrt{\int_V |T_N - T_0|^2 \, dV} \Big/ \sqrt{\int_V |T_0|^2 \, dV}$$

$$\alpha_2(N) = \sqrt{\int_V \left|P_N^R - P_0^R\right|^2 dV} \Big/ \sqrt{\int_V \left|P_0^R\right|^2 dV}$$

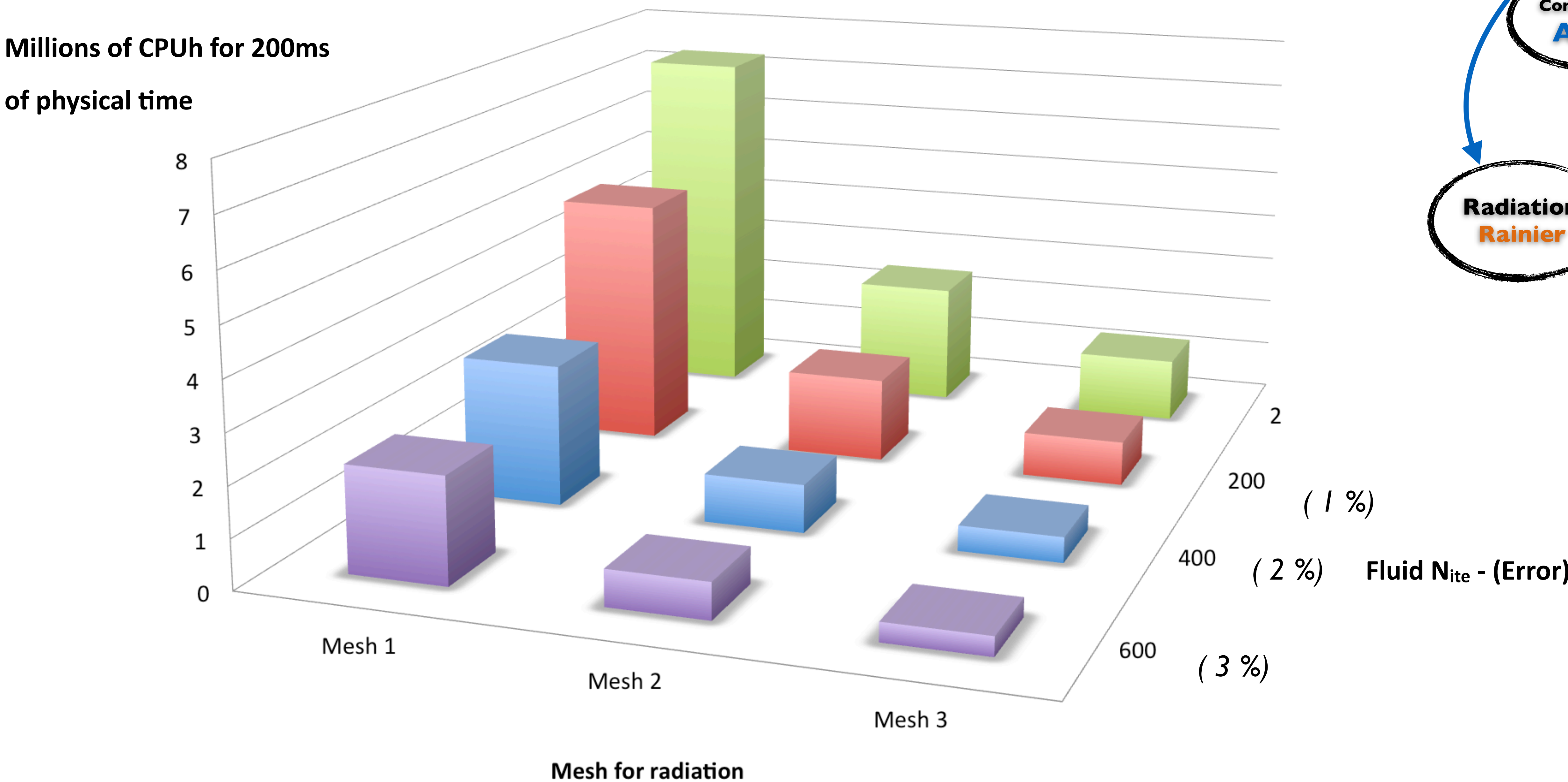
$_0$ = Variable at reference iteration 0

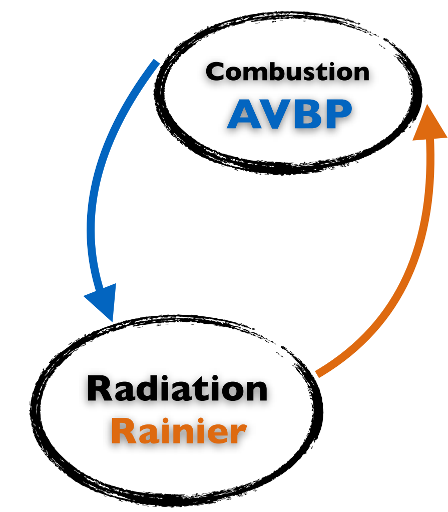
$_N$ = Variable at iteration N of the fluid solver



Coupled Simulations:

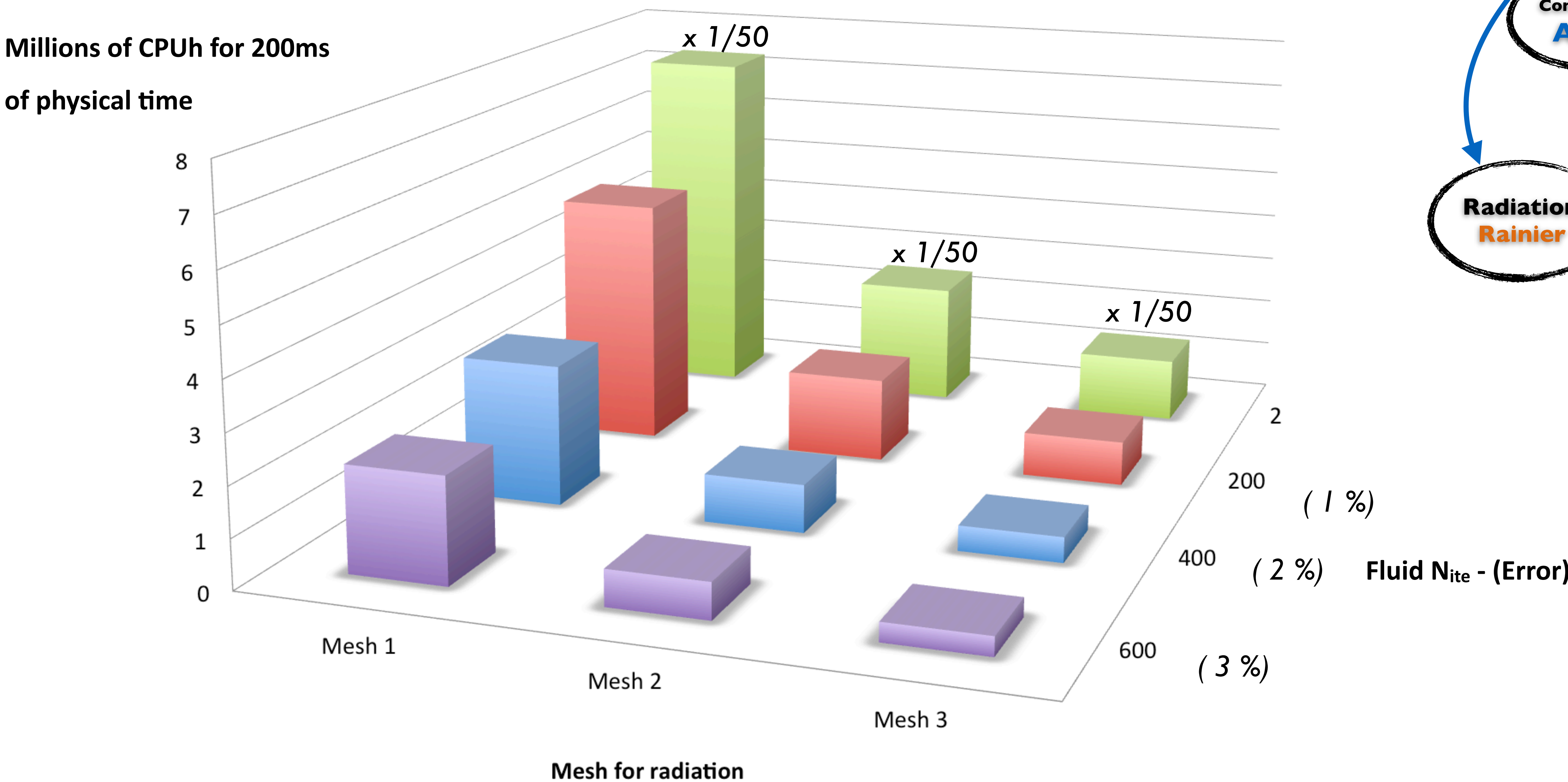
Trade-off CPU cost - accuracy

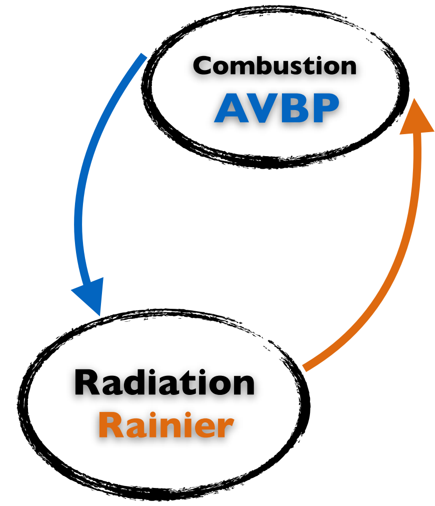




Coupled Simulations:

Trade-off CPU cost - accuracy





Coupled Simulations:

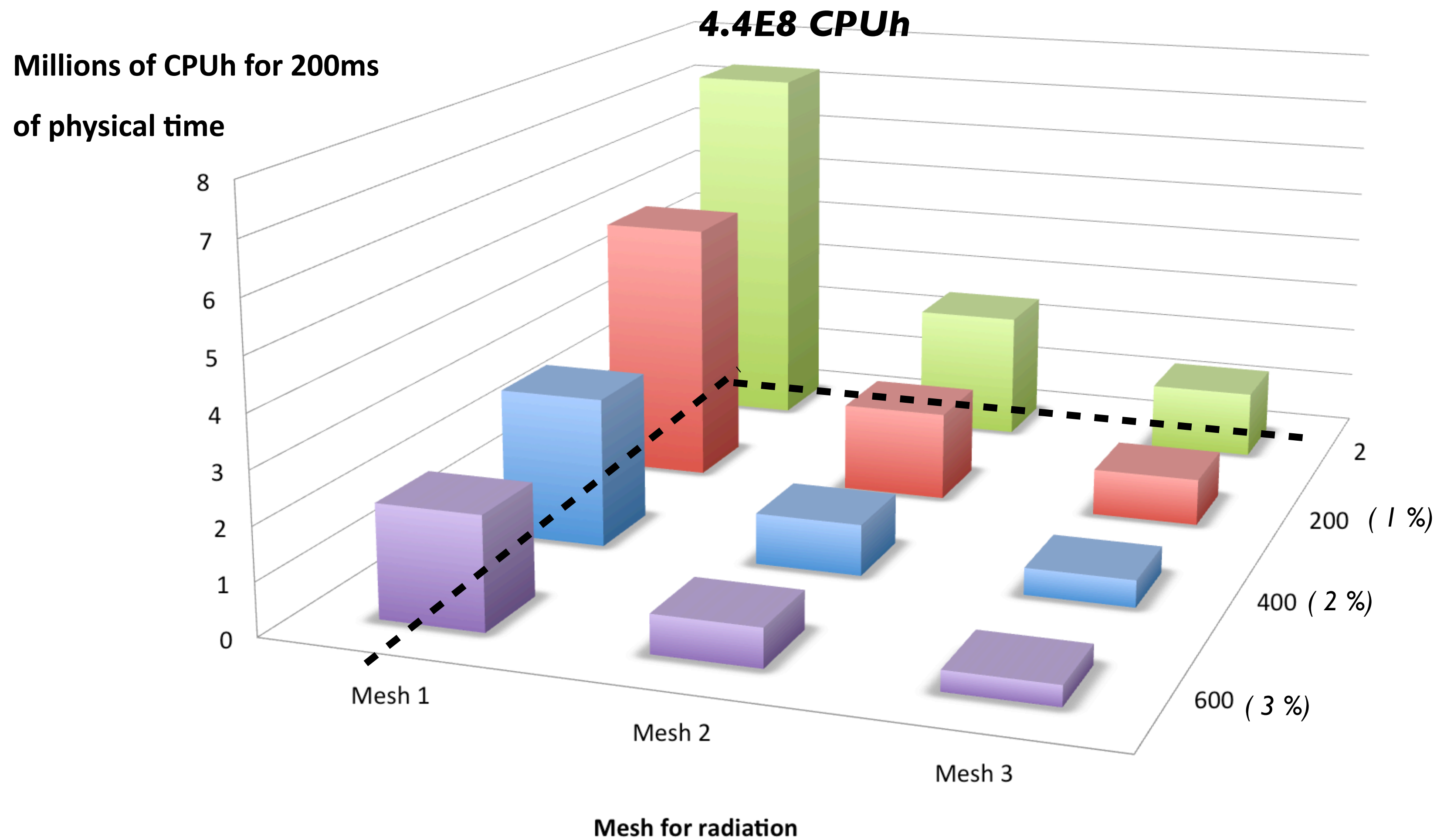
Trade-off CPU cost - accuracy

Scenarios

Optimistic:

Mesh 1 (9M nodes)

Coupling every iteration of fluid solver



Coupled Simulations:

Trade-off CPU cost - accuracy

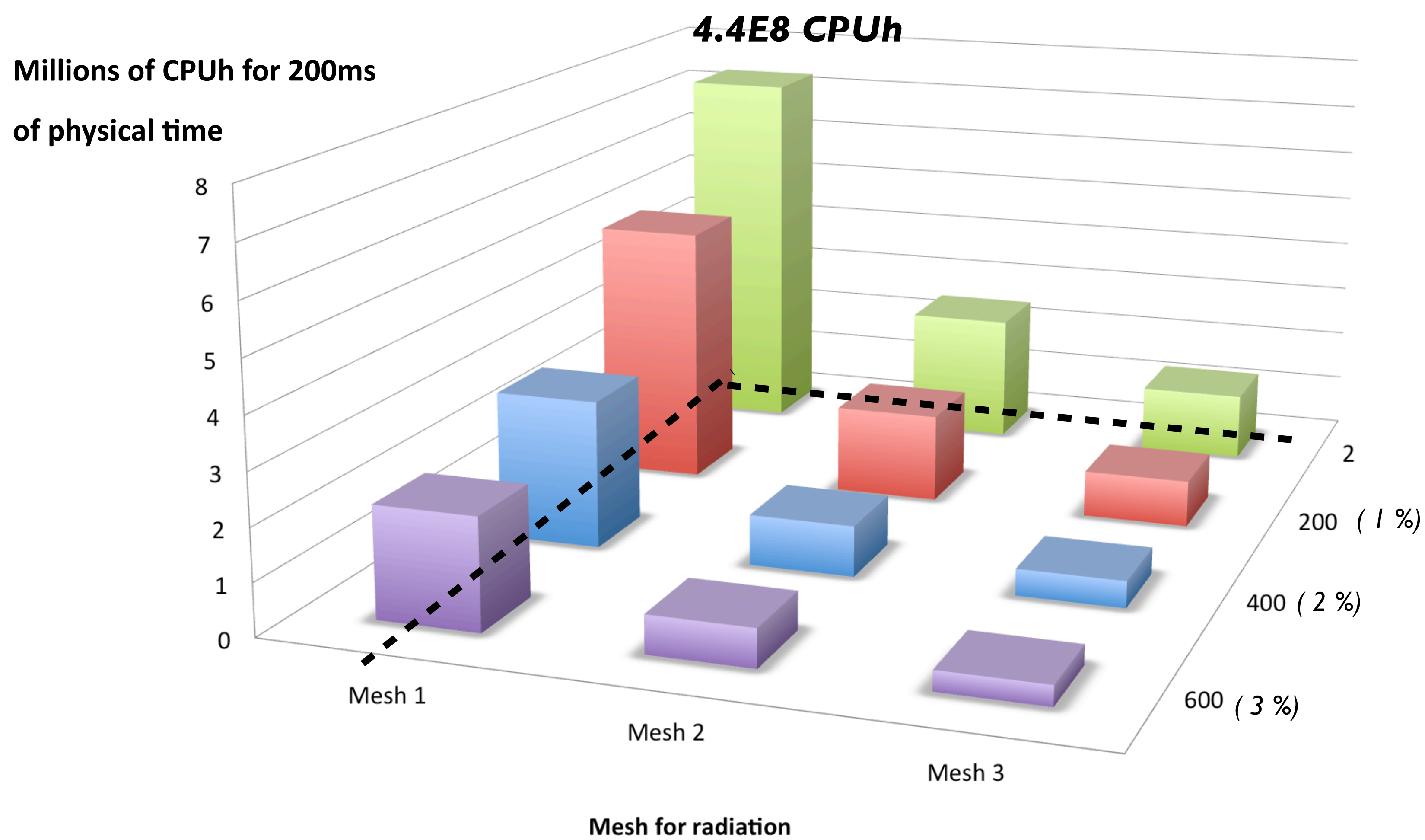
Scenarios

Optimistic:

Mesh 1 (9M nodes)

Coupling every iteration of fluid solver

4.4E8 CPUh = 20 years at 2400 cores



Coupled Simulations:

Trade-off CPU cost - accuracy

Scenarios

Optimistic:

Mesh 1 (9M nodes)

Coupling every iteration of fluid solver

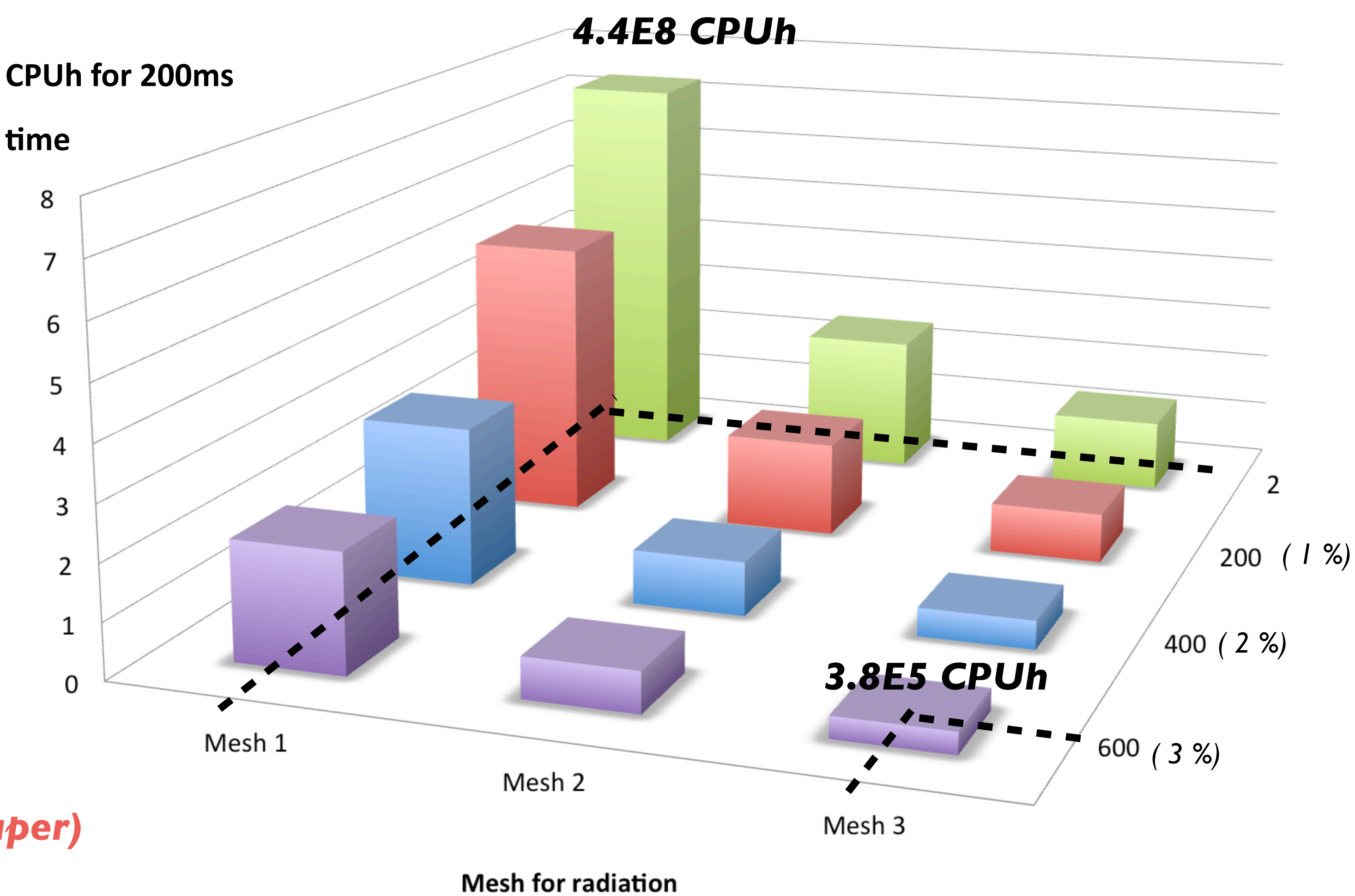
4.4E8 CPUh = 20 years at 2400 cores

Pessimistic:

Mesh 3 (2.7M nodes)

Coupling every 600 iterations of fluid solver

3.8E5 CPUh = 7 days at 2400 cores (1000 times cheaper)



Coupled Simulations:

Trade-off CPU cost - accuracy

Scenarios

Optimistic:

Mesh 1 (9M nodes)

Coupling every iteration of fluid solver

4.4E8 CPUh = 20 years at 2400 cores

Pessimistic:

Mesh 3 (2.7M nodes)

Coupling every 600 iterations of fluid solver

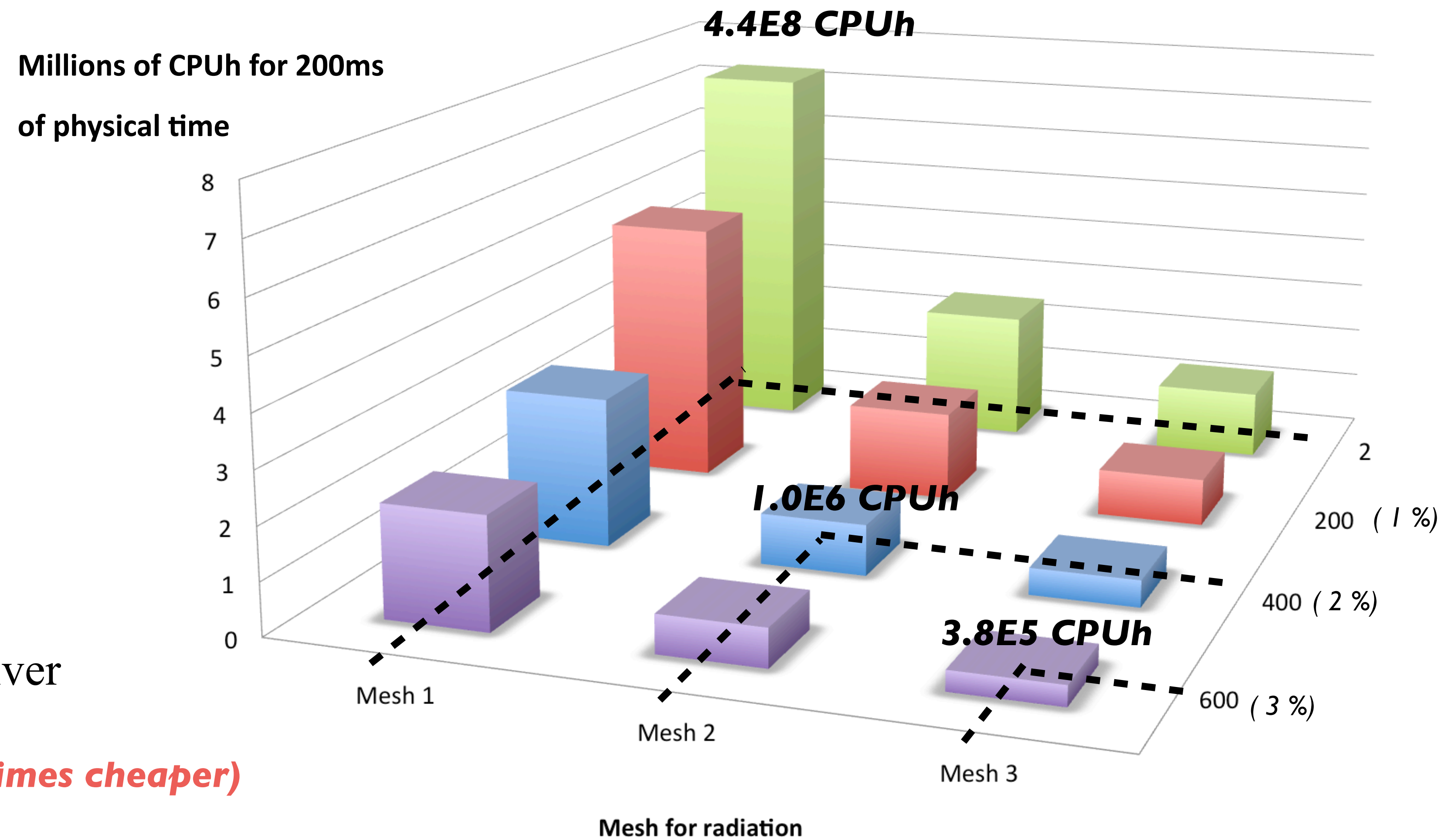
3.8E5 CPUh = 7 days at 2400 cores (1000 times cheaper)

Intermediate:

Mesh 2 (4M nodes)

Coupling every 400 iterations of fluid solver

1E6 CPUh = 20 days at 2400 cores



Coupled Simulations:

Trade-off CPU cost - accuracy

Scenarios

Optimistic:

Mesh 1 (9M nodes)

Coupling every iteration of fluid solver

4.4E8 CPUh = 20 years at 2400 cores

Pessimistic:

Mesh 3 (2.7M nodes)

Coupling every 600 iterations of fluid solver

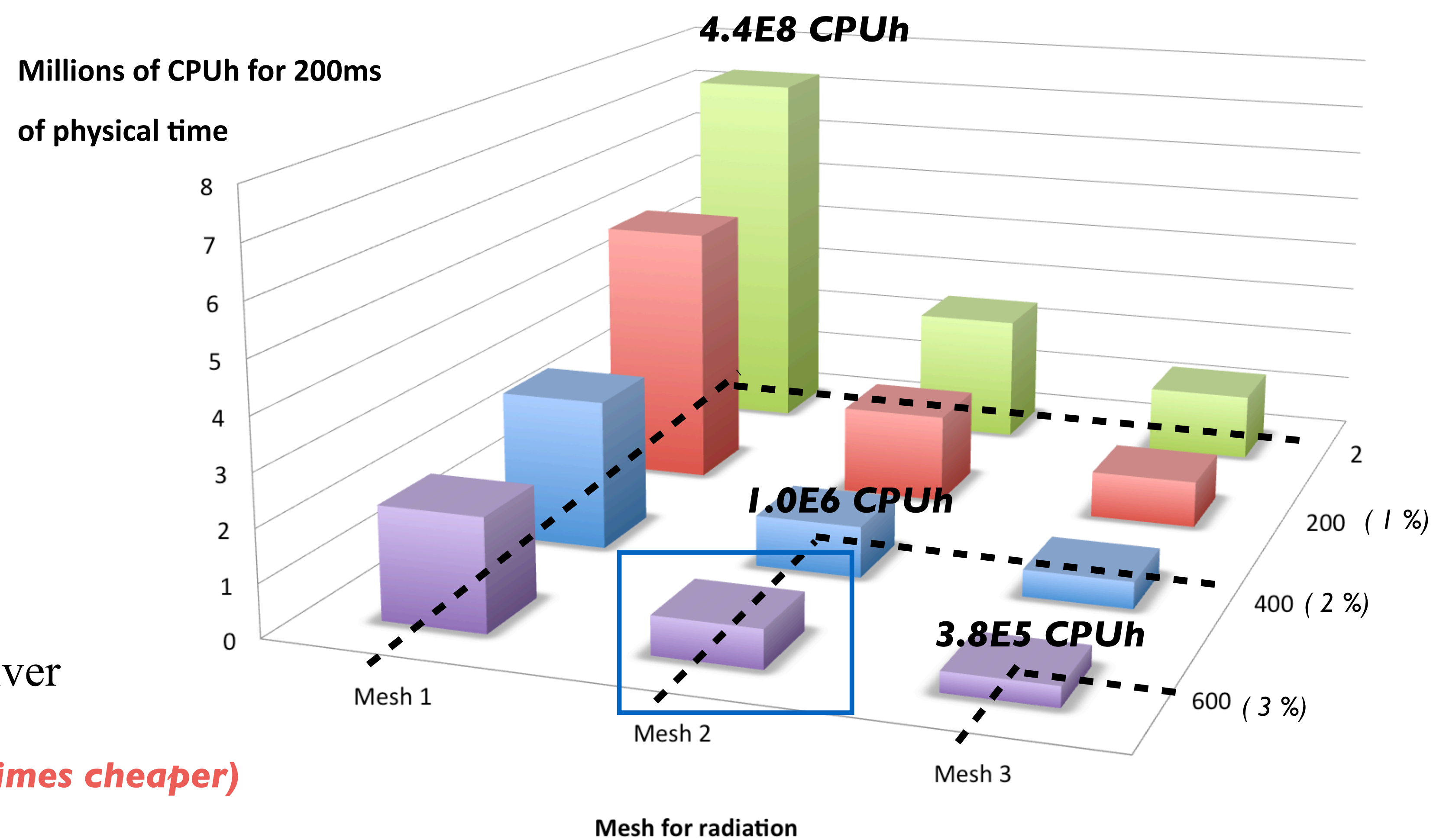
3.8E5 CPUh = 7 days at 2400 cores (1000 times cheaper)

Intermediate:

Mesh 2 (4M nodes)

Coupling every 400 iterations of fluid solver

1E6 CPUh = 20 days at 2400 cores



Chosen scenario:

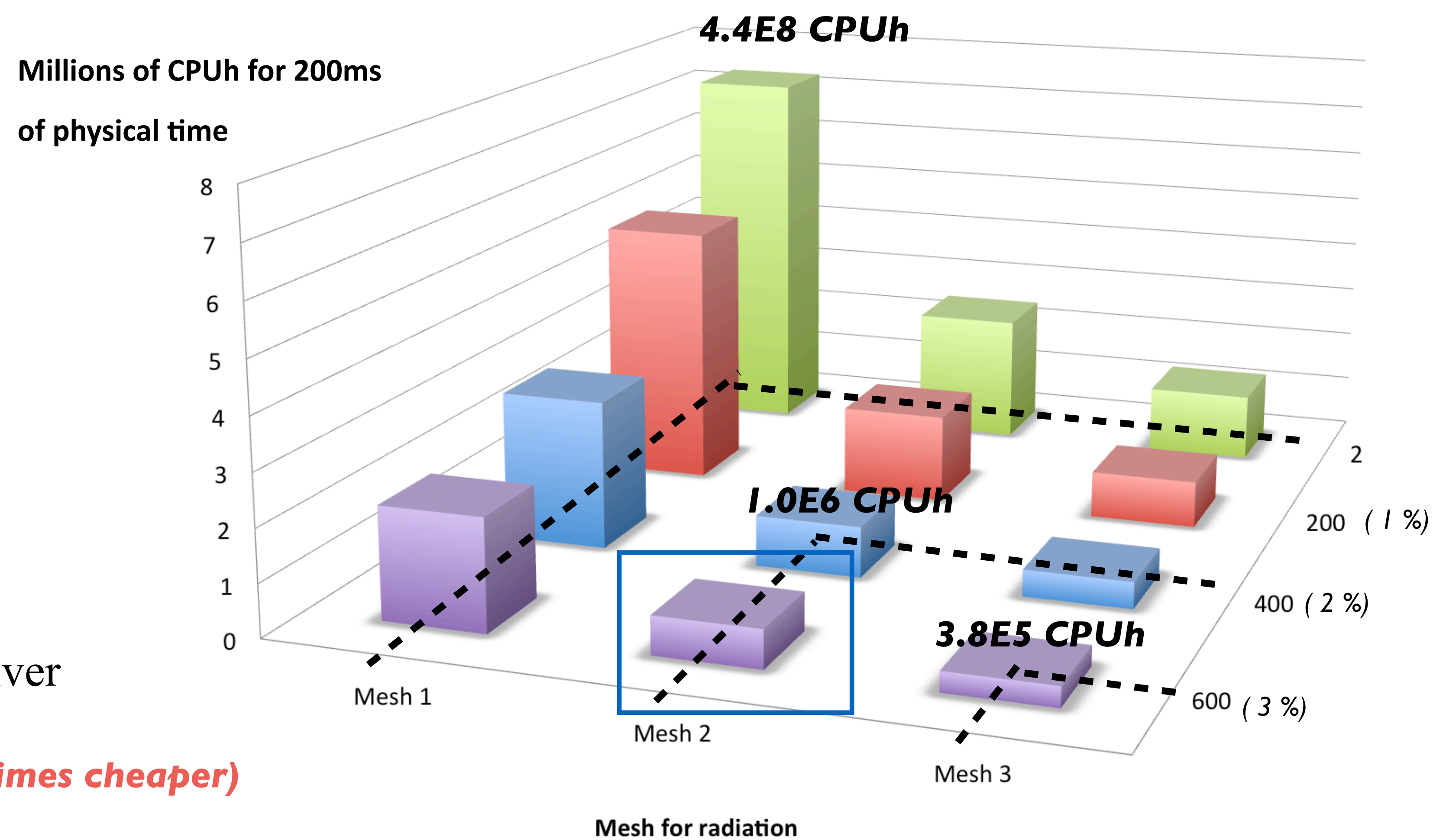
Mesh 2 (4M nodes)

Coupling every 600 iterations of fluid solver

7.2E5 CPUh = 12.5 days at 2400 cores

Coupled Simulations:

Trade-off CPU cost - accuracy



Scenarios

Optimistic:

Mesh 1 (9M nodes)

Coupling every iteration of fluid solver

4.4E8 CPUh = 20 years at 2400 cores

Pessimistic:

Mesh 3 (2.7M nodes)

Coupling every 600 iterations of fluid solver

3.8E5 CPUh = 7 days at 2400 cores (1000 times cheaper)

Intermediate:

Mesh 2 (4M nodes)

Coupling every 400 iterations of fluid solver

1E6 CPUh = 20 days at 2400 cores

Chosen scenario:

Mesh 2 (4M nodes)

Coupling every 600 iterations of fluid solver

7.2E5 CPUh = 12.5 days at 2400 cores

$$\text{Extra Cost} = \frac{\text{CPU time coupled simulation}}{\text{CPU time LES combustion simulation}} = 3.27$$

With QMC

Coupled Simulations:

Trade-off CPU cost - accuracy

Scenarios

Optimistic:

Mesh 1 (9M nodes)

Coupling every iteration of fluid solver

4.4E8 CPUh = 20 years at 2400 cores

Pessimistic:

Mesh 3 (2.7M nodes)

Coupling every 600 iterations of fluid solver

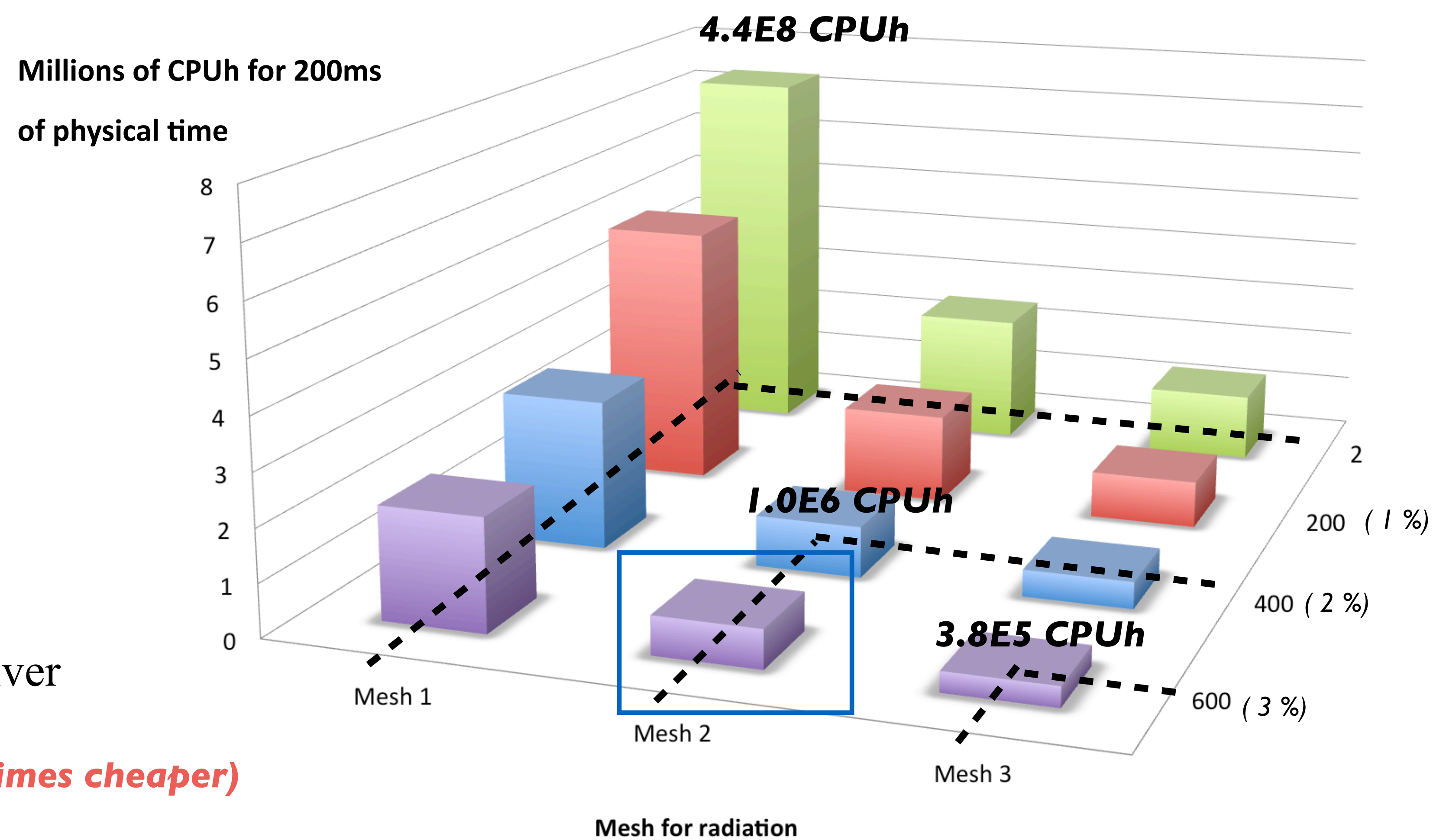
3.8E5 CPUh = 7 days at 2400 cores (1000 times cheaper)

Intermediate:

Mesh 2 (4M nodes)

Coupling every 400 iterations of fluid solver

1E6 CPUh = 20 days at 2400 cores



Chosen scenario:

Mesh 2 (4M nodes)

Coupling every 600 iterations of fluid solver

7.2E5 CPUh = 12.5 days at 2400 cores

$$\text{Extra Cost} = \frac{\text{CPU time coupled simulation}}{\text{CPU time LES combustion simulation}} = 3.27$$

With QMC

$$\text{Extra Cost} > 6$$

With MC

Outline

LES of a premixed swirled flame

- *Presentation of Oxytec chamber*
- *LES results*

Coupled simulations: numerical set-up

- *Monte Carlo solver*
- *CPU cost-accuracy trade off*

→

Conclusions

- *Mesh size for radiation : 4 millions nodes*
- *Coupling frequency : 600 iterations*

First results of coupled simulations

- *Impact of spectral properties of quartz*
- *Radiative heat transfer impact on a methane air flame*

Outline

LES of a premixed swirled flame

- *Presentation of Oxytec chamber*
- *LES results*

Coupled simulations: numerical set-up

- *Monte Carlo solver*
- *CPU cost-accuracy trade off*

→

Conclusions

- *Mesh size for radiation : 4 millions nodes*
- *Coupling frequency : 600 iterations*

First results of coupled simulations

- *Impact of spectral properties of quartz*
- *Radiative heat transfer impact on a methane air flame*

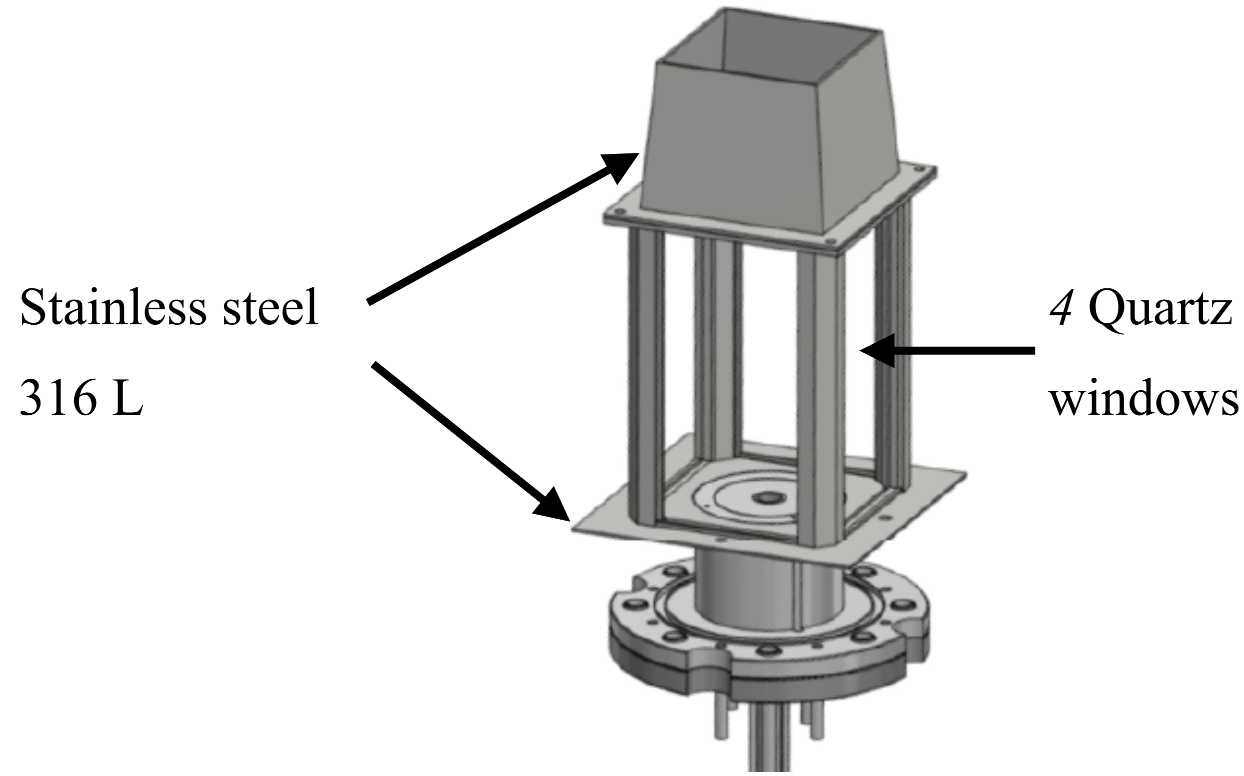
Coupled Simulations:

Boundary Conditions for radiation solver

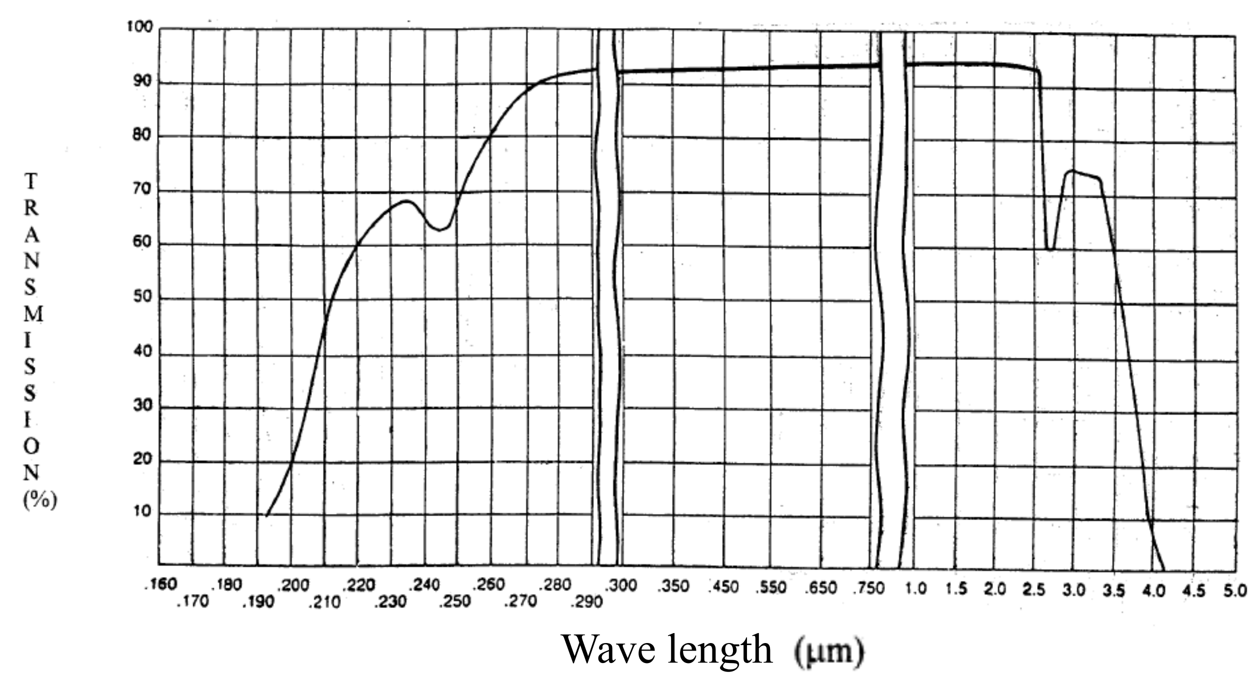
- ***Opaque walls:***
  - *Measured wall temperature*
  - *Stainless Steel emissivity*[1]

    Bottom chamber : 0.28

    Convergent : 0.32



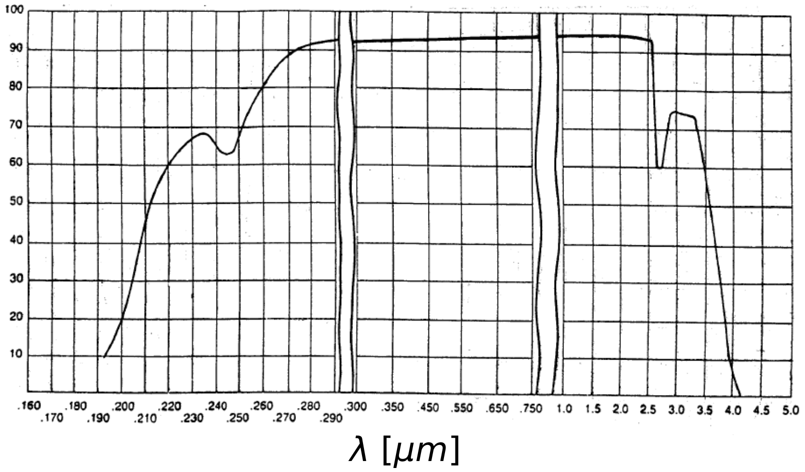
- ***Quartz windows:***
  - *Measured quartz temperature*
  - *Spectral radiative properties*



Transmissivity of a window of fused silica VI 942 between 0.16 and 5.0 micrometers.

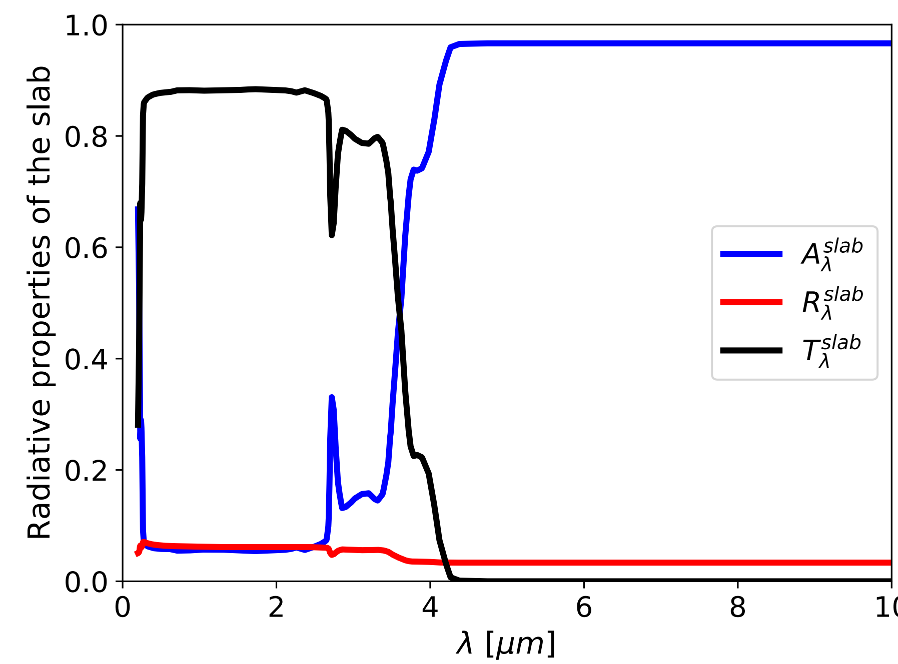
[1] Hunnewell, Tristan S., et al. "Total Hemispherical Emissivity of SS 316L with Simulated Very High Temperature Reactor Surface Conditions." *Nuclear Technology* (2017)

Semi-transparent quartz windows



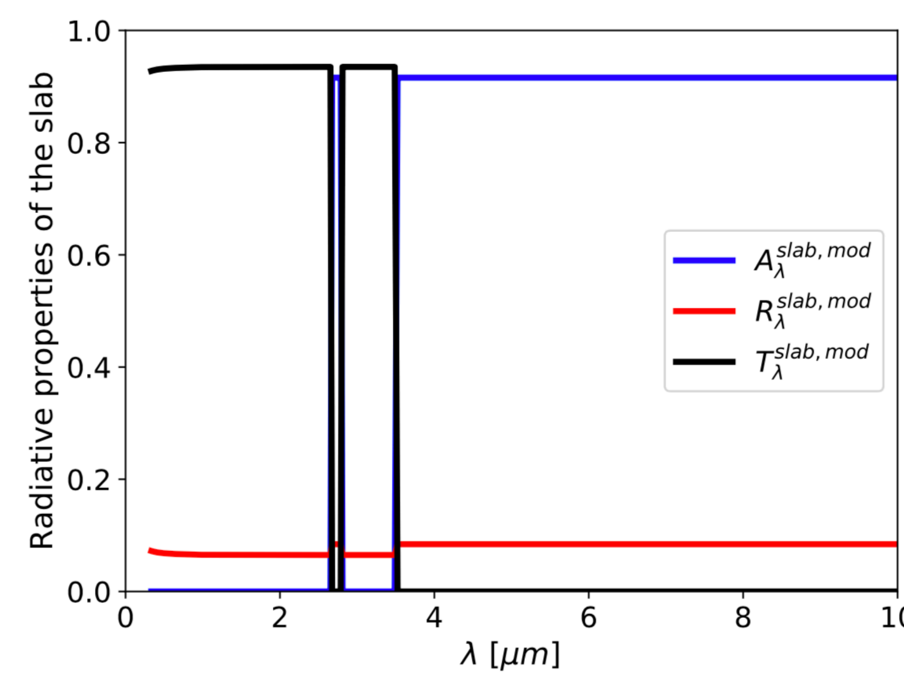
Transmissivity of a window of fused silica VI 942 between 0.16 and 5.0 micrometers.

Slab properties



Simplified band model[1]

T_λ^{slab}	$<$	T_{slab}^{switch}	Opaque
T_λ^{slab}	$>$	T_{slab}^{switch}	Transparent



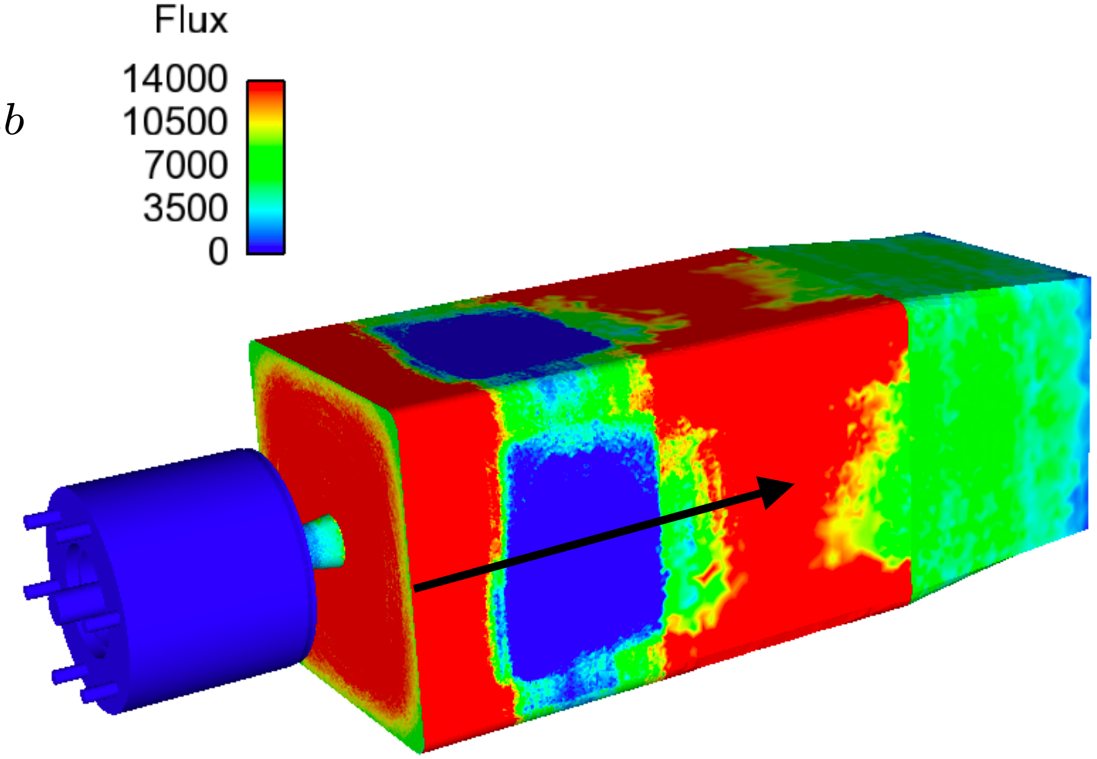
[1] Rodrigues, P., et al. "Assessment of External Heat Transfer Modeling of a Laboratory-Scale Combustor Inside a Pressure-Housing Environment." *ASME Turbo Expo 2018:* 2018.

Impact of quartz spectral properties

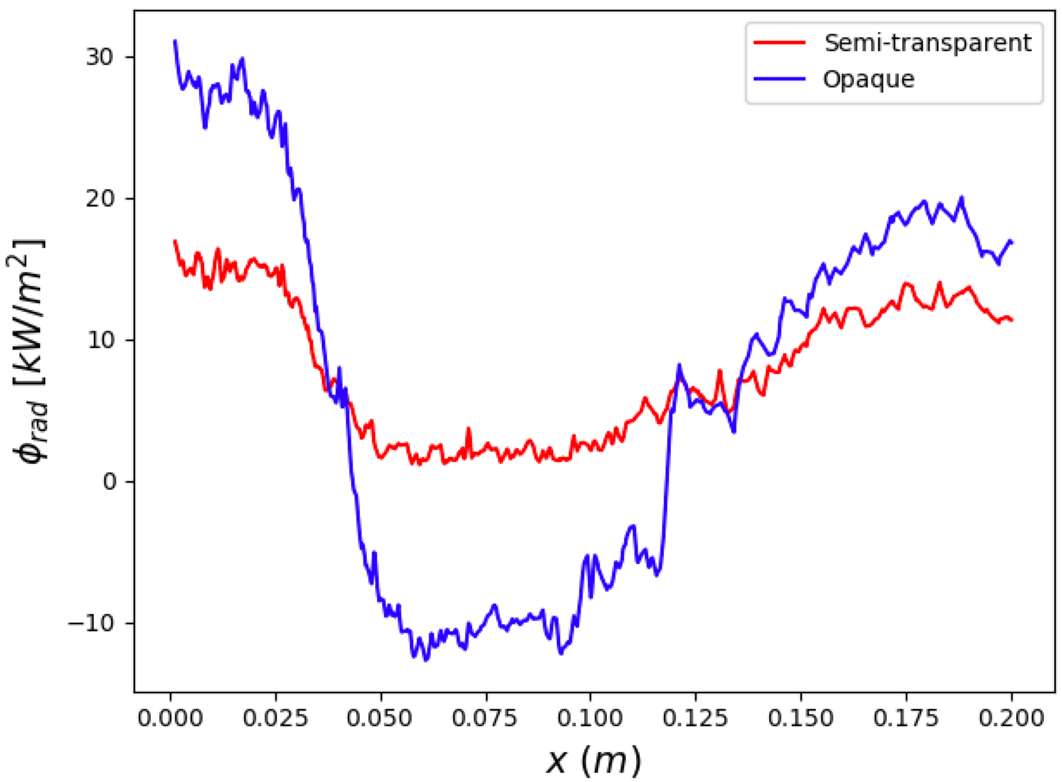
Opaque

$$A_\lambda^{slab} = 1 - R_\lambda^{slab}$$

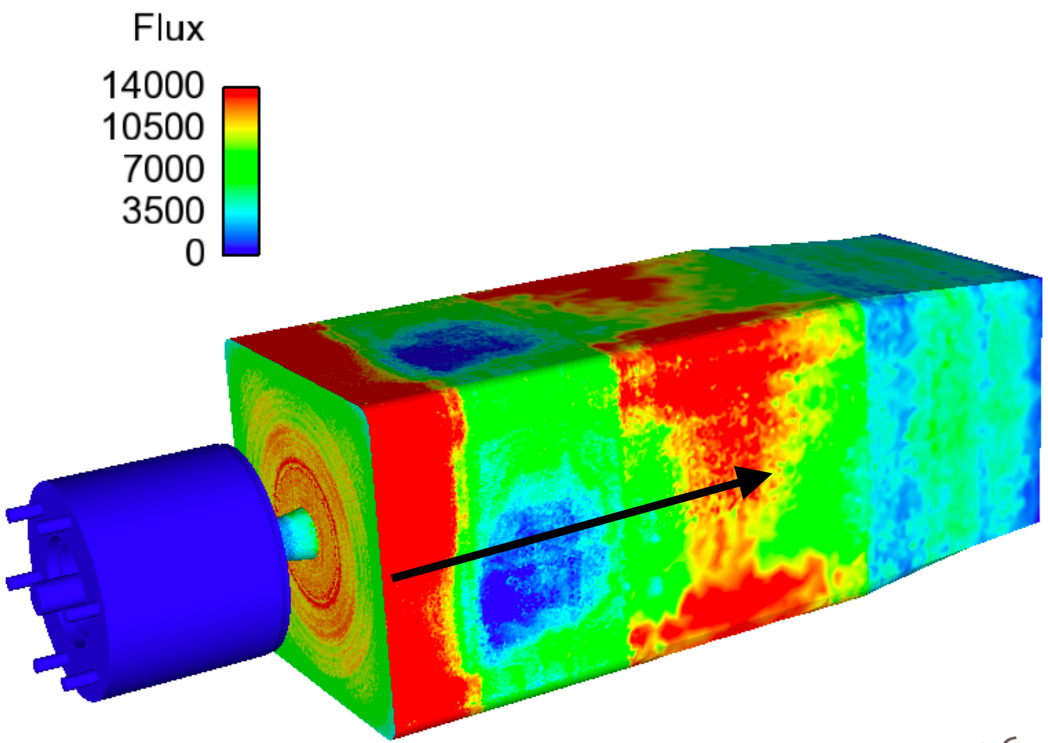
$$T_\lambda^{slab} = 0$$



Radiative Flux



Semi-transparent

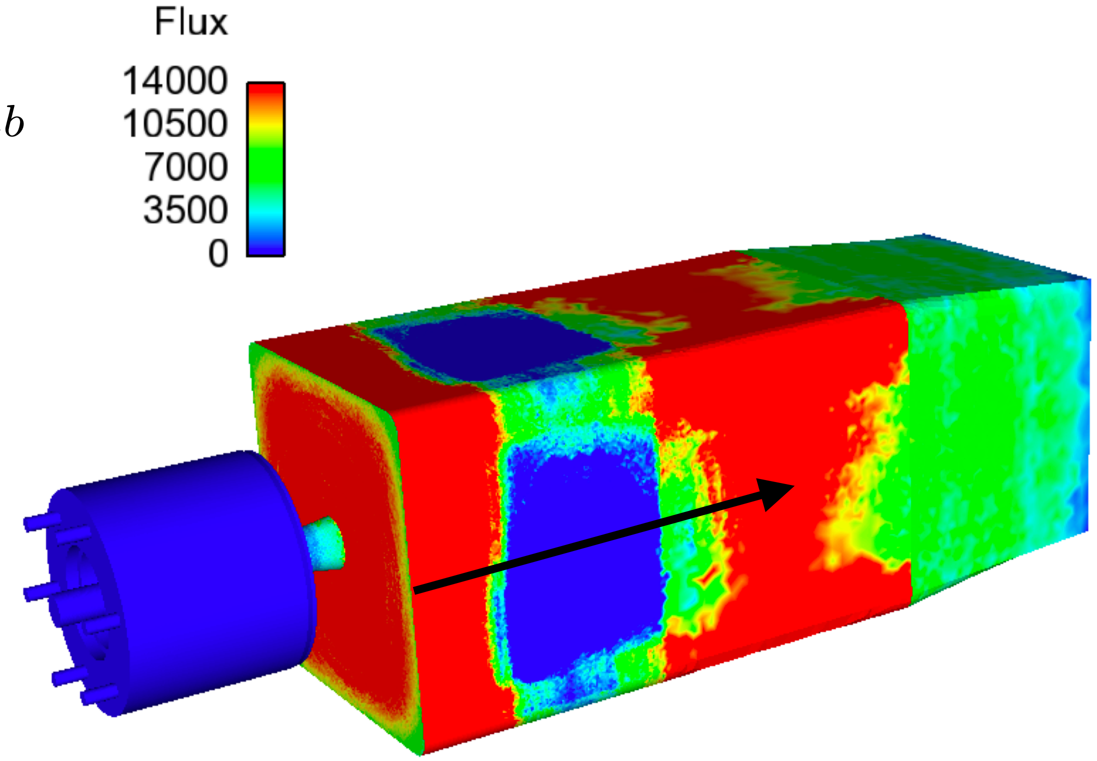


Impact of quartz spectral properties

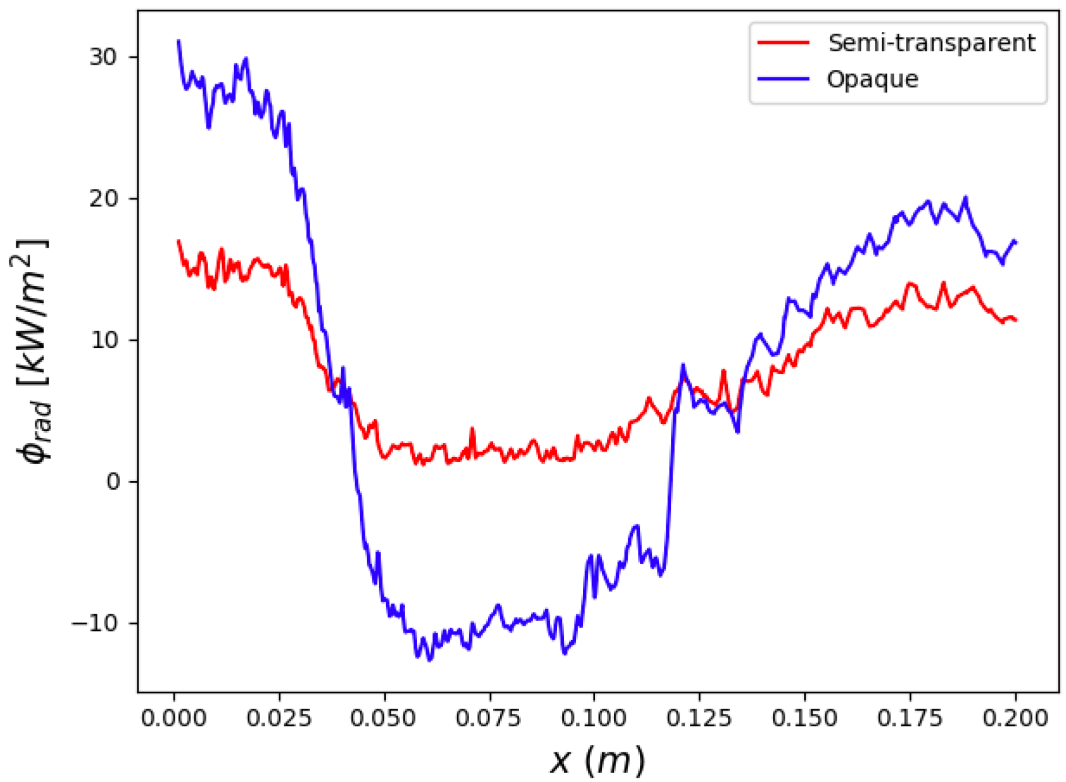
Opaque

$$A_\lambda^{slab} = 1 - R_\lambda^{slab}$$

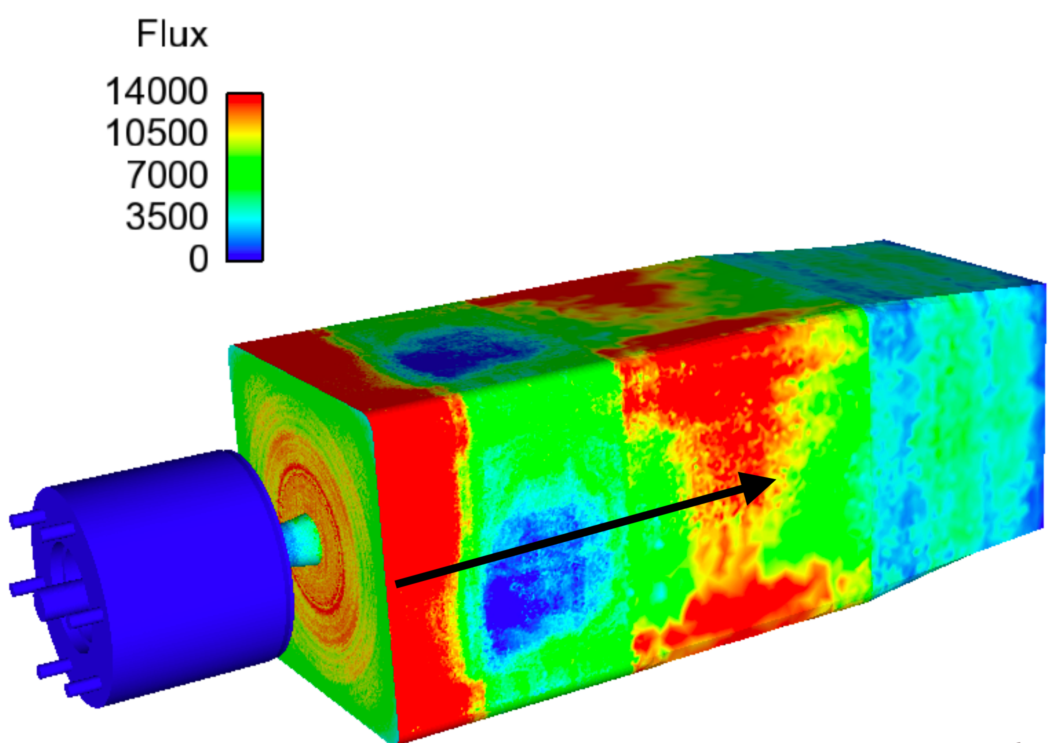
$$T_\lambda^{slab} = 0$$



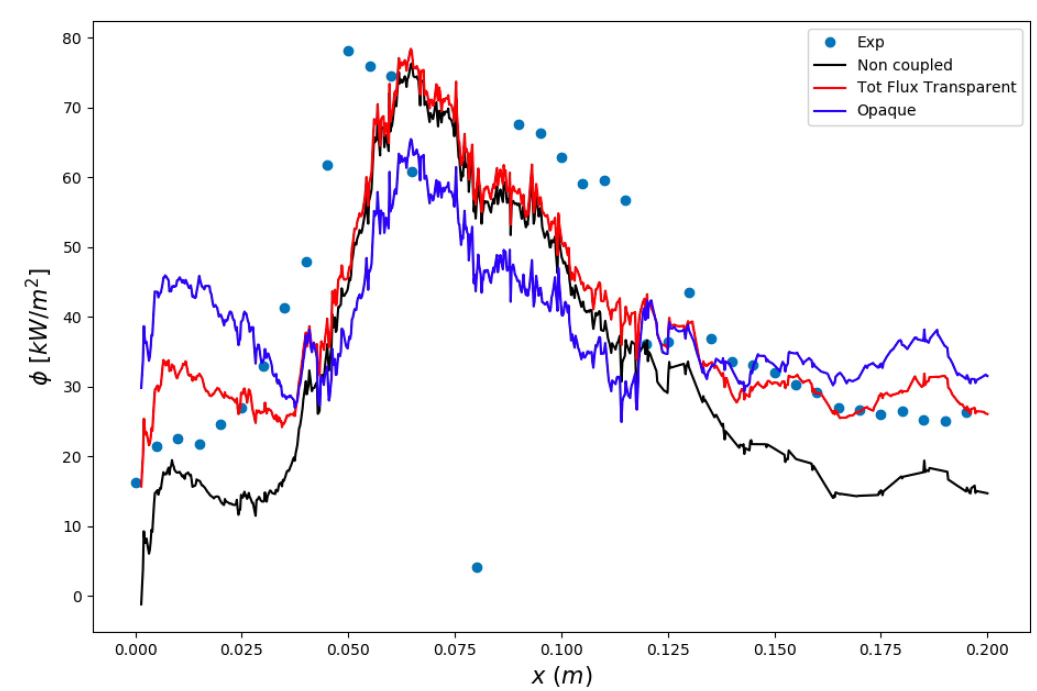
Radiative Flux



Semi-transparent

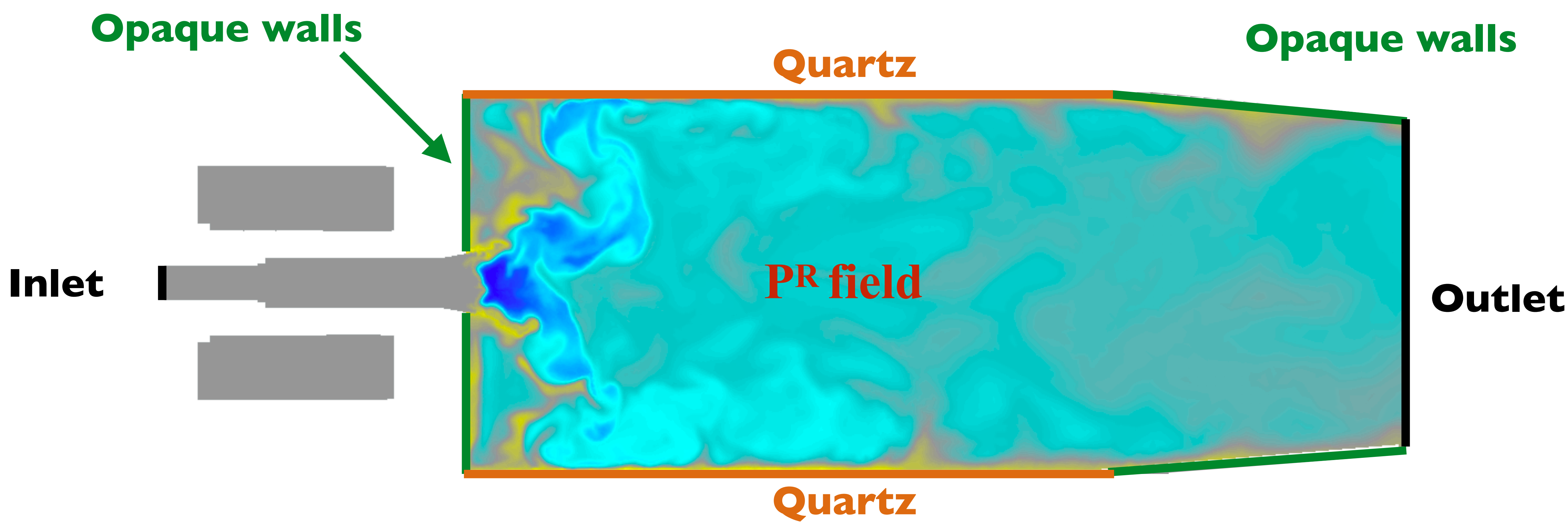


Total wall Flux



Balance of radiative transfer

Instantaneous solution from coupled simulations



$$\int_V -P^R \mathrm{d}V = \int_{\text{inlet}} \varphi_{\text{rad}} \cdot \mathrm{dS} + \int_{\text{outlet}} \varphi_{\text{rad}} \cdot \mathrm{dS} + \int_{\text{opaque walls}} \varphi_{\text{rad}} \cdot \mathrm{dS} + \int_{\text{quartz windows}} \varphi_{\text{rad}} \cdot \mathrm{dS}$$

3185 W | 9 W | 487 W | 466 W | 2223 W

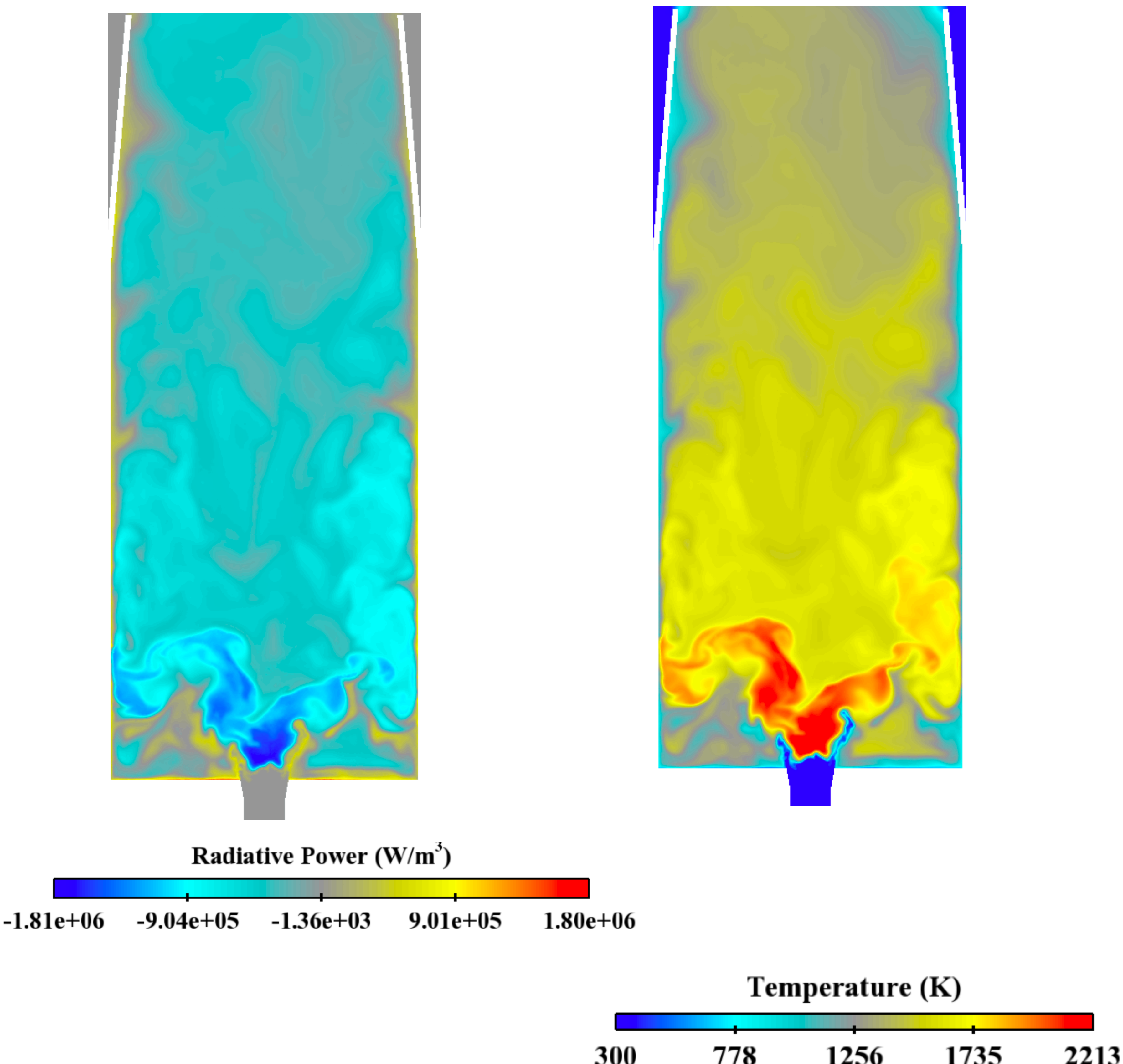
(21% out of flame Pth = 14 kW)

$$\int_{\text{quartz windows}} \varphi_{\text{rad}} \cdot \mathrm{dS}$$

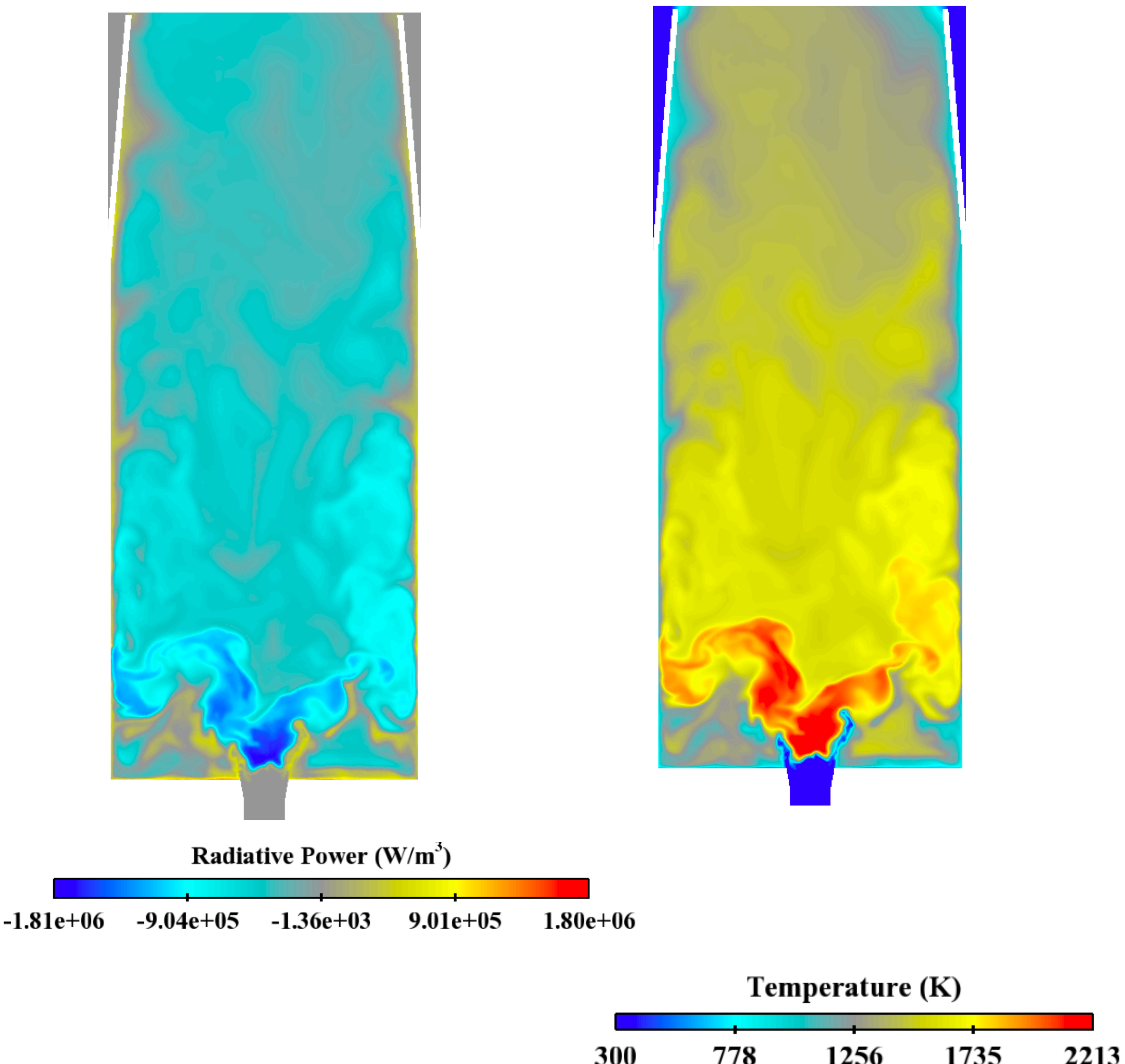
→ Absorbed/emitted = 1696 W (53 % out of P^R)

→ Transmitted = 785 W (24 % out of P^R)

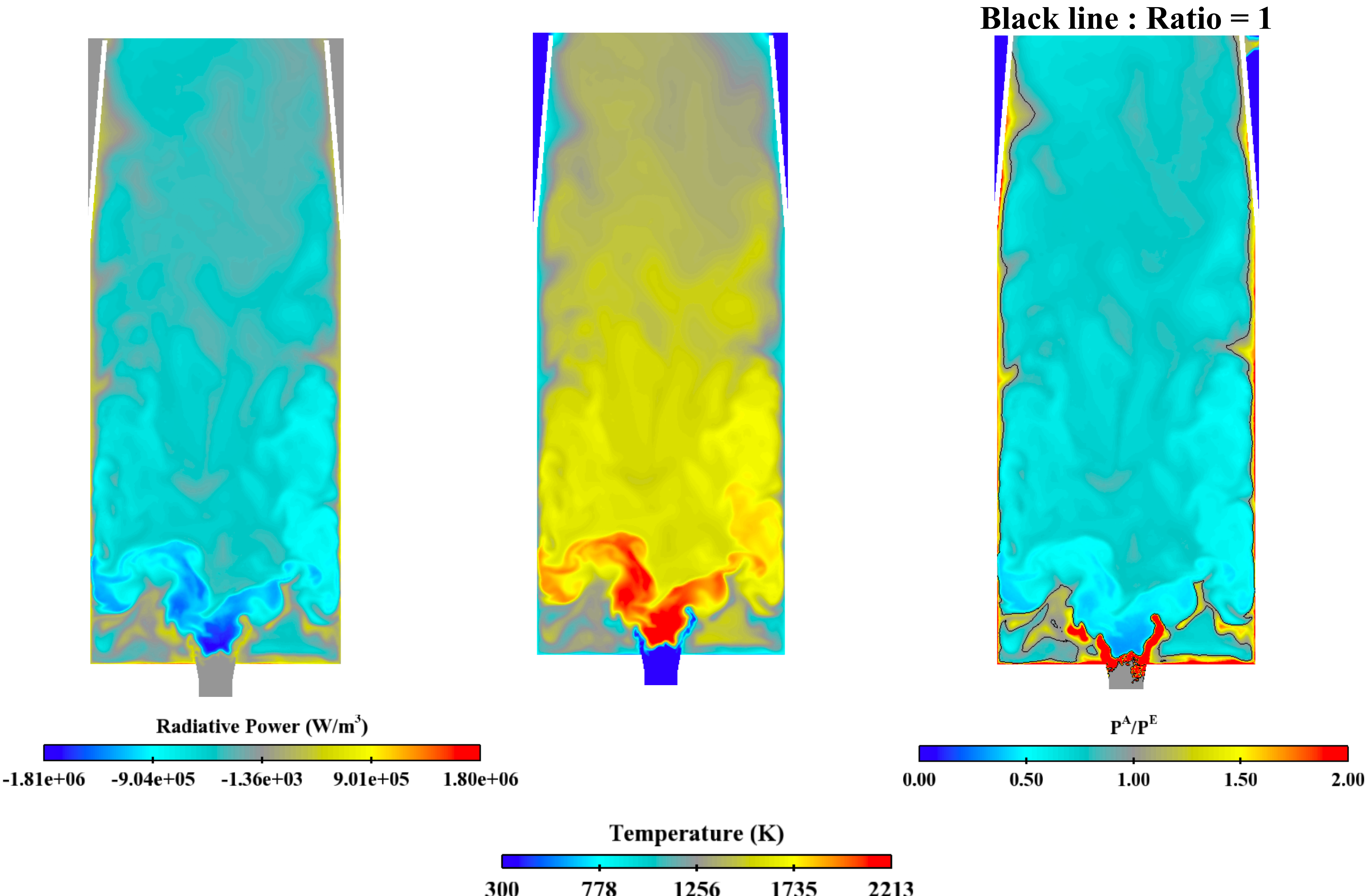
Preliminary coupled results



Preliminary coupled results



Preliminary coupled results



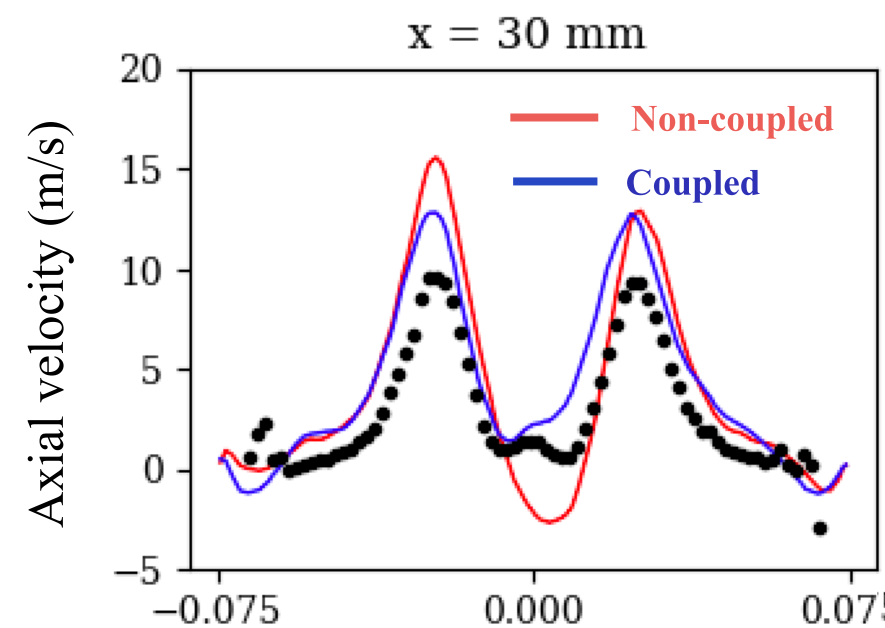
Axial velocity [m/s]

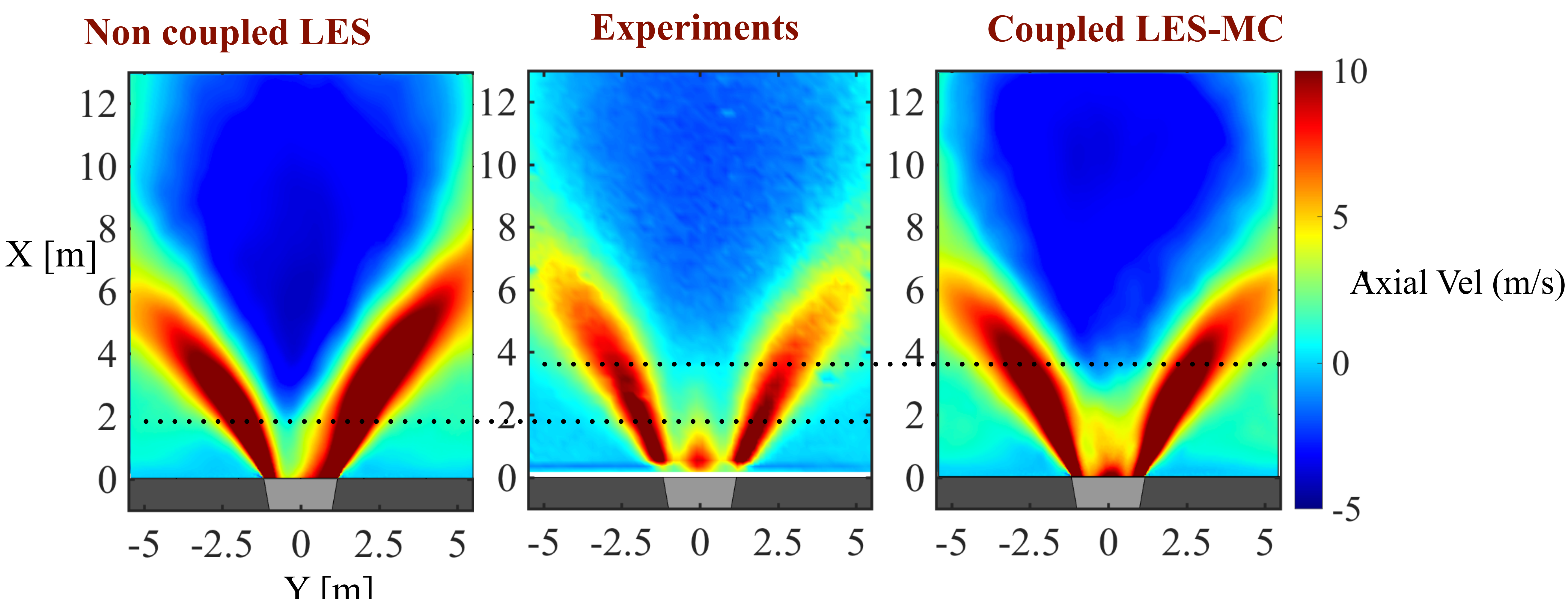
Preliminary results

Impact on velocity field

Flow topology

- Stagnation point position and Recirculation Zone
- Velocity Profiles





Outline

LES of a premixed swirled flame

- *Presentation of Oxytec chamber*
- *LES results*

Coupled simulations: numerical set-up

- *Monte Carlo solver*
- *CPU cost-accuracy trade off*

First results of coupled simulations

- *Impact of spectral properties of quartz*
- *Radiative heat transfer impact on a methane air flame*

Conclusions

Treatment of quartz spectral properties and impact on radiative fluxes

Preliminary results show impact on:

- *Flow topology*
- *Wall fluxes*
- *Flame stabilization*[1]

[1]Pedro Rodrigues, CentraleSupélec *PhD Thesis 2018*

Thank you for your attention

This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska-Curie grant agreement No 643134.

Quasi-Monte Carlo methods

To reduce the MC error:

Alternative sampling method

[1] Halton, J. H. 1960. “On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals”. Numerische Mathematik

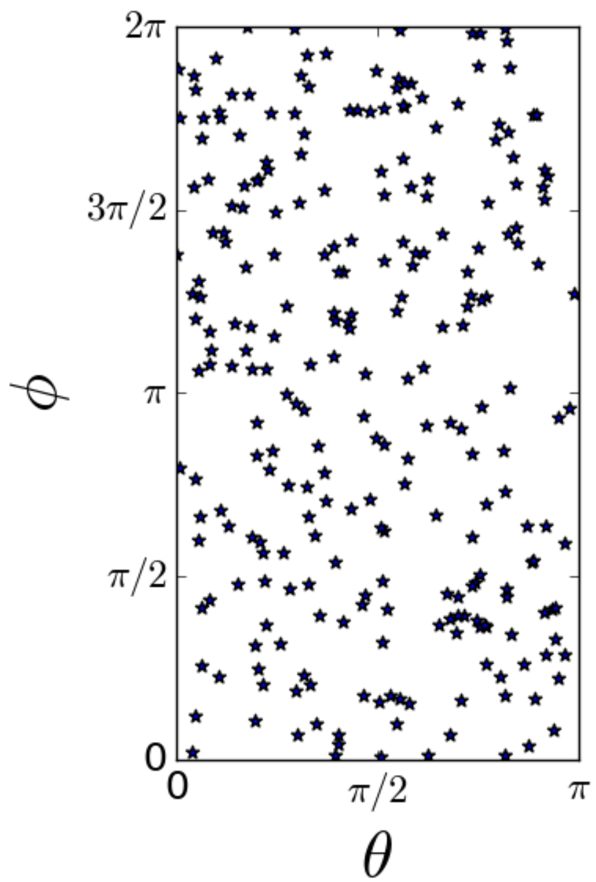
[2] Joe, S., and Kuo, F. Y., 2008. “Constructing Sobol sequences with better two-dimensional projections”. SIAM Journal on Scientific Computing

[3] Faure, H. 1982. “Discrepancy of sequences associated with a numeration system (in s-dimension)”. Acta Arithmetica

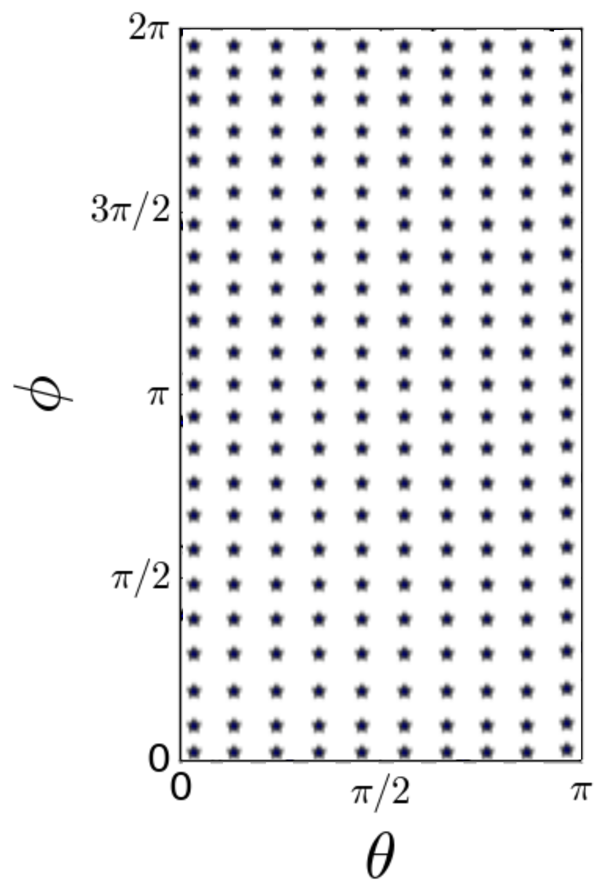
Quasi-Monte Carlo methods

To reduce the MC error:

Alternative sampling method



Pseudo-random sampling MC



Deterministic discretization (Unfeasible in high-D)

[1] Halton, J. H. 1960. "On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals". Numerische Mathematik

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

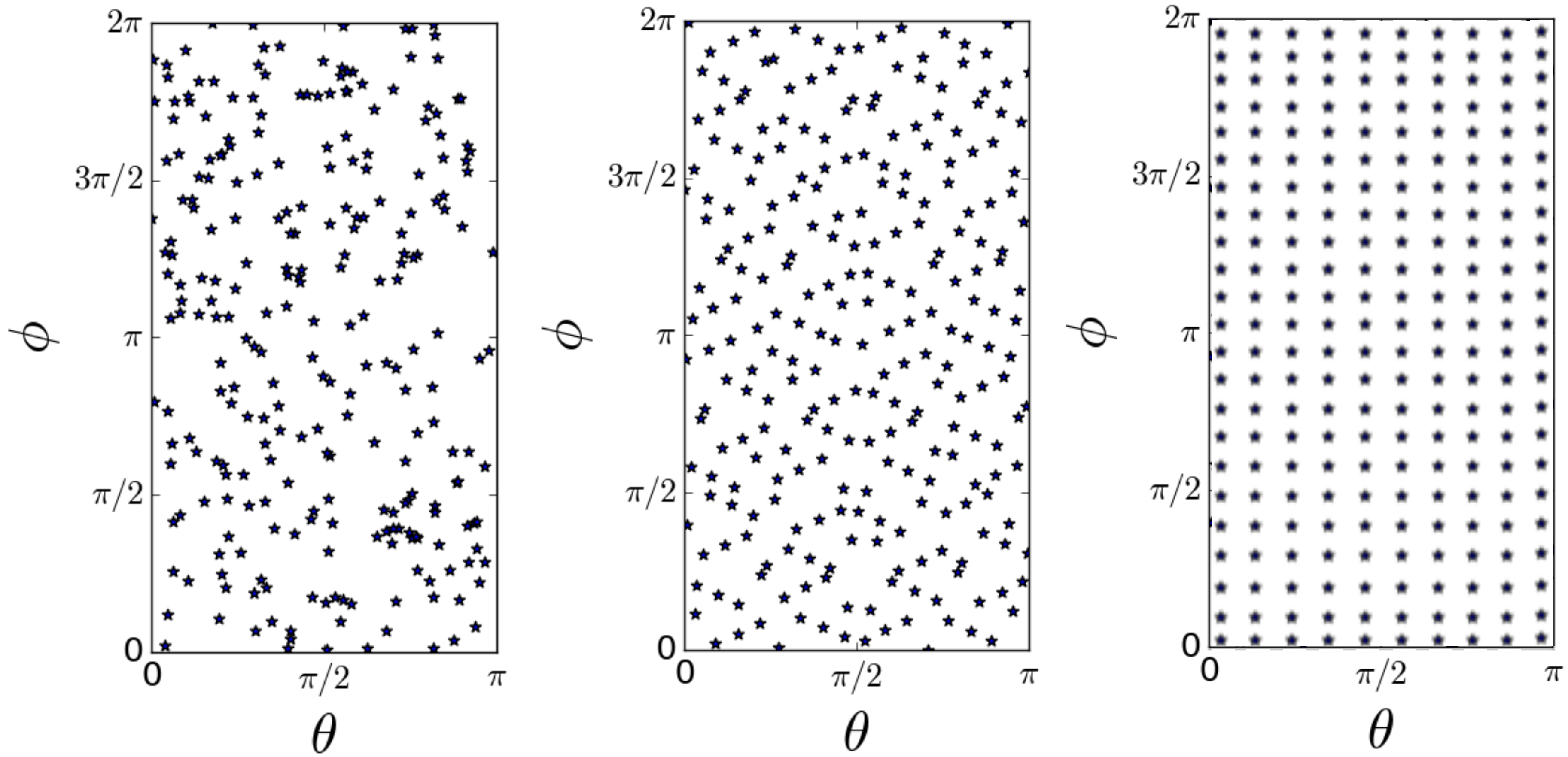
[3] Faure, H. 1982. "Discrepancy of sequences associated with a numeration system (in s-dimension)". Acta Arithmetica

Quasi-Monte Carlo methods

To reduce the MC error:

Alternative sampling method

- *Quasi-random instead of pseudo-random sampling*



Pseudo-random sampling MC

Quasi-random Sampling QMC

Deterministic discretization (Unfeasible in high-D)

[1] Halton, J. H. 1960. "On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals". Numerische Mathematik

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

[3] Faure, H. 1982. "Discrepancy of sequences associated with a numeration system (in s-dimension)". Acta Arithmetica

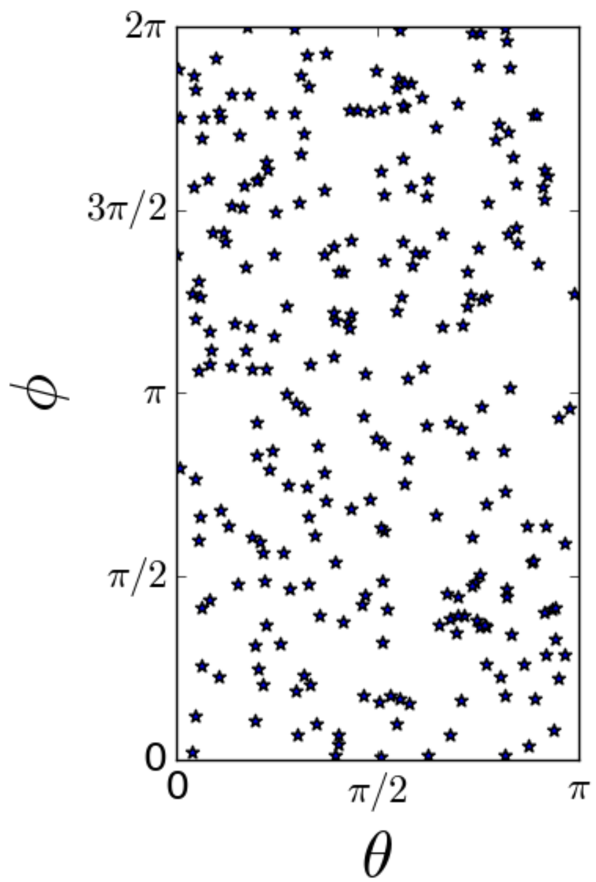
Quasi-Monte Carlo methods

To reduce the MC error:

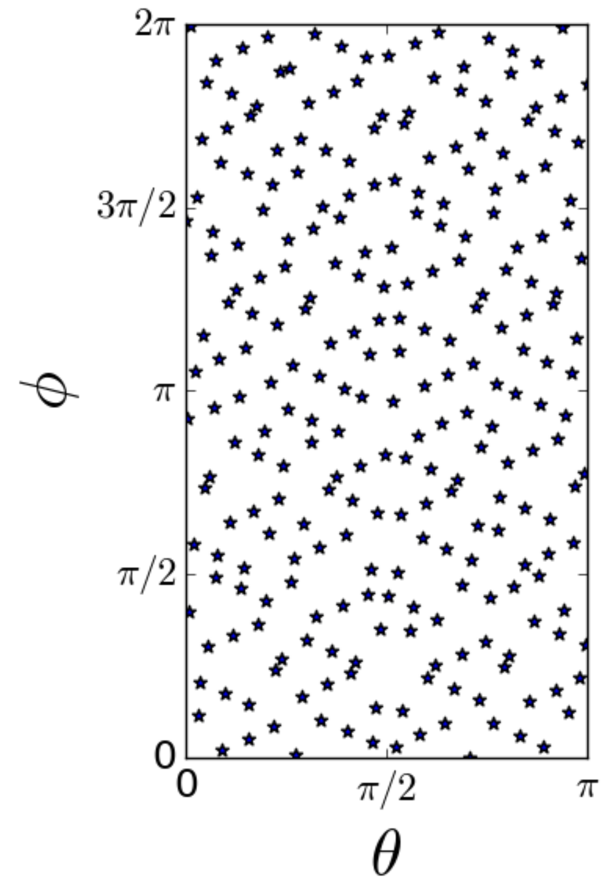
Alternative sampling method

- *Quasi-random instead of*
  pseudo-random sampling

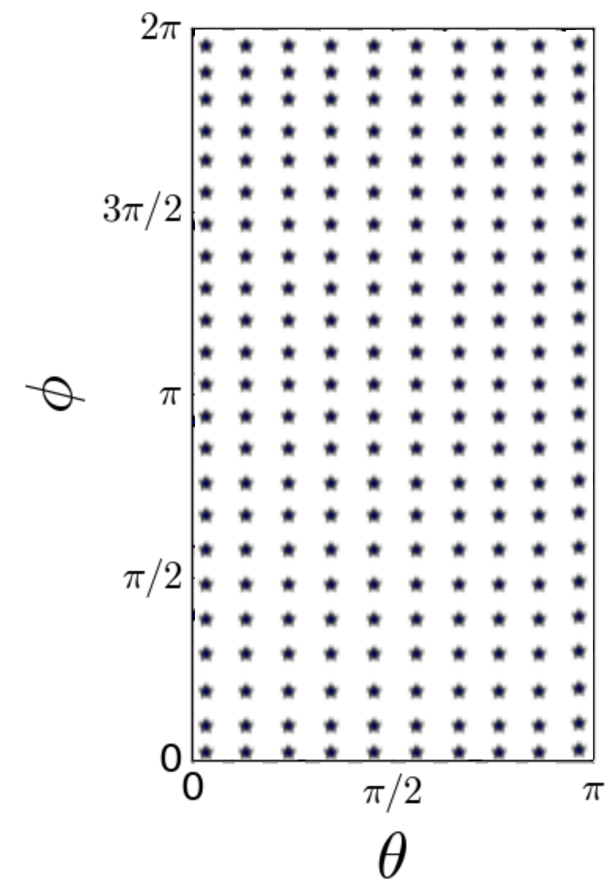
- *Low-discrepancy sequences:*
  Halton[1]
  Sobol[2]
  Faure[3]
  points more uniformly distributed



Pseudo-random sampling MC



Quasi-random Sampling QMC



Deterministic discretization (Unfeasible in high-D)

[1] Halton, J. H. 1960. "On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals". Numerische Mathematik

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

[3] Faure, H. 1982. "Discrepancy of sequences associated with a numeration system (in s-dimension)". Acta Arithmetica

Quasi-Monte Carlo methods

To reduce the MC error:

Alternative sampling method

- *Quasi-random instead of*

  pseudo-random sampling

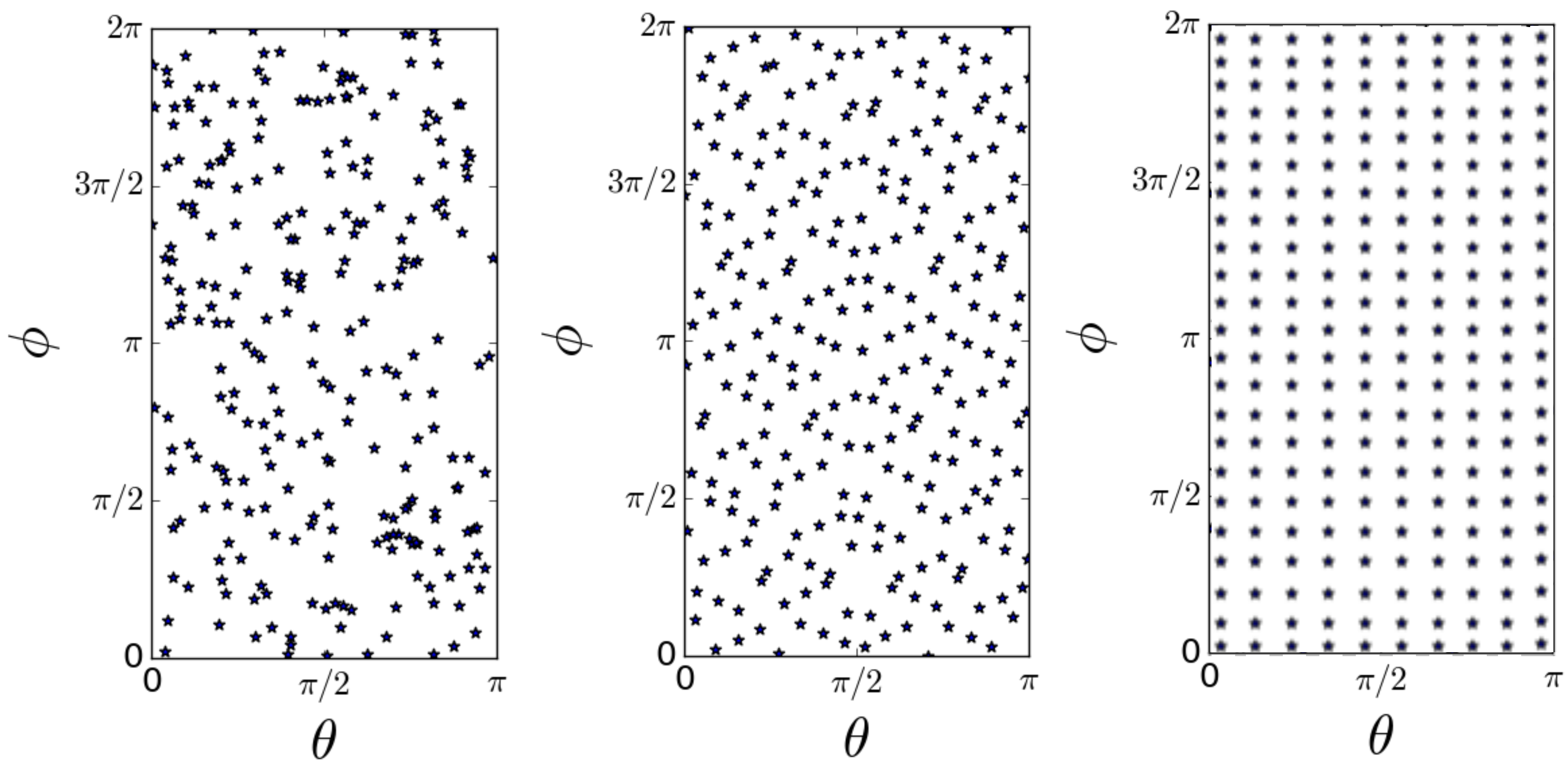
- *Low-discrepancy sequences:*

  Halton[1]

  Sobol[2]

  Faure[3]

  points more uniformly distributed



Pseudo-random sampling MC	***Quasi-random Sampling QMC***	***Deterministic discretization (Unfeasible in high-D)***

[1] Halton, J. H. 1960. "On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals". Numerische Mathematik

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

[3] Faure, H. 1982. "Discrepancy of sequences associated with a numeration system (in s-dimension)". Acta Arithmetica

Quasi-Monte Carlo methods

To reduce the MC error:

Alternative sampling method

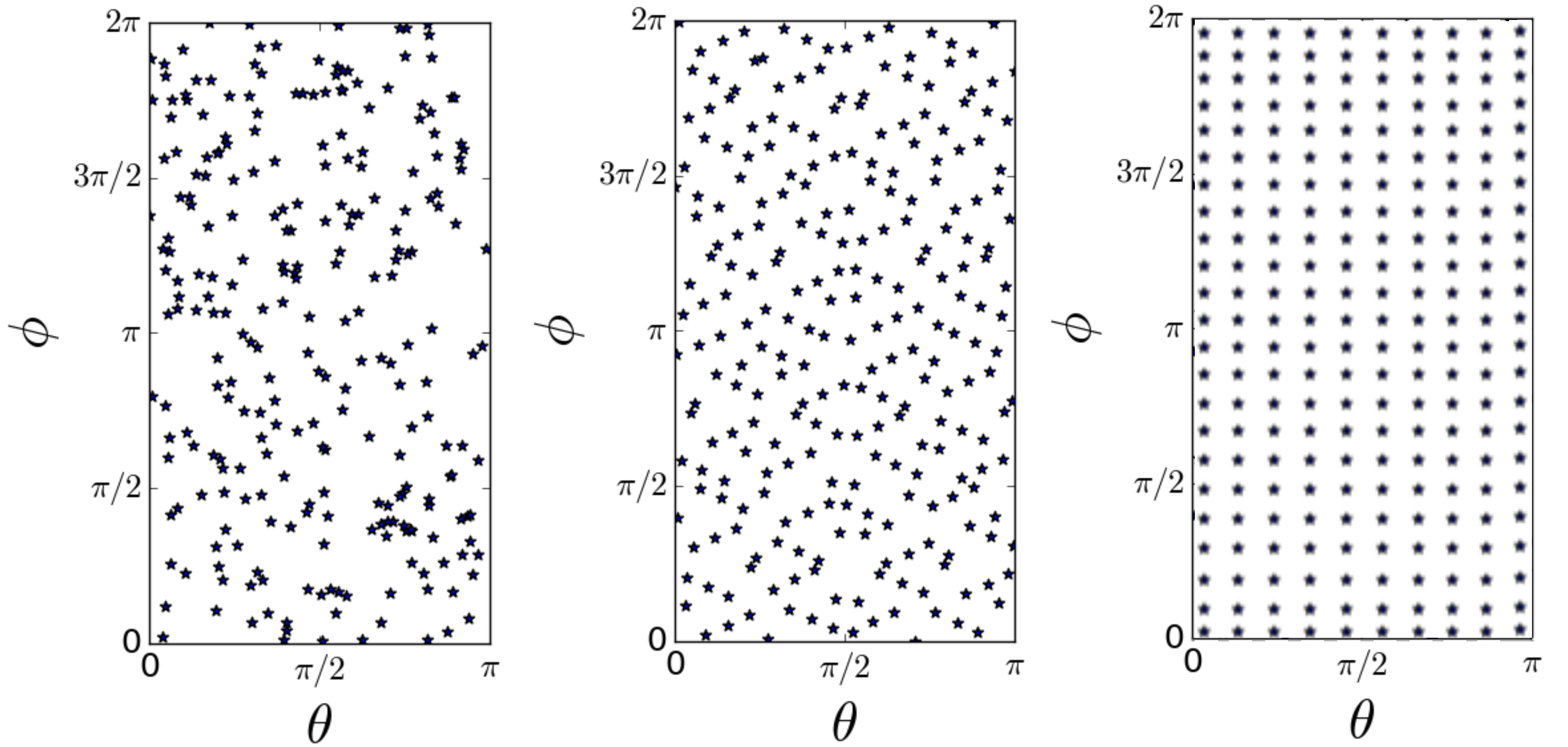
- *Quasi-random instead of pseudo-random sampling*

- *Low-discrepancy sequences:*
  - *Halton[1]*
  - *Sobol[2]*
  - *Faure[3]*

  points more uniformly distributed

- ***Advantage**: convergence rate faster than MC and asymptotically :*

$$\varepsilon \propto \frac{1}{N}$$



Pseudo-random sampling MC

Quasi-random Sampling QMC

Deterministic discretization (Unfeasible in high-D)

[1] Halton, J. H. 1960. "On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals". Numerische Mathematik

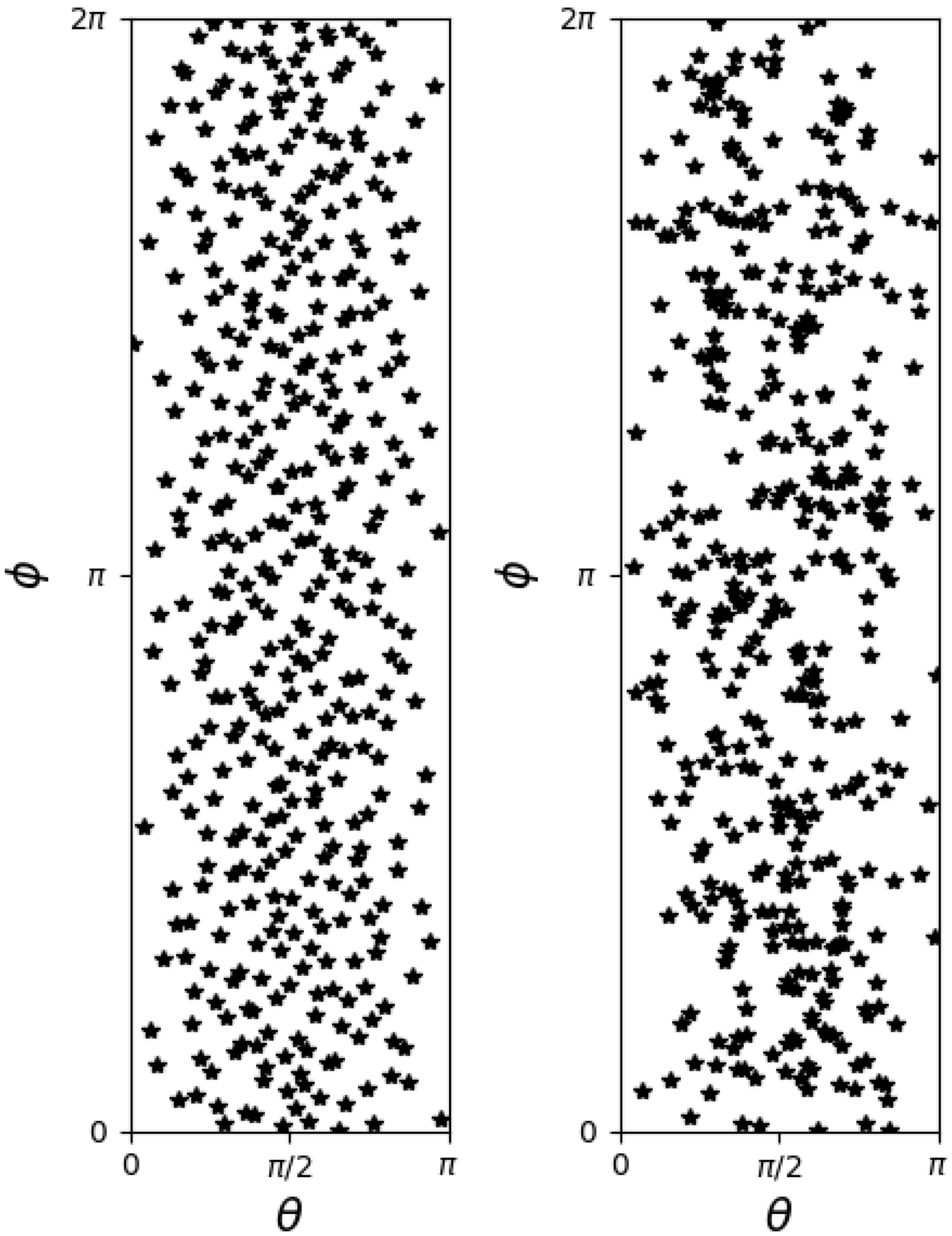
[2] Joe, S., and Kuo, F. Y., 2008. "Constructing Sobol sequences with better two-dimensional projections". SIAM Journal on Scientific Computing

[3] Faure, H. 1982. "Discrepancy of sequences associated with a numeration system (in s-dimension)". Acta Arithmetica

Quasi-Monte Carlo methods

Koksma-Hlawka inequality :

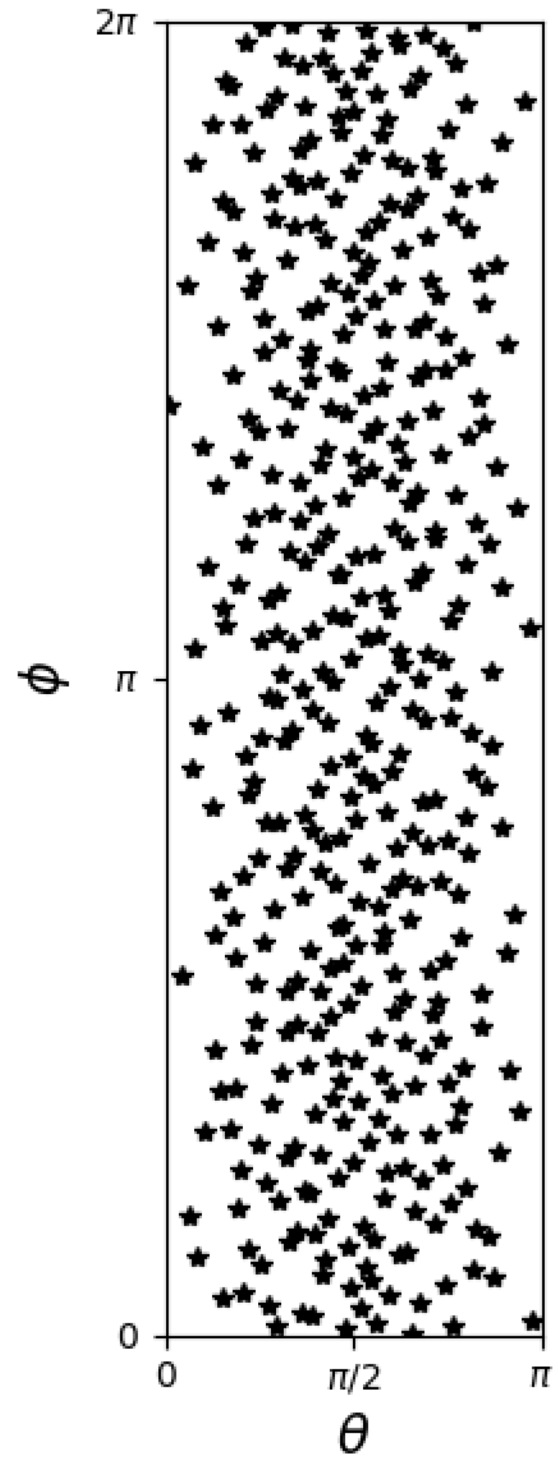
$$\epsilon[f] \leq CV[f]\frac{(ln\ n)^d}{n}$$



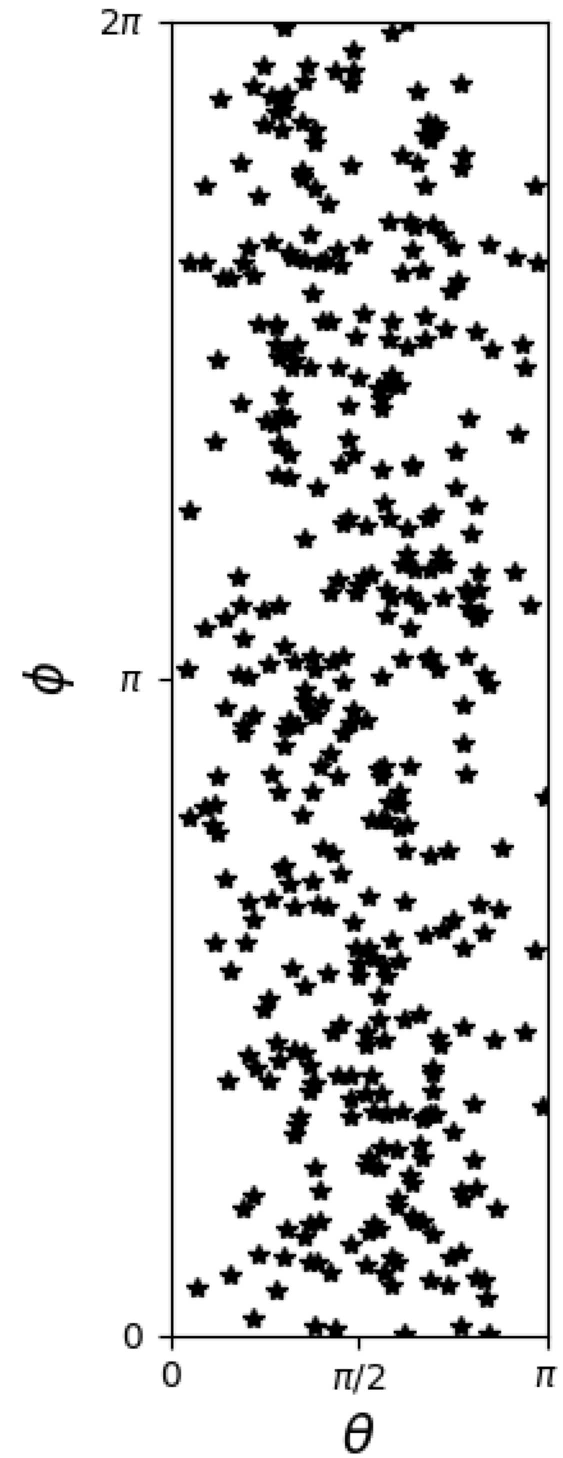
Quasi-Monte Carlo methods

Koksma-Hlawka inequality :

$$\epsilon[f] \leq CV[f]\frac{(ln\ n)^d}{n}$$



Pseudo-random sampling MC



Quasi-random Sampling QMC

Quasi-Monte Carlo methods

QMC convergence rate faster than MC but no error estimation

In order to get error estimation

↓

Randomization *of quasi-random sequences*

↓

Randomized Quasi-Monte Carlo

[1] Tezuka, S., and Faure, H., 2003. "I-binomial scrambling of digital nets and sequences". Journal of complexity.

Quasi-Monte Carlo methods

QMC convergence rate faster than MC but no error estimation

In order to get error estimation

↓

Randomization *of quasi-random sequences* ↗

↓

Randomized Quasi-Monte Carlo

Randomization methods:

Shifting

Full Scrambling

Linear Scrambling[1]

[1] Tezuka, S., and Faure, H., 2003. "I-binomial scrambling of digital nets and sequences". Journal of complexity.

Quasi-Monte Carlo methods

QMC convergence rate faster than MC but no error estimation

In order to get error estimation

↓

Randomization *of quasi-random sequences*

↓

Randomized Quasi-Monte Carlo

Randomization methods:

Shifting

Full Scrambling

Linear Scrambling[1]

[1] Tezuka, S., and Faure, H., 2003. "I-binomial scrambling of digital nets and sequences". Journal of complexity.

Quasi-Monte Carlo methods

QMC convergence rate faster than MC but no error estimation

In order to get error estimation

Randomization *of quasi-random sequences*

Randomization methods:

Shifting

Full Scrambling

Linear Scrambling[1]

Randomized Quasi-Monte Carlo

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

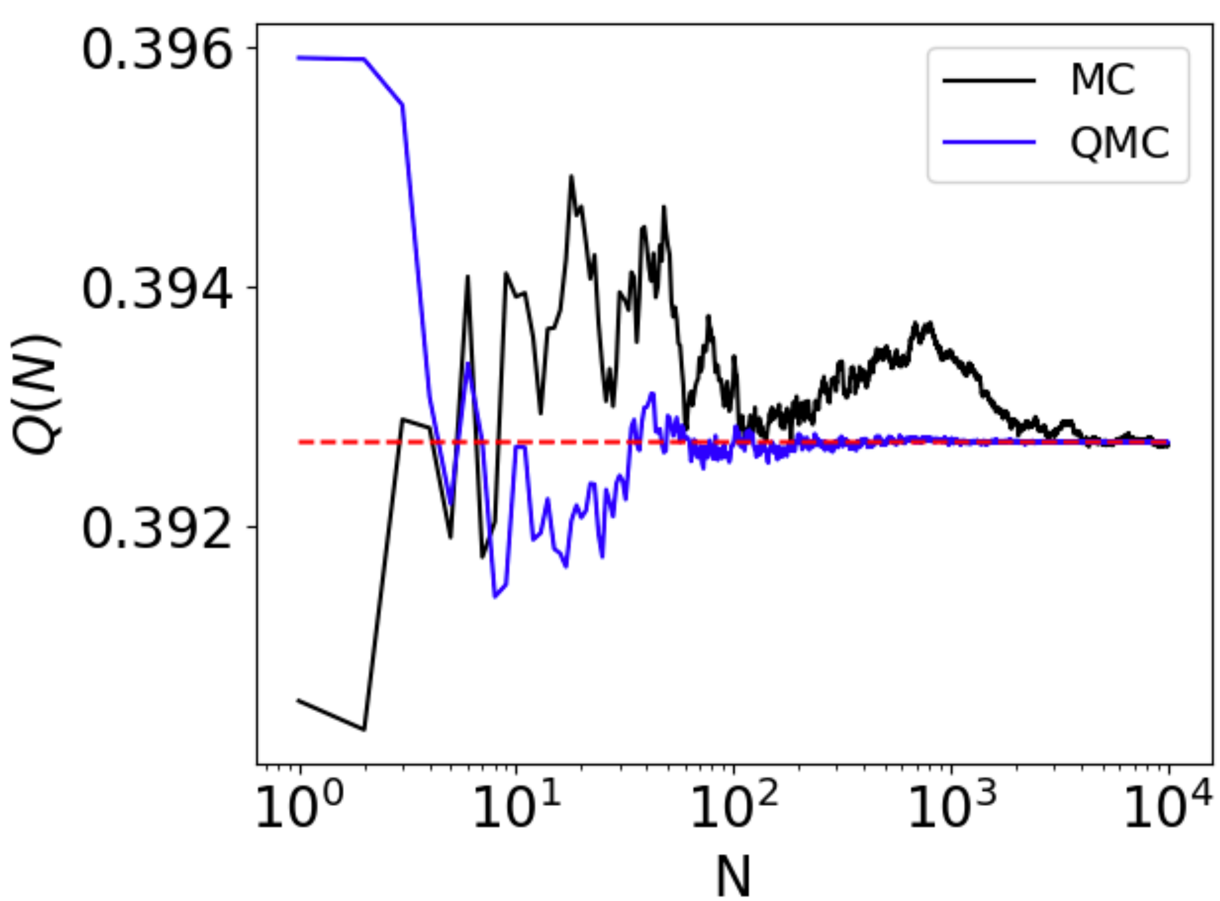
QMC applied in a real 3-D application

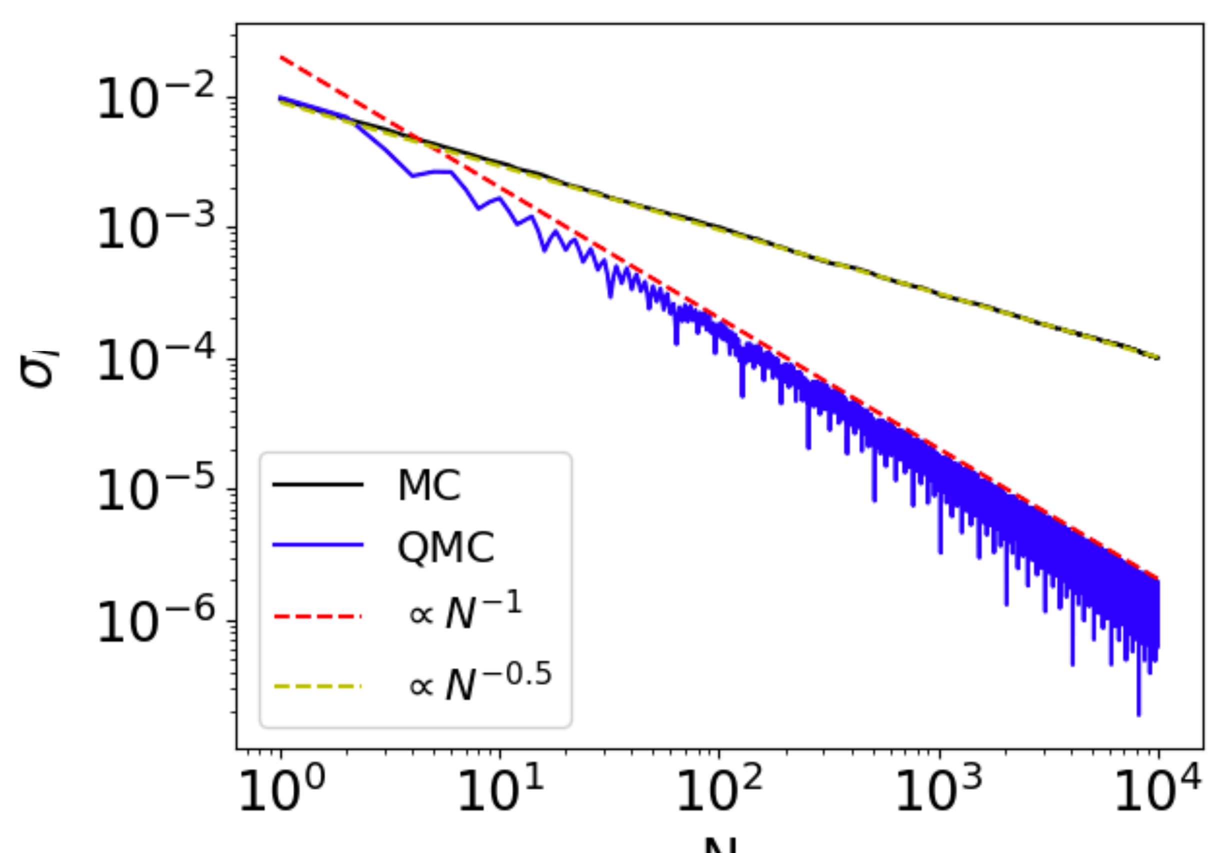
[1] Tezuka, S., and Faure, H., 2003. "I-binomial scrambling of digital nets and sequences". Journal of complexity.

Quasi-Monte Carlo methods

2D integral

$$I = \int_0^{2\pi} \int_0^{\pi} \frac{1}{4\pi} sin^2(\phi/2) sin^2\theta d\theta d\phi$$





Coupled simulations

Approaches used in this work

Fluid solver	Radiation solver	Gas radiative properties
DNS	MC	LBL
LES	DOM	Narrow band
RANS	P1	Global models

Accuracy
CPU cost

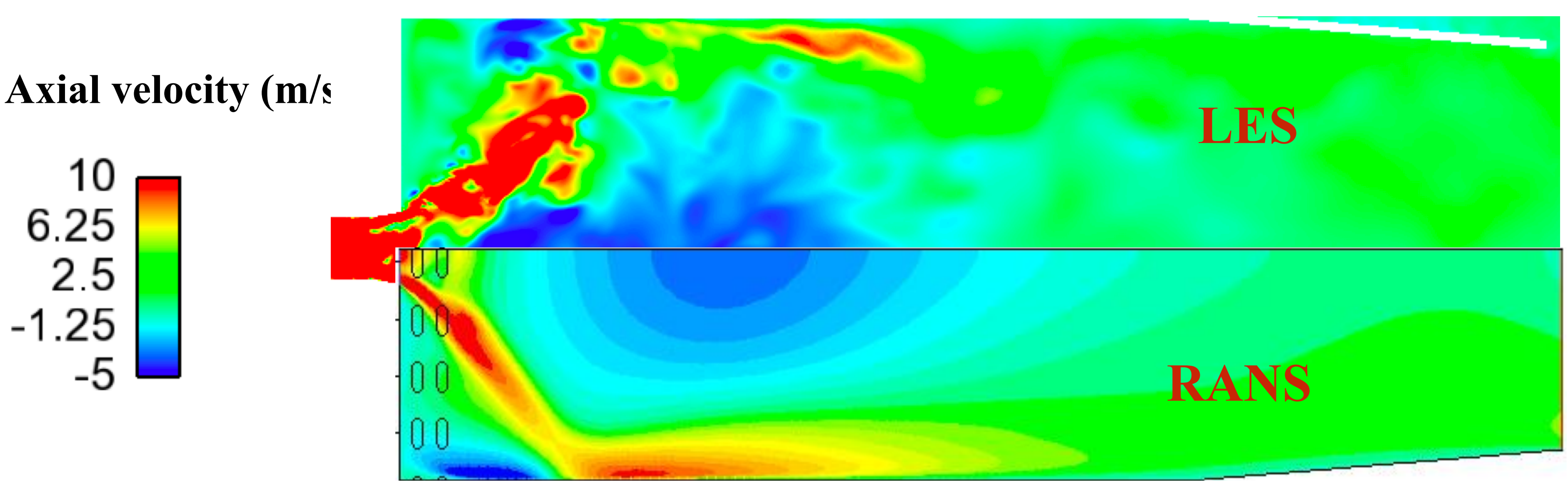
Coupled simulations

Approaches used in this work

Why LES?	Fluid solver	Radiation solver	Gas radiative properties
Not affordable for real configs	**DNS**	MC	LBL
CPU cost - accuracy trade off	**LES**	DOM	Narrow band
Modelling uncertainties	**RANS**	P1	Global models

Accuracy

CPU cost



Coupled simulations

Approaches used in this work

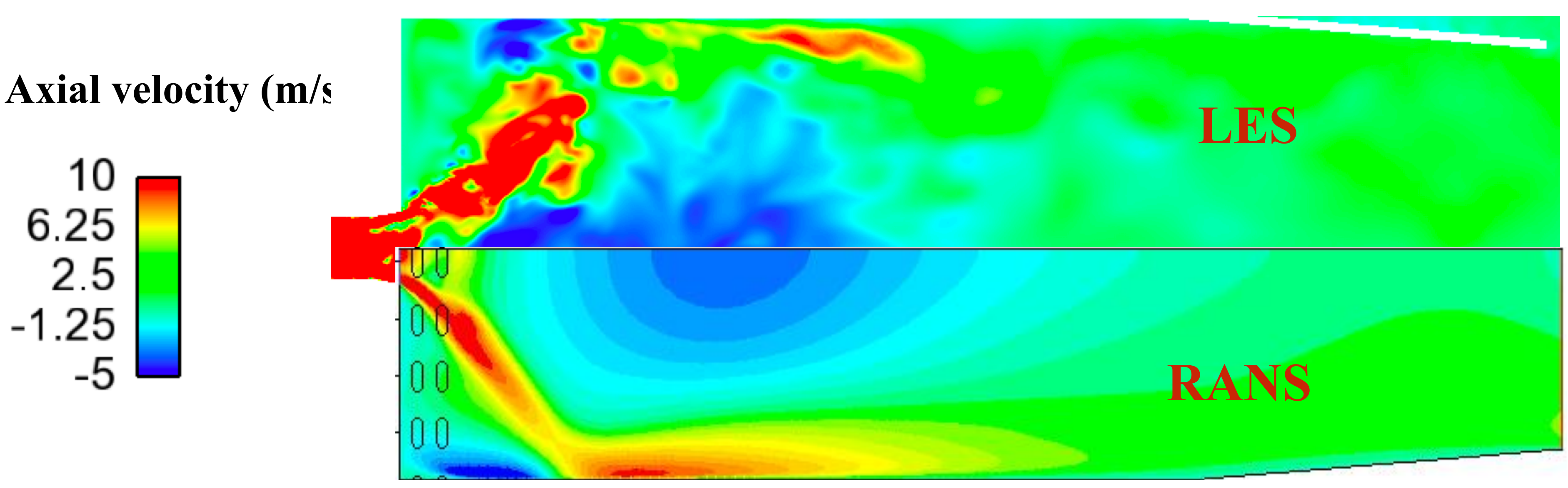
Why MC?

More accurate method

Fluid solver	Radiation solver	Gas radiative properties
DNS	MC	LBL
LES	DOM	Narrow band
RANS	P1	Global models

Accuracy

CPU cost



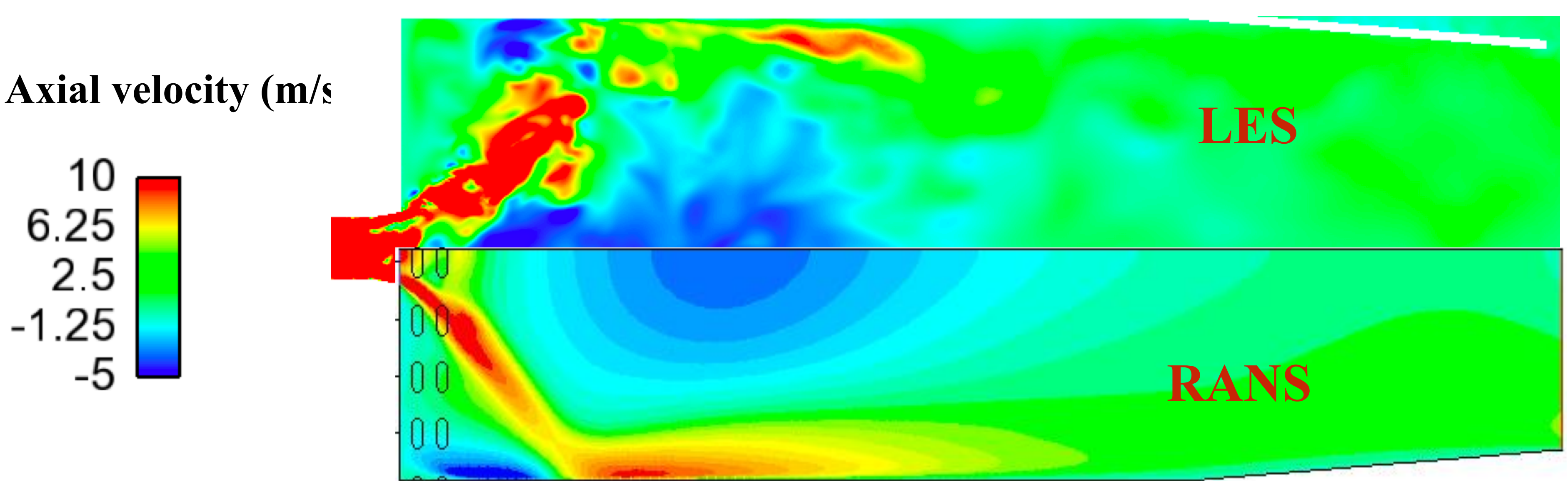
Coupled simulations

Approaches used in this work

	Fluid solver	Radiation solver	Gas radiative properties
Why Narrow band model?			
Not affordable	DNS	MC	LBL
Easily handle with semi-transparent walls BC	LES	DOM	Narrow band
	RANS	P1	Global models

Accuracy

CPU cost

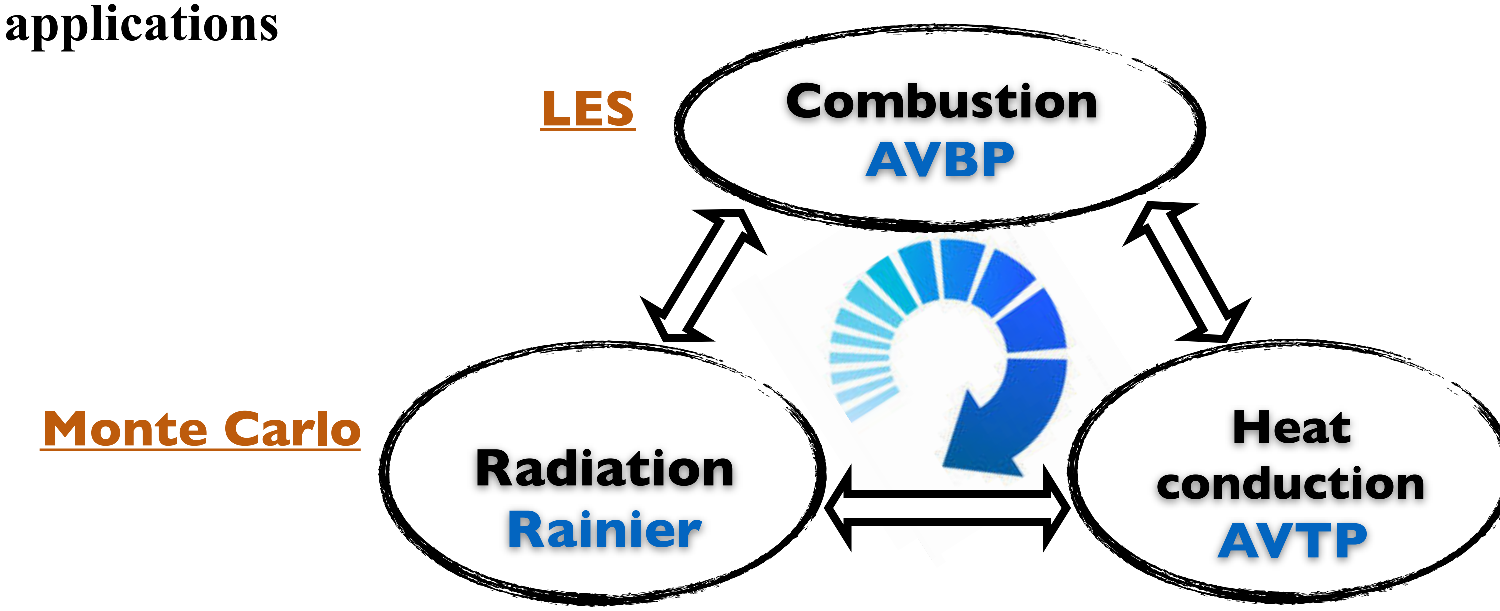


Context (3/3)

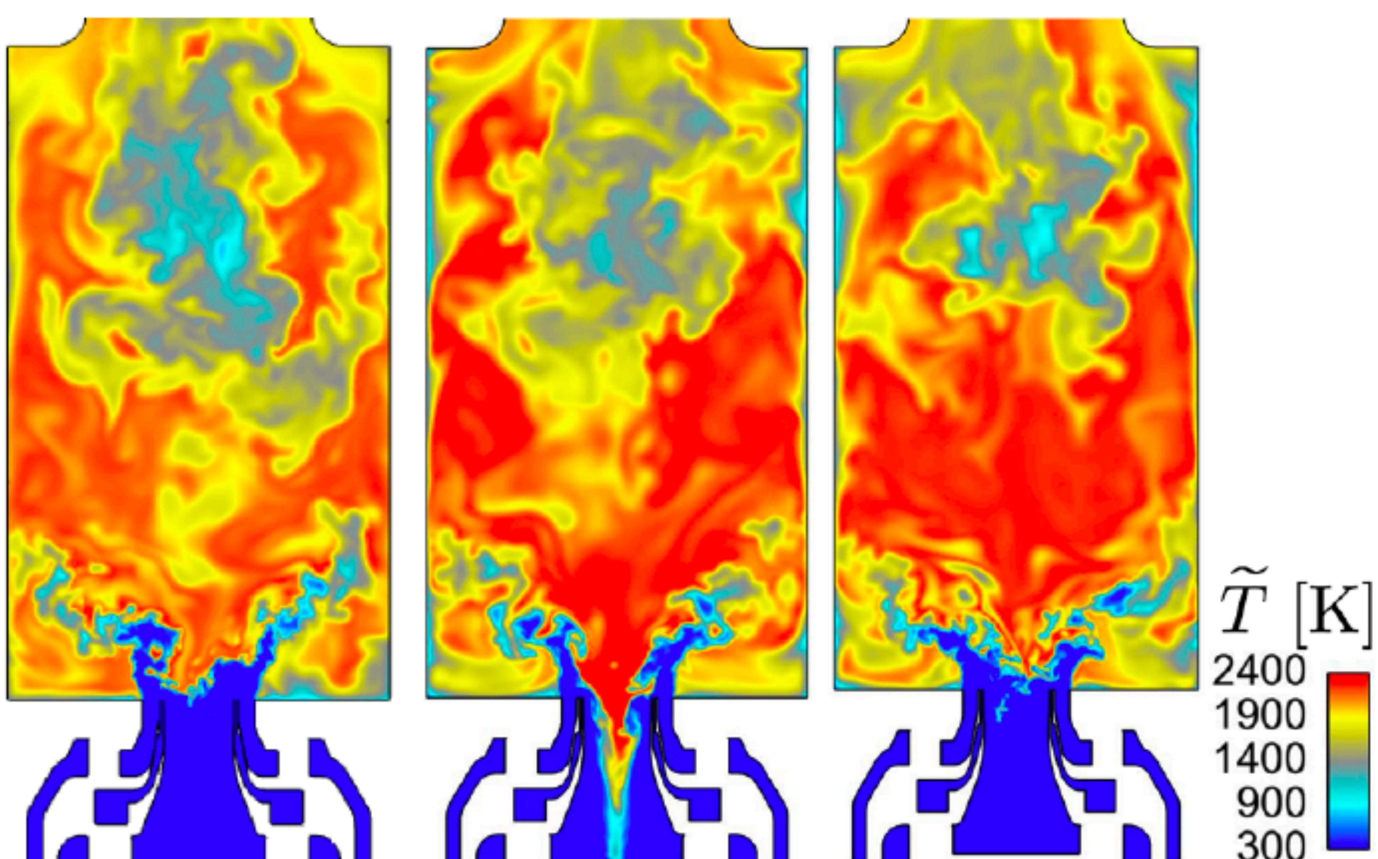
Importance of radiative heat transfer in combustion applications

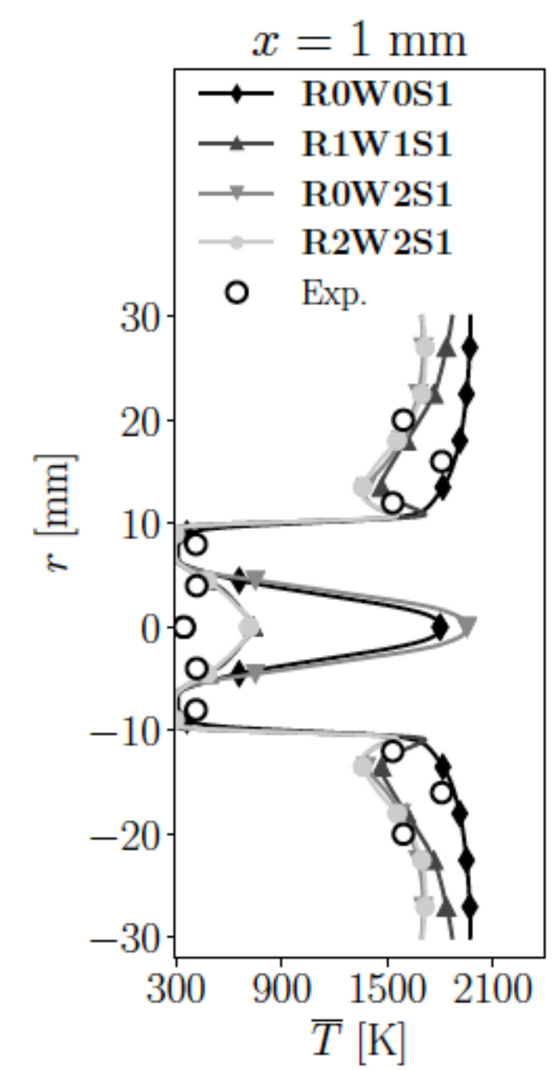
Confined-pressurized sooting flame

- Fully coupled methodology
- Radiation important for:
  - Flame stabilization
  - Temperature field



Optically thin **No radiation** **Detailed radiation**





[1]Rodrigues, P., Gicquel, O., Darabiha, N., Geigle, K. P., & Vicquelin, R.. *ASME Turbo Expo 2018*.