

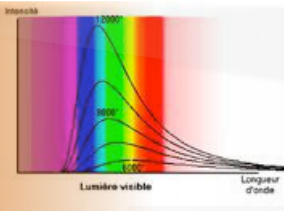


# Formation PRISSMA

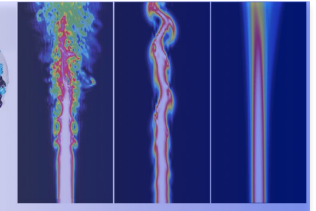
8 novembre 2011

Damien Poitou  
[poitou@cerfacs.fr](mailto:poitou@cerfacs.fr)

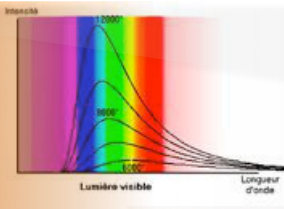




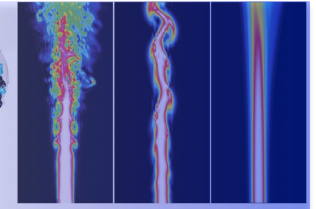
# Programme



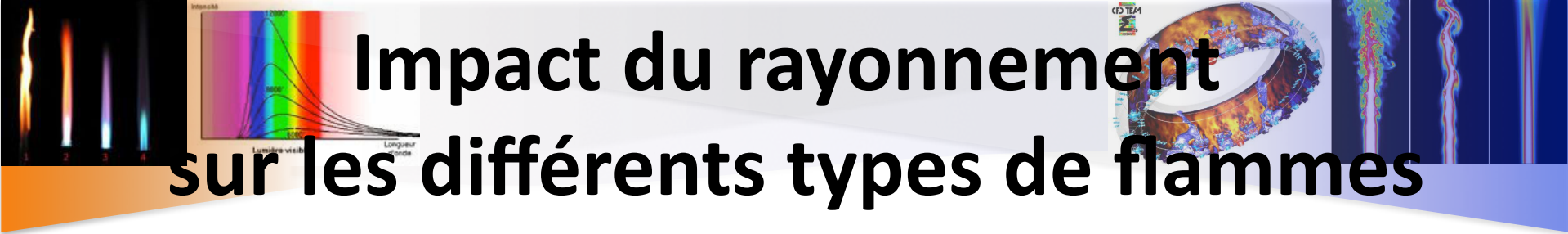
1. Contexte et théorie
2. Le code PRISSMA
3. Parallélisme
4. Modèles spectraux
5. Vers le couplage...



# Programme



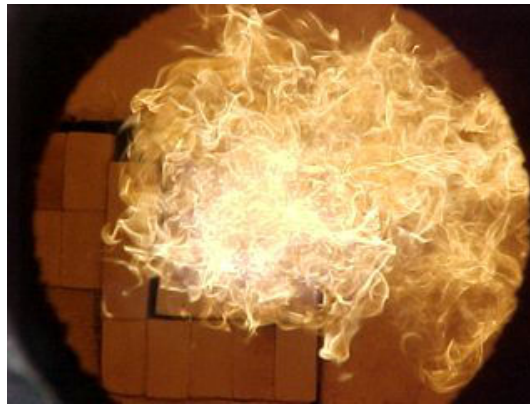
- 1. Contexte et théorie**
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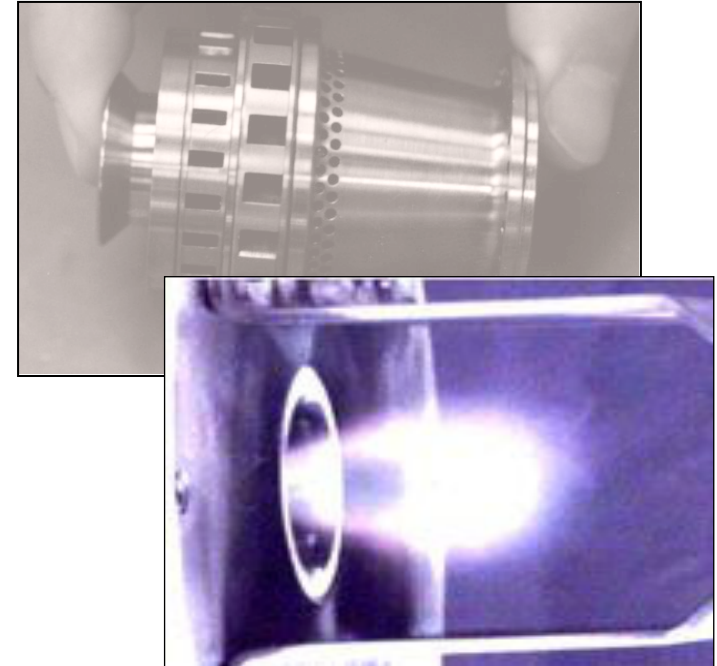
# Impact du rayonnement sur les différents types de flammes



Incendies: propagation par rayonnement (surtout suies, ex. flashover)



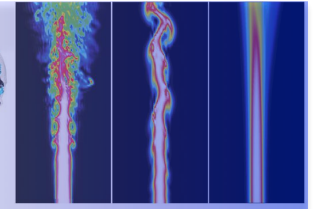
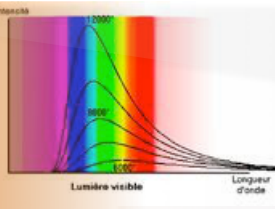
Fours, flammes torches:  
flammes de grande taille  
-non optiquement minces  
-effets radiatifs importants sur la structure de flamme, flux aux parois.



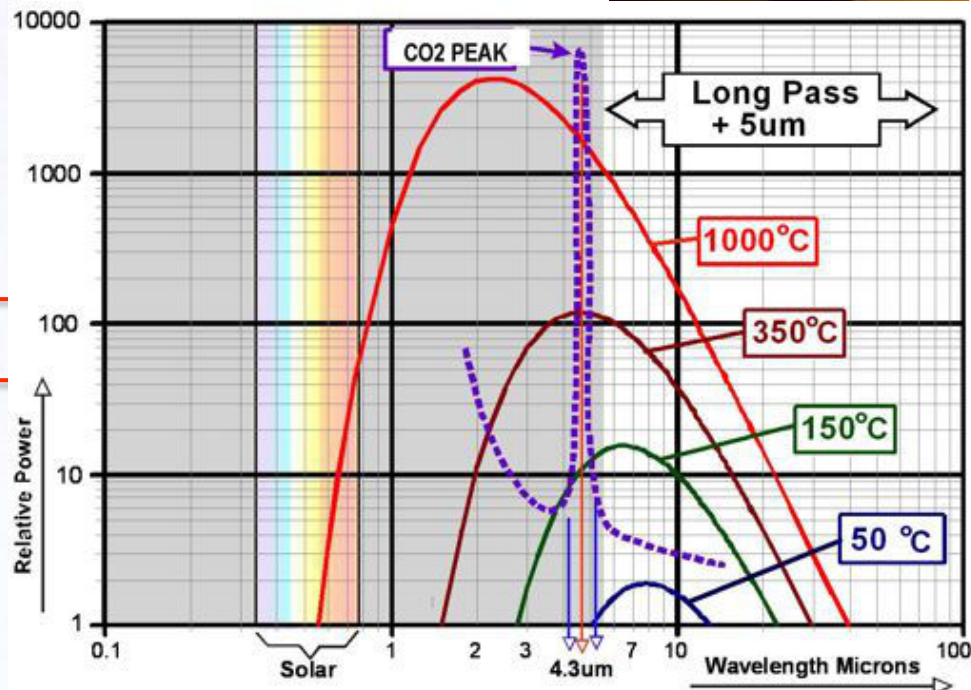
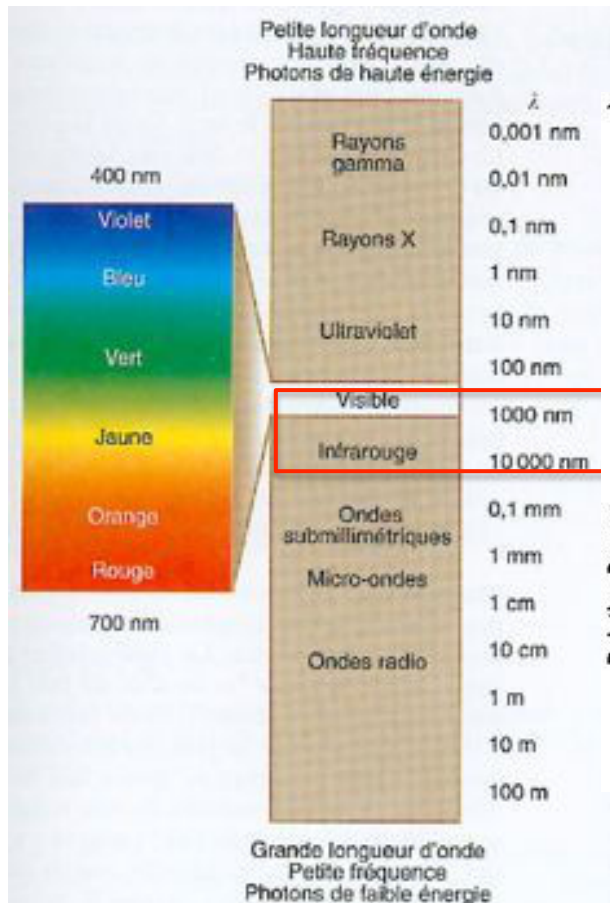
Propulsion :  
flammes de petite taille  
-optiquement minces sauf suies.  
-effet sur les  $\text{NO}_x$  et les flux thermiques pariétaux.



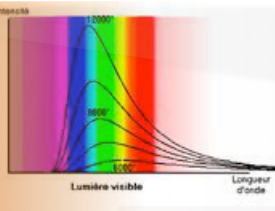
# Physique du rayonnement



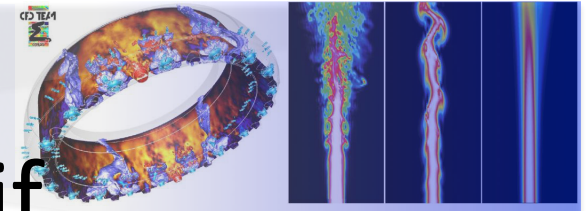
Mécanisme d'échange **à distance** :  
 -> Effet directionnel



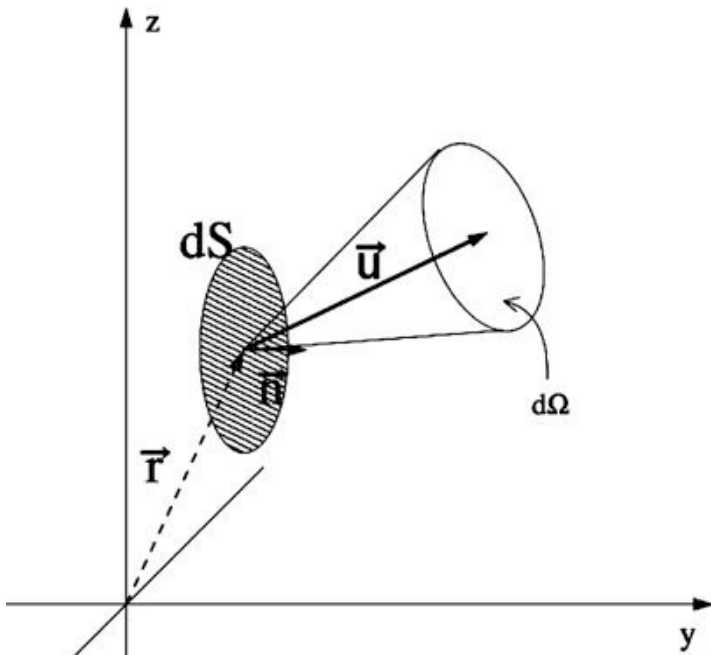
Forte dépendance **à la longueur d'onde** :  
 -> Rayonnement thermique = Infrarouge



# Modélisation du transfert radiatif

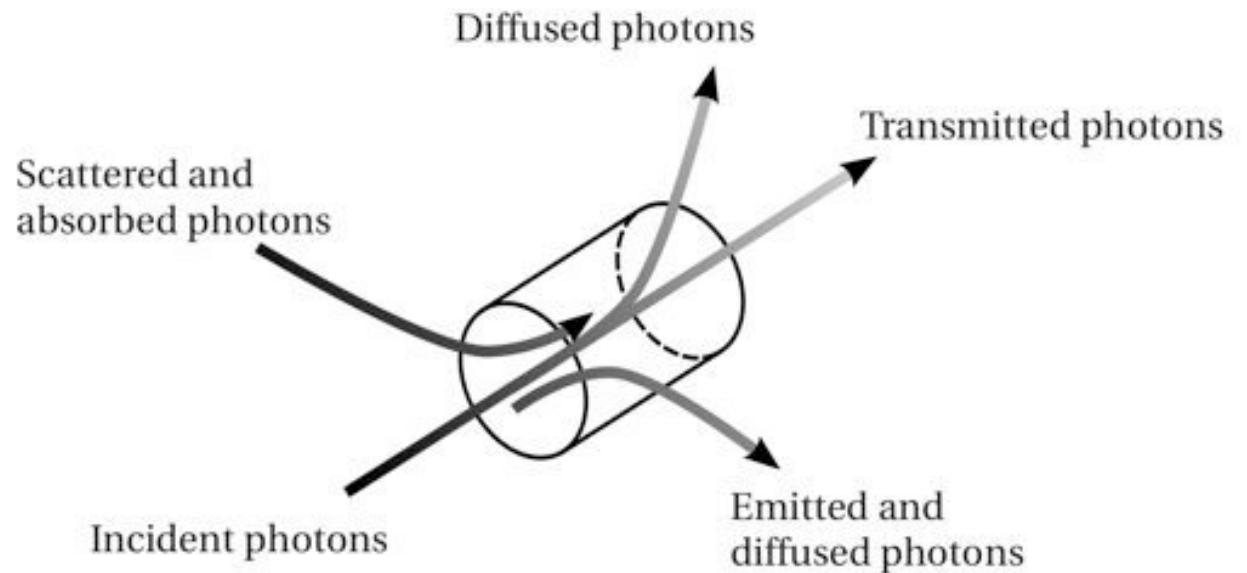


Luminance: densité surfacique de flux dans la direction  $\mathbf{u}$  à 1 fréquence

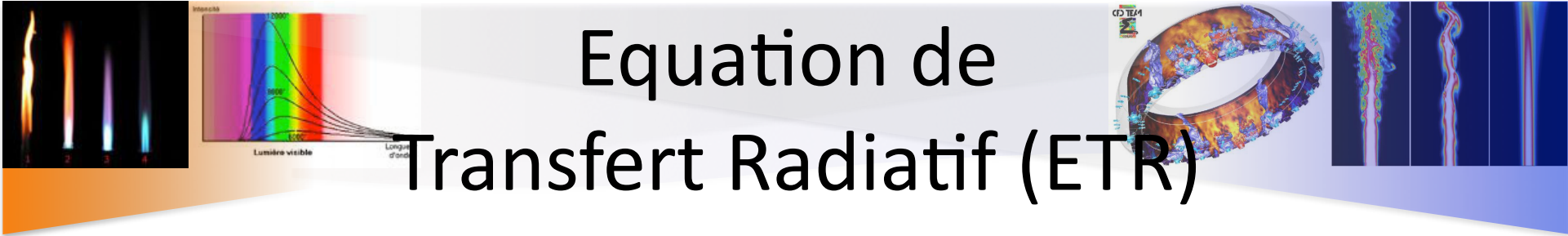


$$L_\nu(\mathbf{x}, \mathbf{u}, t) = \frac{d\phi(\mathbf{u}, t)}{\mathbf{u} \cdot \mathbf{n} d\Omega dt dS}$$

Contributions:



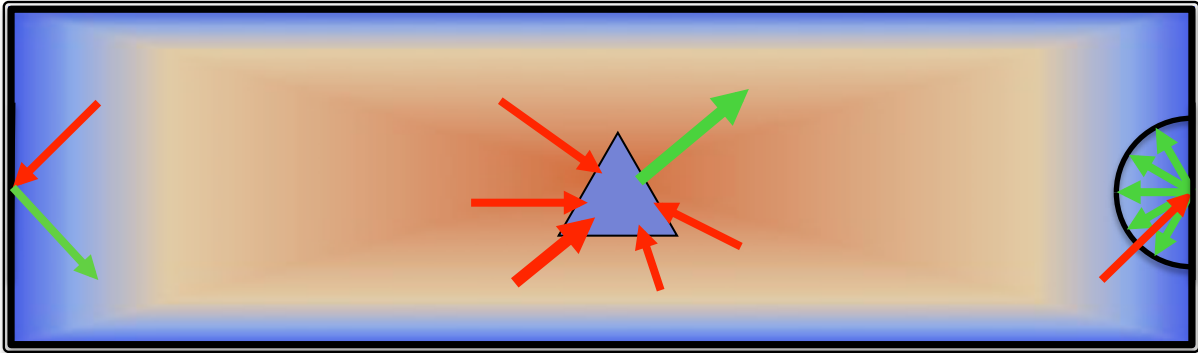
Combustion : Milieu participant, diffusion négligée



# Equation de Transfert Radiatif (ETR)

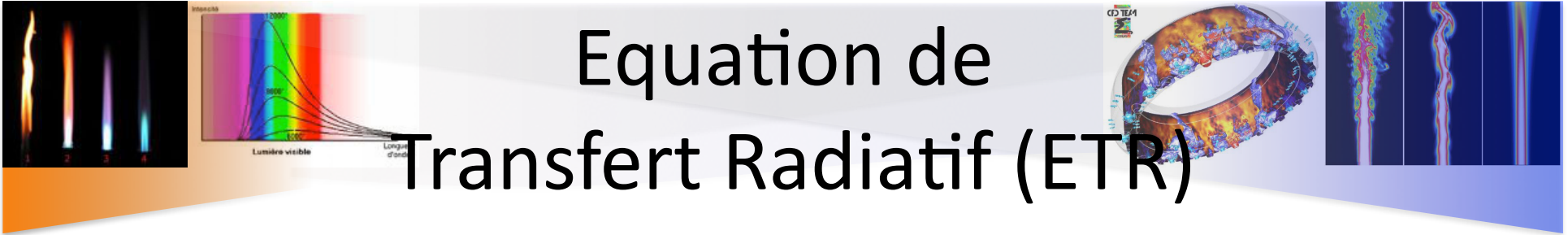
$$\frac{dL_\nu(\mathbf{x}, \mathbf{u})}{ds} = \kappa_\nu \left[ \underbrace{L_\nu^0(\mathbf{x})}_{\text{Fonction de Planck}} - \underbrace{L_\nu(\mathbf{x}, \mathbf{u})}_{\text{Luminance incidente}} \right]$$

Conditions limite  $L_\nu(\mathbf{x}_w, \mathbf{u}) = \underbrace{\epsilon_\nu(\mathbf{x}_w)L_\nu^0(\mathbf{x}_w)}_{\text{Partie émise}} + \underbrace{\rho_\nu(\mathbf{x}_w)L_{\nu,incident}(\mathbf{x}_w, \mathbf{u})}_{\text{Partie réfléchie}}$



Terme source radiatif  $S_r(\mathbf{x}) = \int_0^\infty \underbrace{\kappa_\nu}_{\text{Modèle Spectral}} \left[ 4\pi L_\nu^0(\mathbf{x}) - \int_{4\pi} L_\nu(\mathbf{x}, \mathbf{u}) d\Omega \right] d\nu$

Intégration **Angulaire**



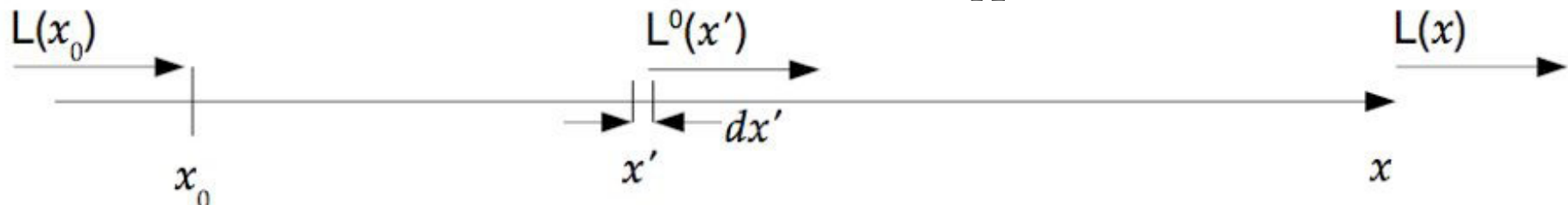
# Equation de Transfert Radiatif (ETR)

Formulation intégrale : intégration sur les chemin optiques

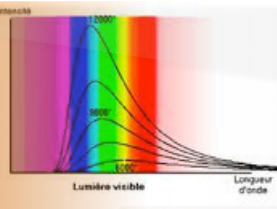
$$L_\nu(\mathbf{x}, \mathbf{u}) = L_\nu(\mathbf{x}_0, \mathbf{u}) \mathbf{T}_\nu(\mathbf{x}_0 \rightarrow \mathbf{x}) + \int_{\mathbf{x}_0}^{\mathbf{x}} L_\nu^0(\mathbf{x}') \frac{\partial \mathbf{T}_\nu(\mathbf{x}' \rightarrow \mathbf{x})}{\partial \mathbf{x}'} d\mathbf{x}'$$

Transmittance :  $\mathbf{T}_\nu(\mathbf{x}' \rightarrow \mathbf{x}) = \exp(-\tau_\nu(\mathbf{x}' \rightarrow \mathbf{x}))$

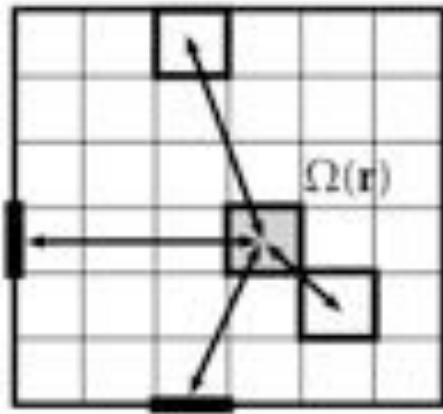
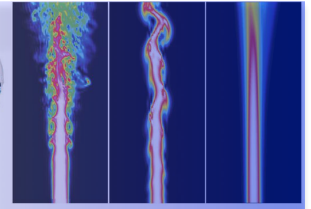
Épaisseur optique :  $\tau_\nu(\mathbf{x}' \rightarrow \mathbf{x}) = \int_{\mathbf{x}'}^{\mathbf{x}} \kappa_\nu(x'') dx''$



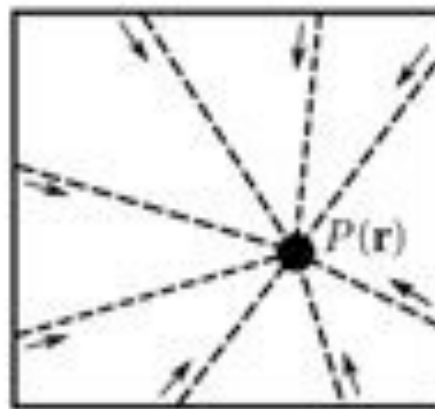




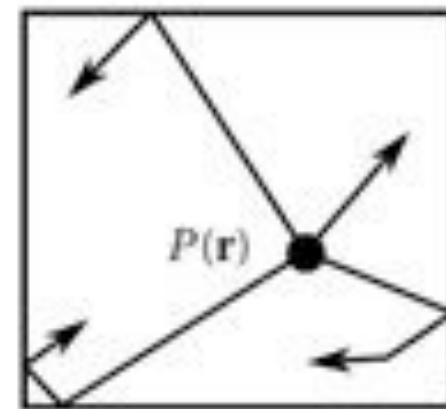
# Méthodes usuelles



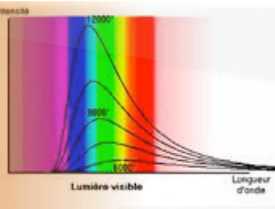
(a) Zonal method



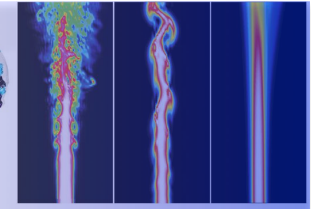
(b) Ray tracing



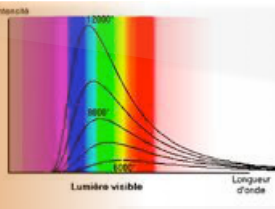
(c) Monte Carlo method



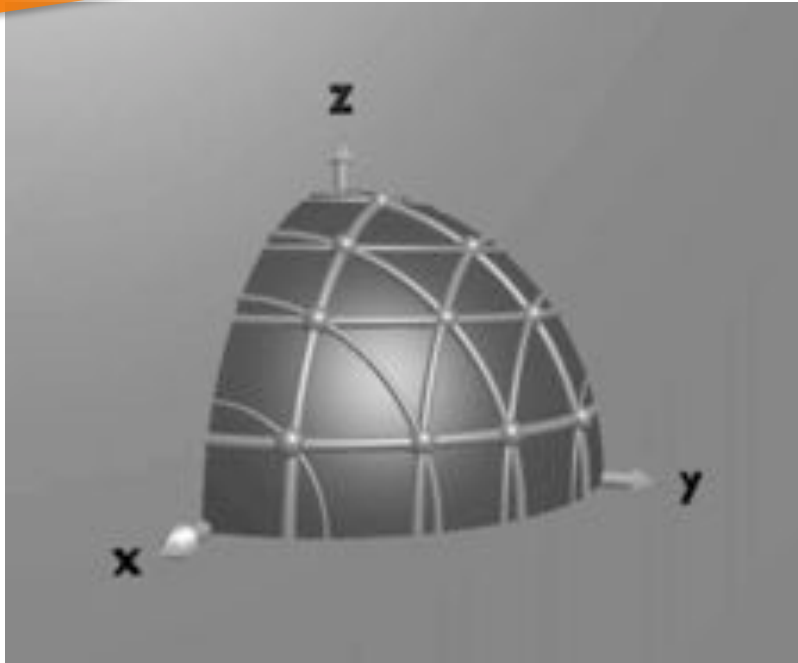
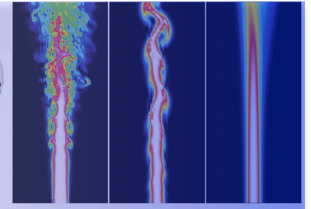
# Méthodes usuelles



	Avantages	Inconvénients
Méthode des zones (Hottel, 1958)	Formulation proche physique	Lourde, coûts CPU
Harmoniques sphériques, $P_N$ (Jeans, 1917.)	Formulation :EDP simples	Non adaptée aux milieux minces
Monte Carlo (Fleck, Howell, Modest, ...)	Solutions de réf. Avec variance statistique	Coûts CPU
Discrete Ordinates Méthod $S_N$ (Chandrasekhar, 1960.)	Formulation / Couplage CFD facile	- Effets de rayon - Diffusion num.
Discrete Transfer Method (Lockwood & Shah, 1981.)	Assez implantée codes CFD	- Effets de rayon, - coûts CPU (milieux non gris, réflexions parois..)



# Méthode aux ordonnées discrètes



$$\int_{4\pi} f(\mathbf{s}) d\Omega \approx \sum_{i=1}^{N_{dir}} \omega_i f(\mathbf{s}_i)$$

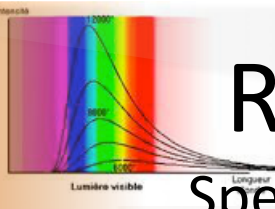


Jeu de quadratures  $\left\{ \begin{array}{l} \mathbf{s}_i \{ \mu_i, \eta_i, \xi_i \} \\ \omega_i \end{array} \right\}$

Ex: Quadrature S8

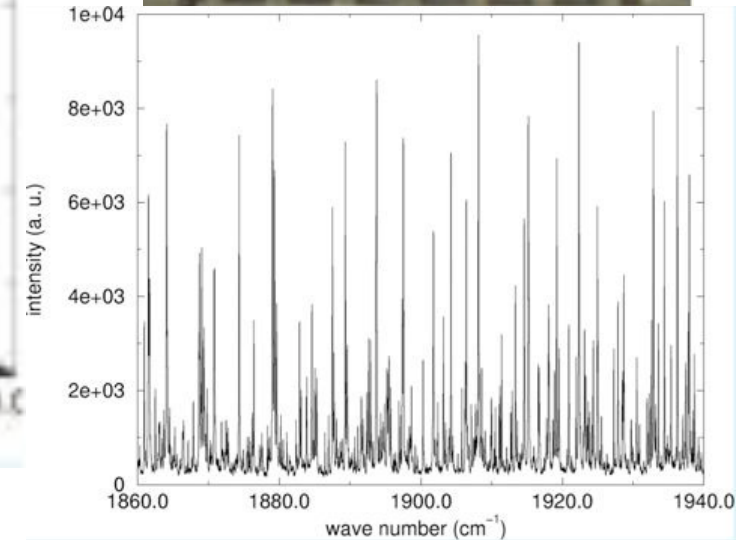
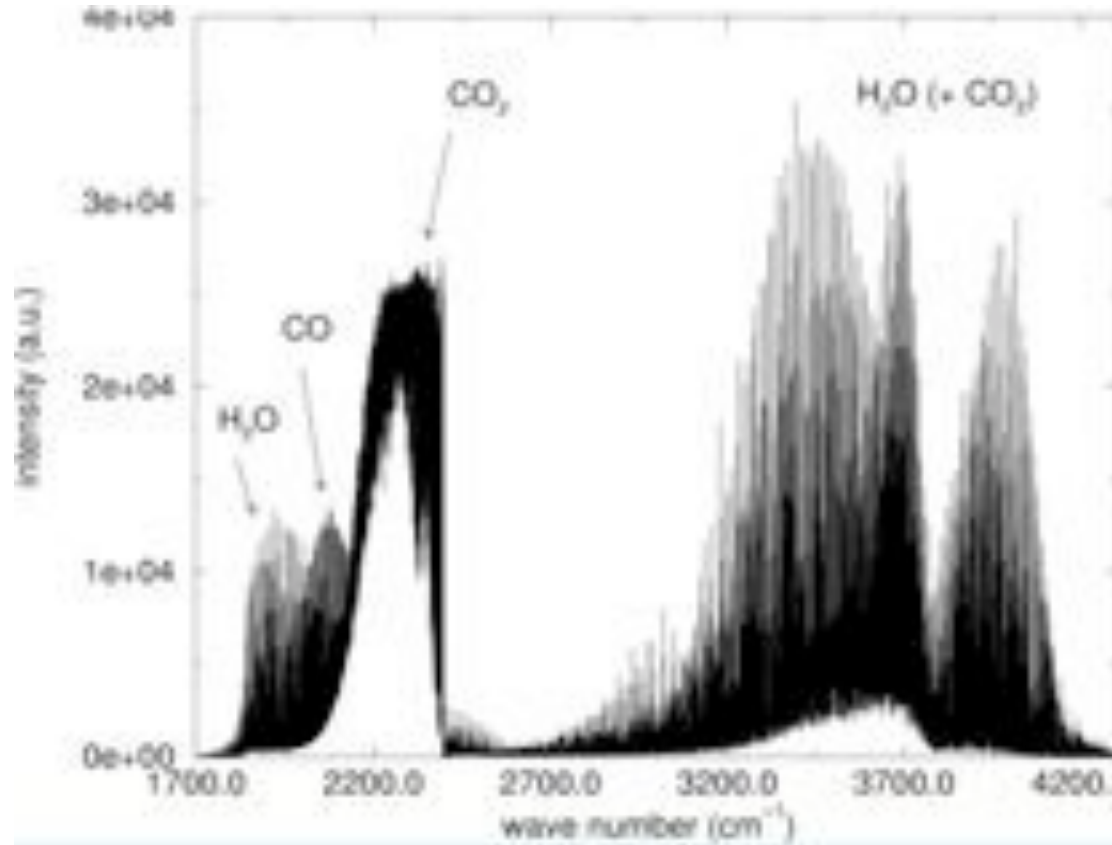
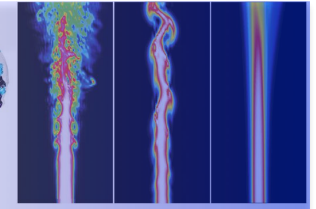
Les plus courantes : quadrature SN, quadrature TN, quadrature Polaire/Azimuthale (FVM)

➔ Effet de rayon



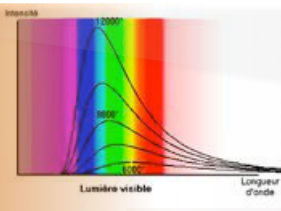
# Rayonnement des gaz :

Spectre d'émission typique d'une flamme

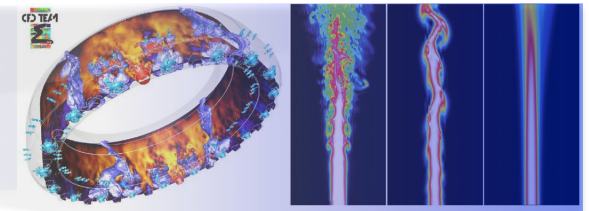


Spectre d'émission expérimental d'une flamme CH<sub>4</sub>/air à 2160K  
(spectroscopie d'émission FTIR; Soufiani et al. 2002)





# Modèles spectraux



- Modèle Raie-par-raie

=>  $10^6$  résolutions/direction

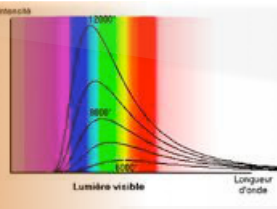
$$\kappa_\nu = \sum_{\text{espèces}} \sum_{\text{transition } i} \frac{h\nu}{c} F_i(\nu - \nu_i) B_{ul}^i \left( \frac{g_u^i}{g_l^i} n_u^i - n_l^i \right)$$

- Modèles à Bandes étroites : SNBCK

=>  $10^3$  résolutions/direction

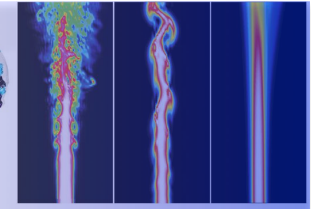
- Modèles Globaux : WSGG, FSK, FSCK

=>  $10^1$  résolutions/direction

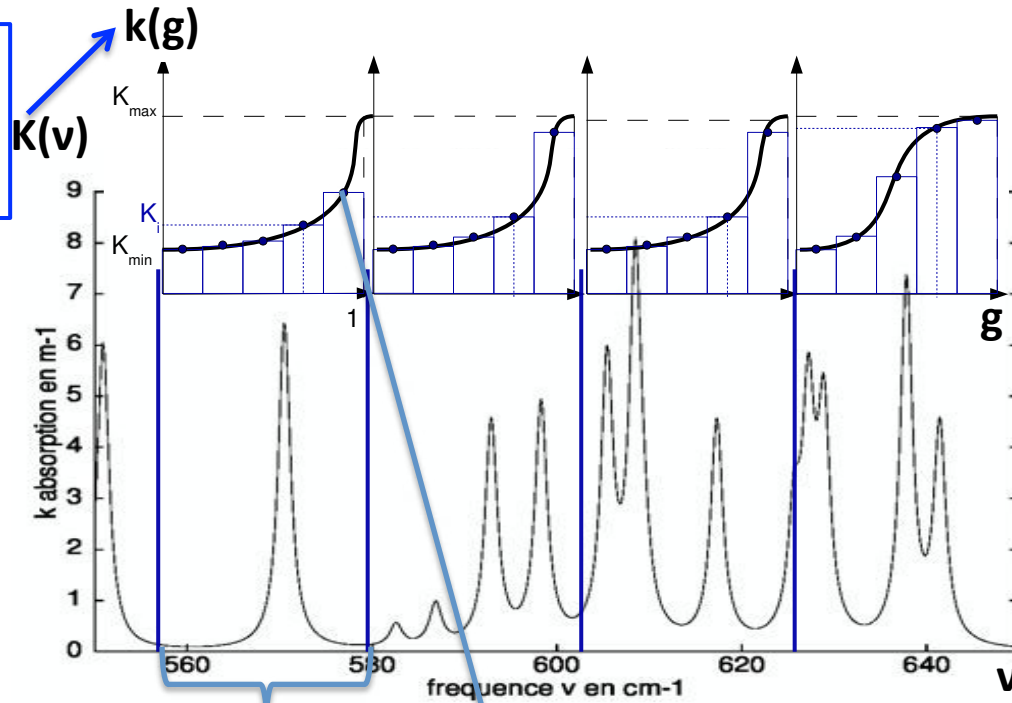


# Modèles spectraux

## Bandes étroites



Réordonnement  
Statistique par bande  
(CK)

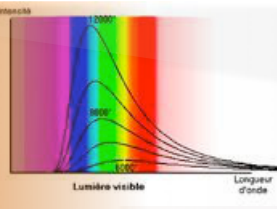


Bande étroite  $i$

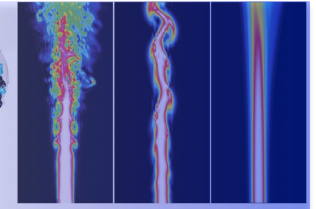
Point de quadrature  $g_j$

$$S_r(\mathbf{x}) \simeq \sum_{i=1}^{N_{band}} \Delta v_i \left[ \sum_{j=1}^{N_{quad}} \omega_j \kappa_{ij} \left( 4\pi \overline{L_{\Delta v_i}^0(\mathbf{x})} - \sum_{k=1}^{N_{dir}} \omega_k^a L_{i,j}(\mathbf{x}, \mathbf{u}_k) \right) \right]$$

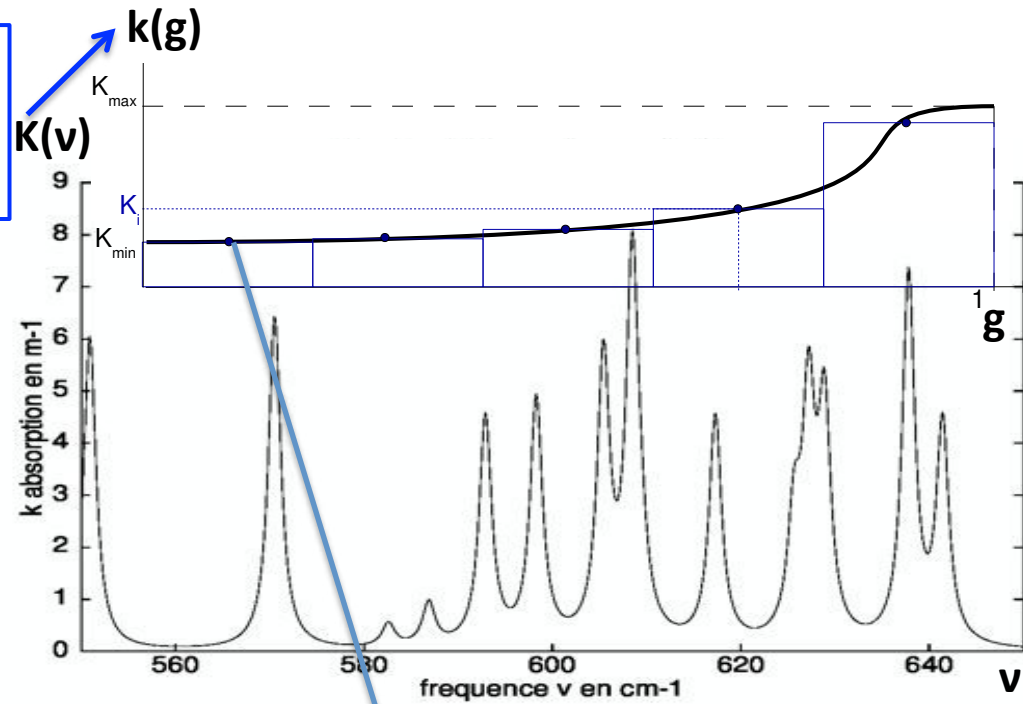
371\*5 ≈ 1800 intégrations/direction



# Modèles globaux



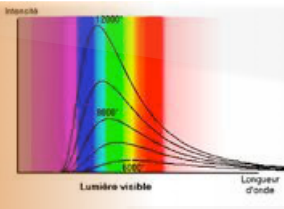
Réordonnement  
Statistique sur tout le  
spectre (FSK, FSCK)



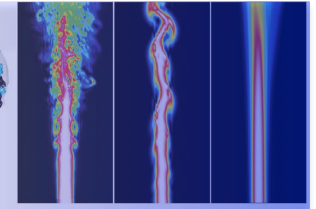
Point de quadrature  $g_j$

$$S_r(\mathbf{x}) \simeq \sum_{j=1}^{N_q} \omega_j K_j \left( 4\pi\sigma T^4(\mathbf{x}) - \sum_{k=1}^{N_{dir}} \omega_k^a L_j(\mathbf{x}, \mathbf{u}_k) \right)$$

3-15 intégrations/direction



# Programme



1. Contexte et théorie
2. Le code PRISSMA
3. Parallélisme
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5. Vers le couplage...



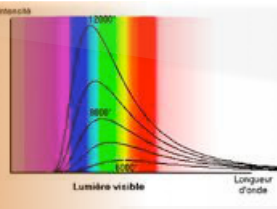


Collaboration : École des Mines d'Albi, CERFACS

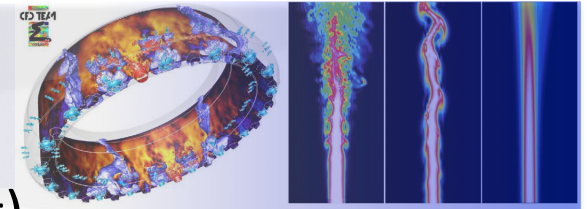
⇒ D. Joseph, J. Amaya, D. Poitou, M. El Hafi, B. Cuenot, ...

- Solveur adapté au traitement de géométries complexes :  
*Maillages hybrides, non structurés,*
- Compatible AVBP : maillage (V5.X), solution initiale,
- Suivi de version : svn,
- cas test automatisés,
- Orienté couplage : *instructions PALM*
- web <http://www.cerfacs.fr/prissma>

• Memory usage for 1 000 000 cells:	
PREPROCESSING	-> 2,1 Gb
PRISSMA	-> 495 Mb (CK)
	-> 485 Mb (Global);



# Ordonnement des cellules (sweeping)



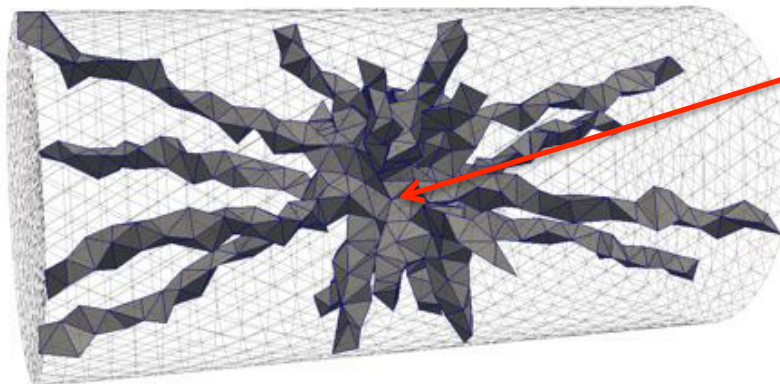
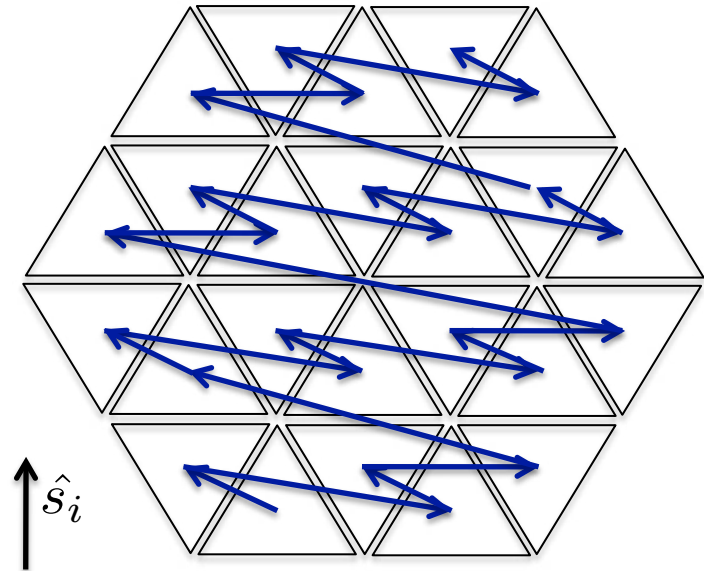
- Difficulté de parallélisation par sous domaine :

$$S_r(\mathbf{x}) \simeq \sum_{j=1}^{N_q} \omega_j \kappa_i \left( 4\pi\sigma T^4(\mathbf{x}) - \sum_{k=1}^{N_{dir}} \omega_k^a L_j(\mathbf{x}, \mathbf{u}_k) \right)$$

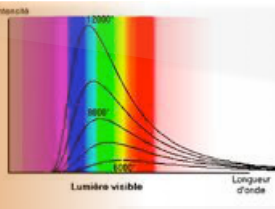
$L_j$  : échanges à distance.

Les cellules sont ordonnées tel que la luminance de la cellule précédente soit connue

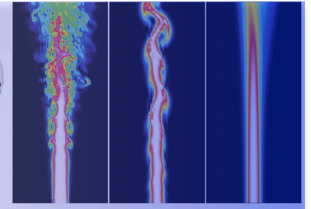
→ **algorithme séquentiel**



Exemple des chemins optiques incidents au centre  
→ Tool **quad\_tracing**



# Calcul Radiatif



## PRE PROCESSING

- Building geometrie and sweeping

## RADIATIVE CALCULATION

- Mesh partitionning

Do  $i_{\text{coupl}} = 1, N_{\text{coupl}}$

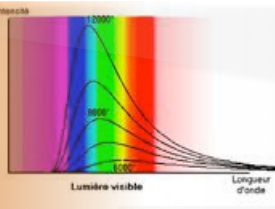
- Get fluid fields from the fluid solver

$$\Phi = (T, P, X_{CO_2}, X_{H_2O}, X_{CO}, f_{v,soot})$$

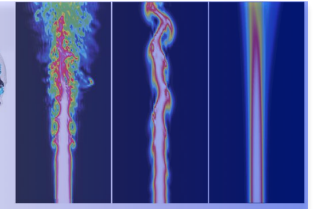
Spectral Calculation

Angular integration

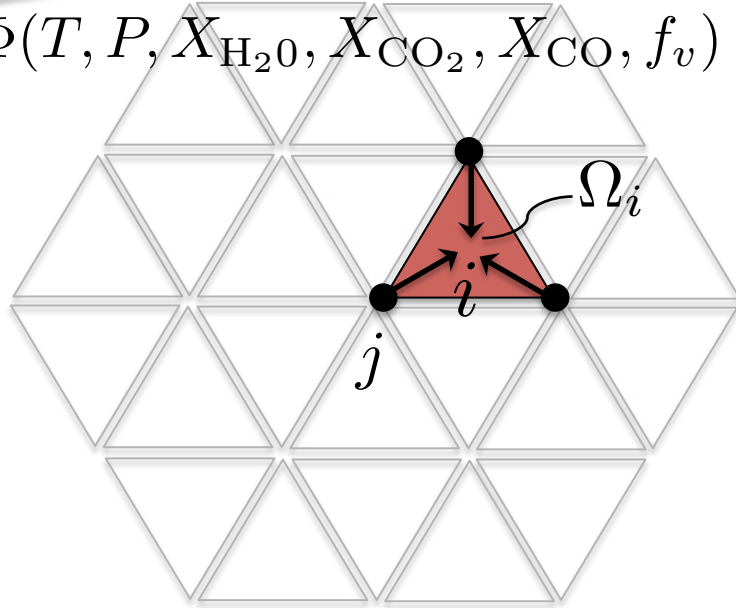
- Postprocessing results
- Send  $S_r$  and  $Q_w$  to the fluid solver
- EndDo



# Calcul Radiatif



$$\Phi(T, P, X_{\text{H}_2\text{O}}, X_{\text{CO}_2}, X_{\text{CO}}, f_v)$$



Solution initiale aux nœuds

-> Modèle global :

Calcul spectral aux nœuds  $\kappa_j(\Phi_j), L_j^0(T_j)$

Puis gather

$$\kappa_j \rightarrow \kappa_i$$

-> Modèle bande étroite : Boucle sur les bandes (371)

Gather données physiques  $\Phi_j \rightarrow \Phi_i$

Calcul spectral aux cellules  $\kappa_i, L_i^0$

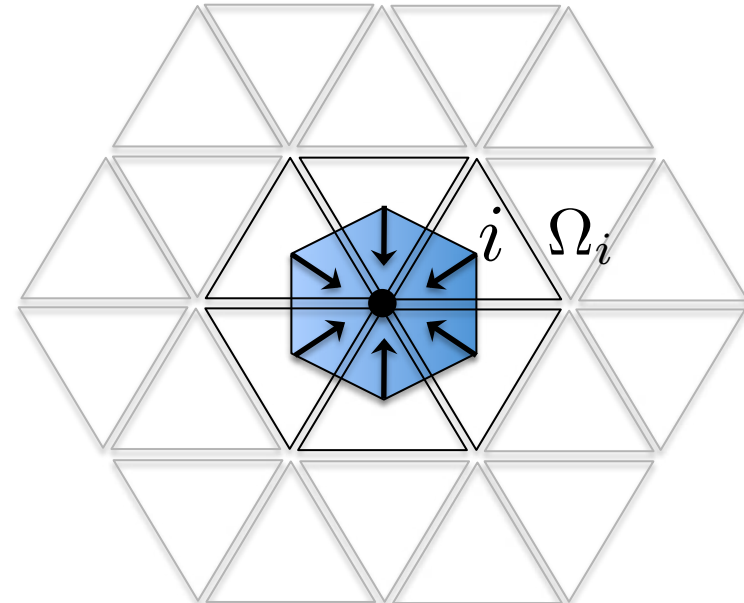
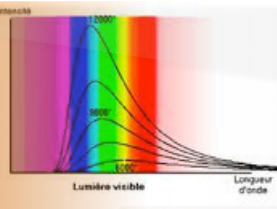


Schéma cell-center : calcul aux cellules

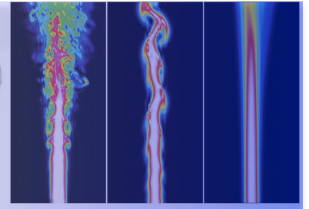
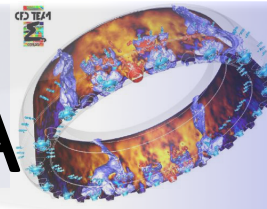
Scatter : Solution stockée aux nœuds

$$S_{r,i} \rightarrow S_{r,j}$$





# Solveur PRISSMA

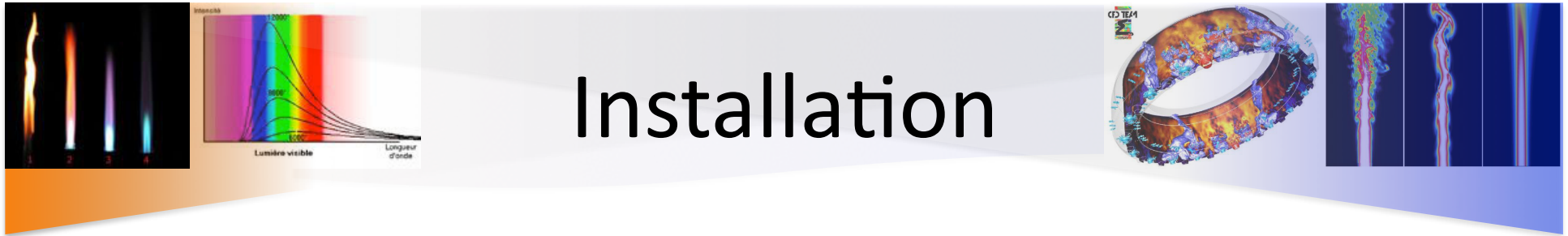


- ETR sans diffusion
- Type volumes finis, Schéma spatial DMFS/STEP (David Joseph et al. 2004)
- Discrétisation angulaire : quadrature type  $S_N$ ,  $LC_{11}$

Modèles Spectraux		Précision	Coût
Bandes étroites	CK	+++	1000
Globaux	WSGG	-	1
	FSK / TFSK	+ (hyp. Homogène)	10 / 3 Tabulé
	FSCK / TFSCK	++ (état de référence)	10 / 3 Tabulé

Base de données : SNB (**EM2C**) : SNB-CK, SNB-FSCK, ...  
 NBKM (**CETHIL**) : NBKM-CK, NBKM-FSCK, ...

- Parallélisation hybride : Taches (directions, fréquence; MPI & OpenMP),  
Sous-domaines (MPI)



# Installation

**Login** : user et password -> form01 à form10

## Downloading source files:

@CERFACS : `svn co svn+ssh://login@nuage/home/cfd1/prisma/svn/PRISSMA/version INSTALL_DIR`

Extérieur `svn co http://www.cerfacs.fr/prissmasvn/version INSTALL\_DIR`

## Source code :

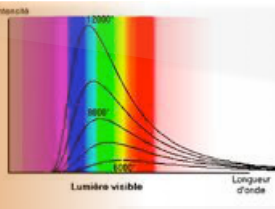
-> **version**='tags/PRISSMA\_V2.0'

-> *Set Environnement Variables* : <http://www.cerfacs.fr/prisma/index.php?body=installing>

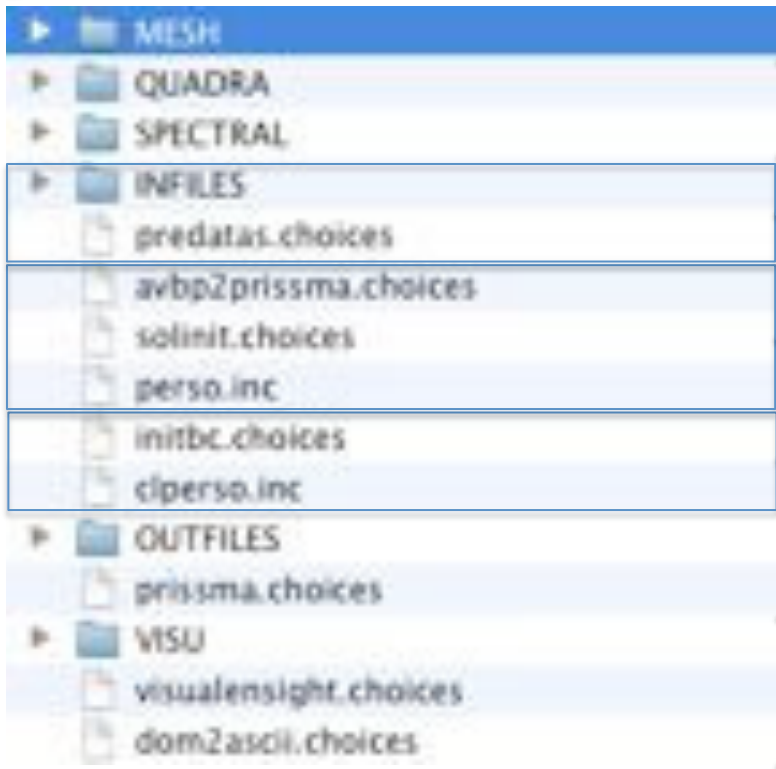
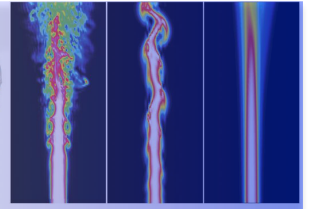
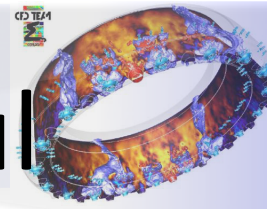
**AVBP** : source /home/form00/FORMATION\_PRISSMA/path\_AVBP

**Cas test** : **version**='branches/TEST\_CASES'

**Cas d'application** : /home/form00/RUNS\_PRISSMA



# Exemple de calcul



Maillage : AVBP 5.X / Gambit

Données DOM & Spectrales : **createdomcase**

Fichiers d'entrée PRISSMA

1-> **predatas** balayage de la géométrie

2-> Solution initiale : **avbp2prisma**  
ou **solinit** (perso.inc)

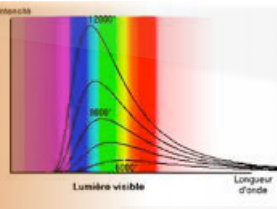
3-> **inibc** Conditions limite

4-> **run\_para** PRISSMA!

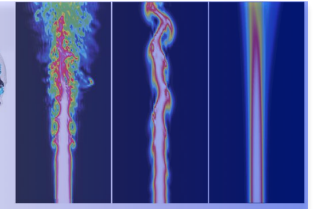
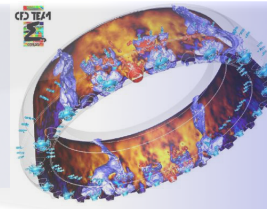
Visualisation : **visu** (ensight) ou **dom2ascii**

=> Champs de  $S_r$ ,  $Q_r$  et  $Q_w$

Site web : <http://www.cerfacs.fr/prisma> : documentation, cas tests, flowchart, ...



# Exemple de calcul



- predatas.choices

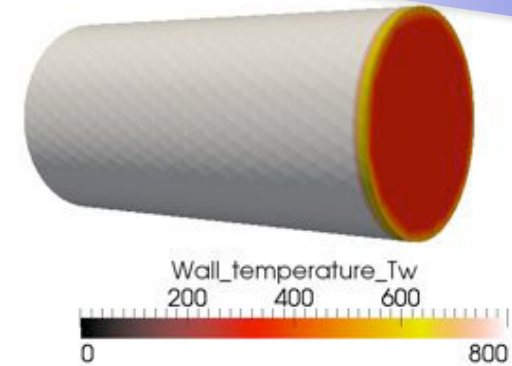
```
'./meshes/cyl_coarse.neu' | Mesh file name
'./QUADRA' | Quadrature definition directory
2 | Mesh type (1-AVBP, 2-GAMBIT)
'./INFILES/' | Output path
SNDOM | Quadrature type [SNDOMIFVMITNDOMIPERSO]
4 | Quadrature order
2 | Number of directions if PERSO quadrature
1. 0. 0. | 1st direction for PERSO quadrature
-1. 0. 0. | 2nd direction ...
```

- prissma.choices

```
'./INFILES' | Path to *.in files
'./SPECTRAL' | Path to spectral data
'./OUTFILES' | Output path
DMFS | Spatial discretization [ DMFS | SMFS | EXPON ]
SNB | Narrow band data base [ SNB | NBKM ]
CK | Spectral model [ CK | (T)FSCK | (T)FSK | MSGG | GRAY ]
5 | Spectral quadrature points (CK:5, FS(C)K:5->15)
1.e-2 | Convergence criterion (Reflection and subdomains)
NO | Homogeneous system [ NO | YES ]
0 | Print directions [ 1 | 0 ]
1 | Number of subdomains (Ndomains < Nprocs)
1 | Number of threads (Nthreads < Ndirs )
```

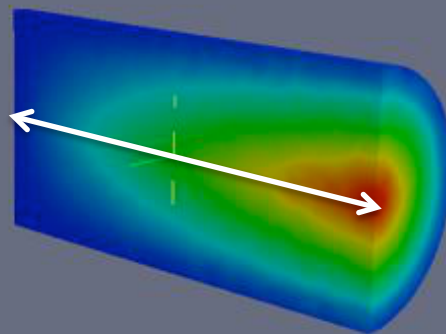
# Cas test 1

- Maillage GAMBIT, Configuration cylindrique
  - Solution analytique avec profil de température et de concentration.
  - $R=0,3\text{m}$   $L=1,2\text{m}$ , Maillage 27749 cellules
  - $T_w=300\text{K}$  partout sauf en  $x=1,2\text{m}$   $T_w=800\text{K}$
- Parois noires  $\epsilon = 1$ ,

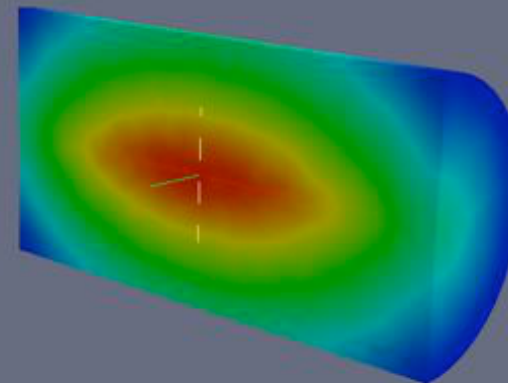


Energie radiative : 18,53 kW

Temperature  
2004.2  
1697.2  
1390.1  
1083.1  
776.00

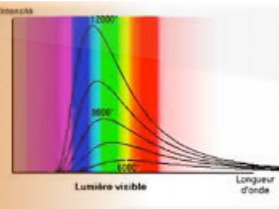


XH2O  
0.094483  
0.077573  
0.060663  
0.043754  
0.026844

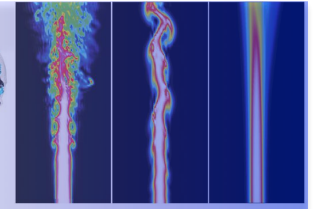


COELHO *et al.* 2003. Numerical Heat Transfer, Part B: Fundamentals 43:425 - 444.



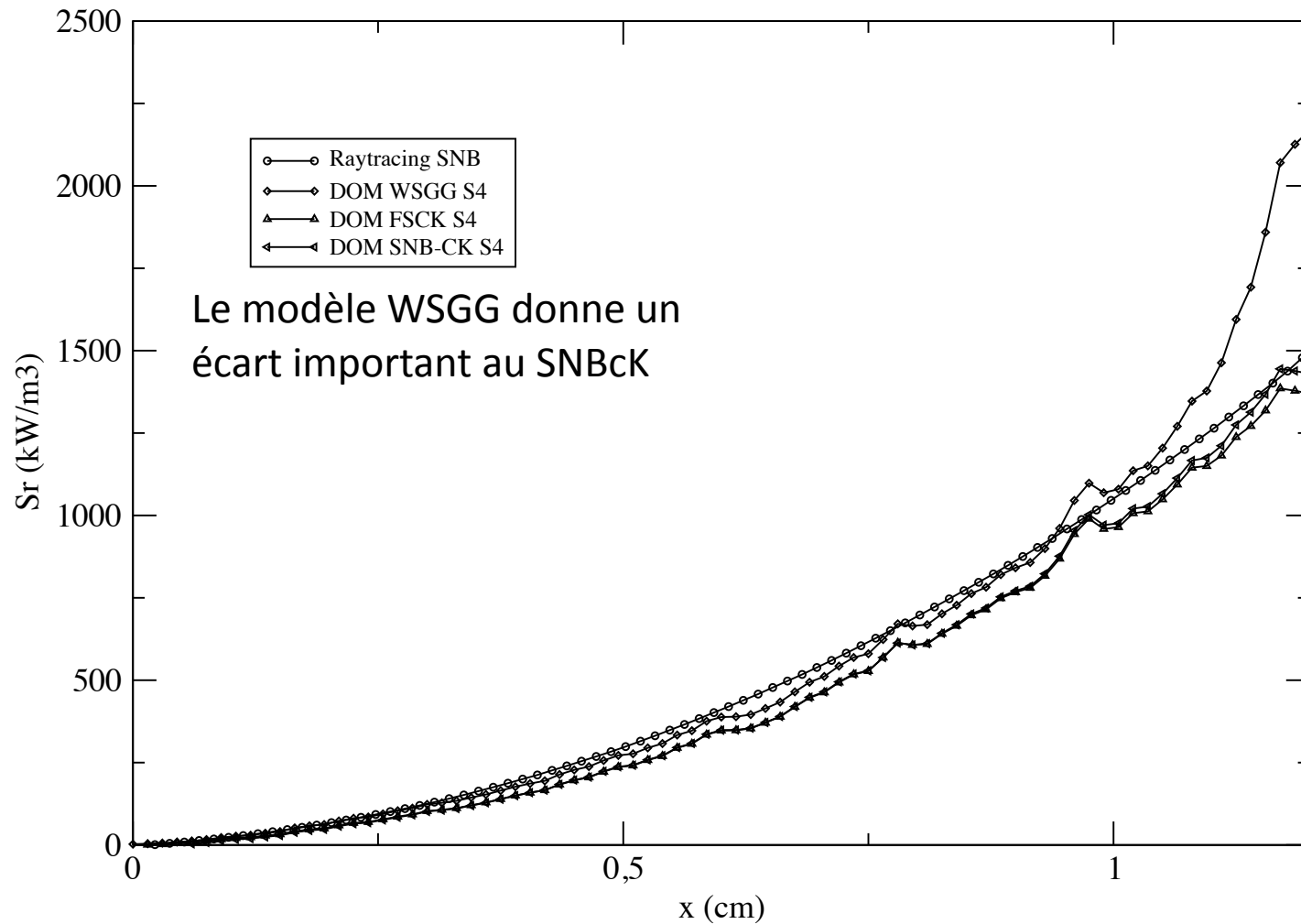


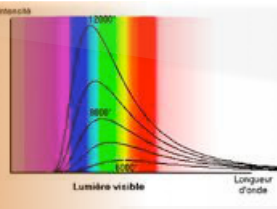
# Cas test 1



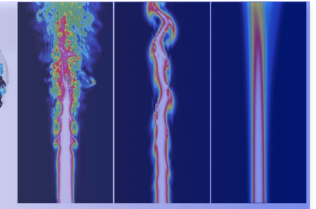
## *Spectral models - DOM DMFS S4*

Inhomogeneous cylinder  $X_{\text{soot}} = 1.e-7$



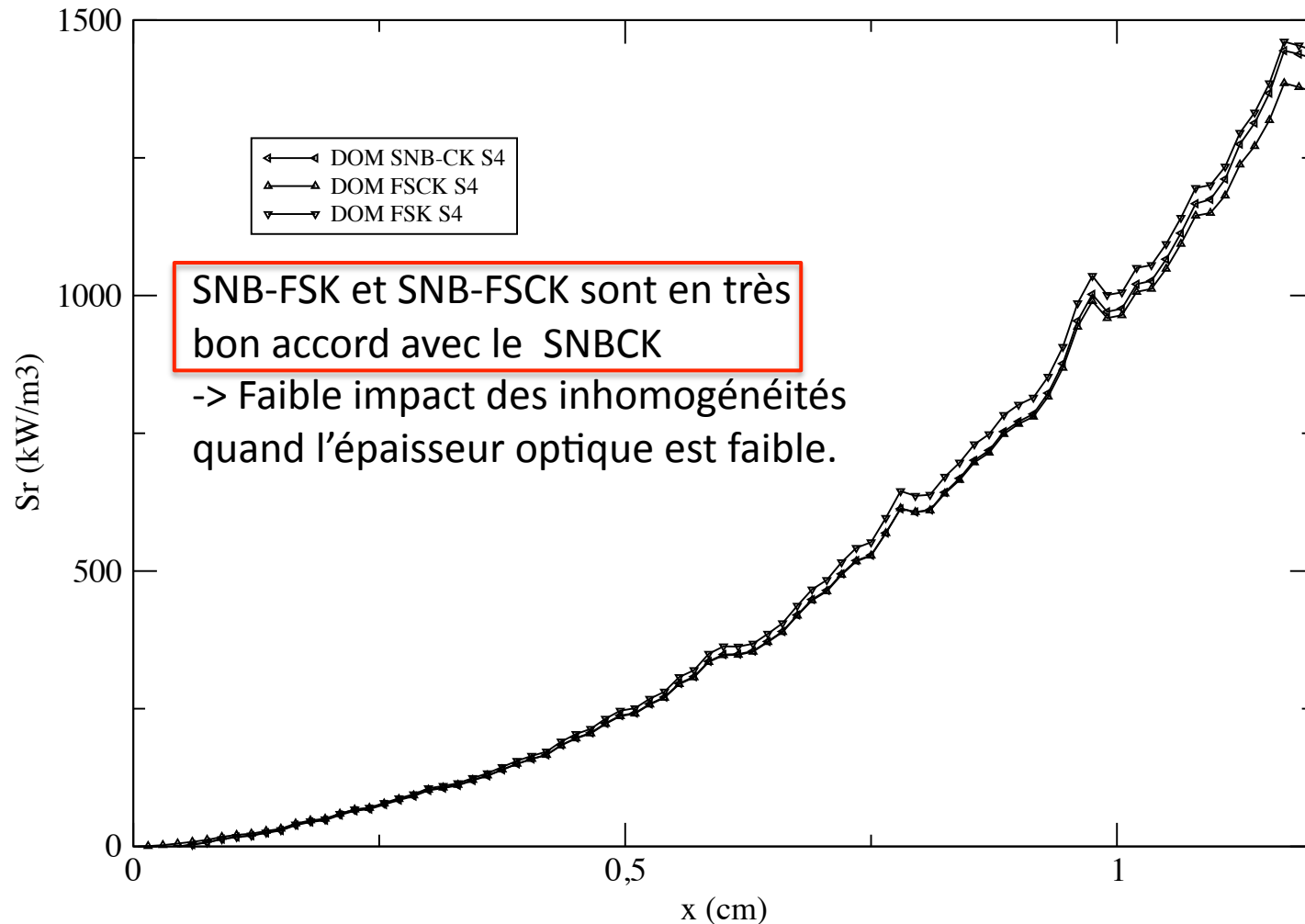


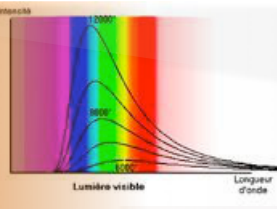
# Cas test 1



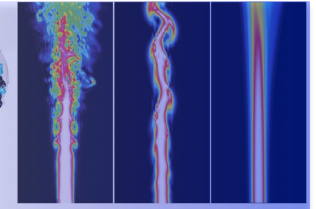
## *Spectral models - DOM DMFS S4*

Inhomogeneous cylinder  $X_{\text{soot}} = 1.e-7$

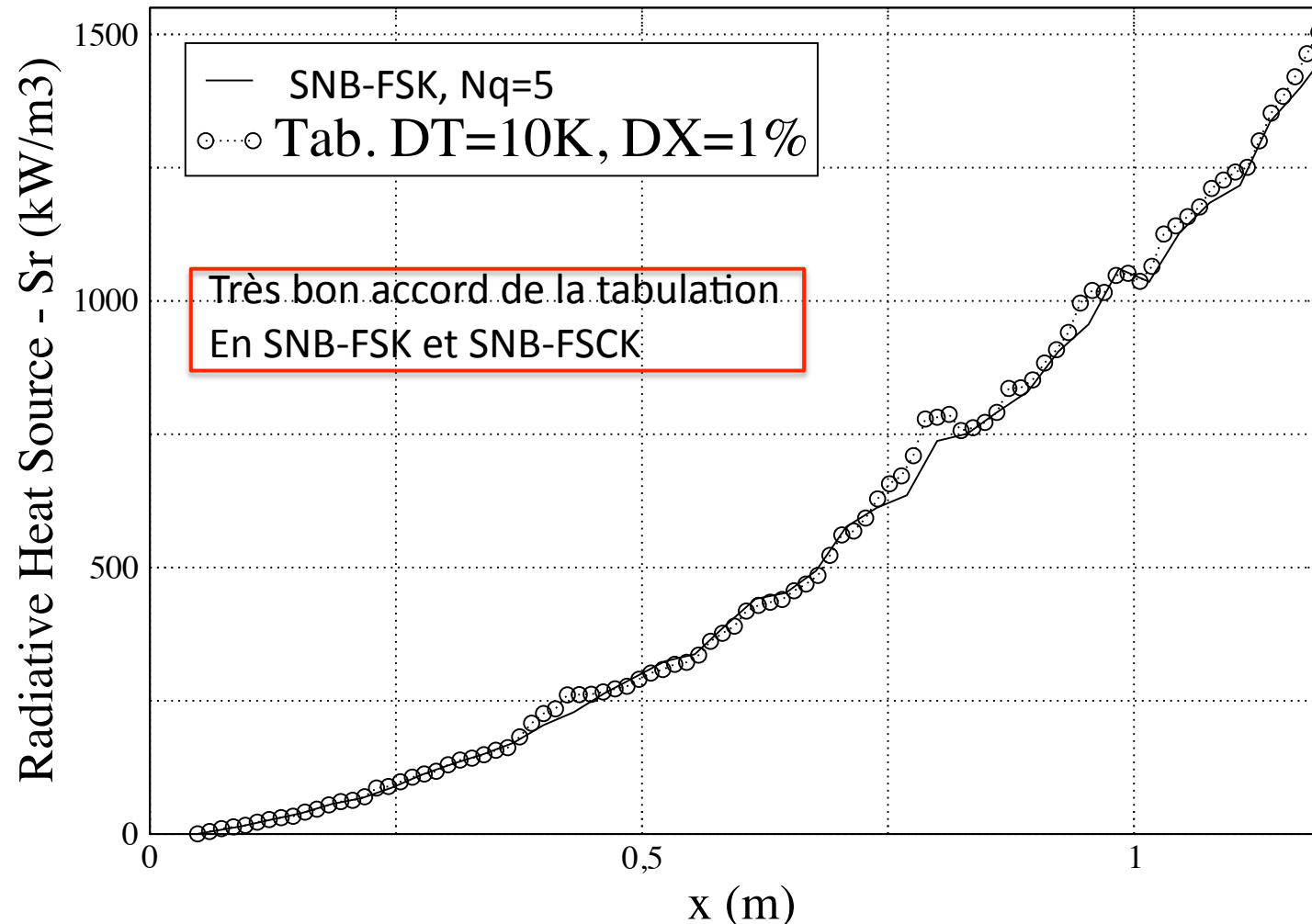


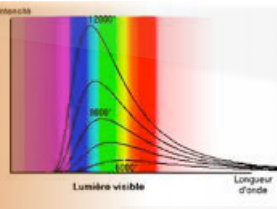


# Cas test 1

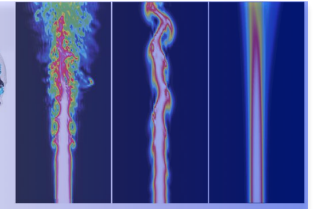


Cylinder with temperature profile  
XSoot =  $1e-7$

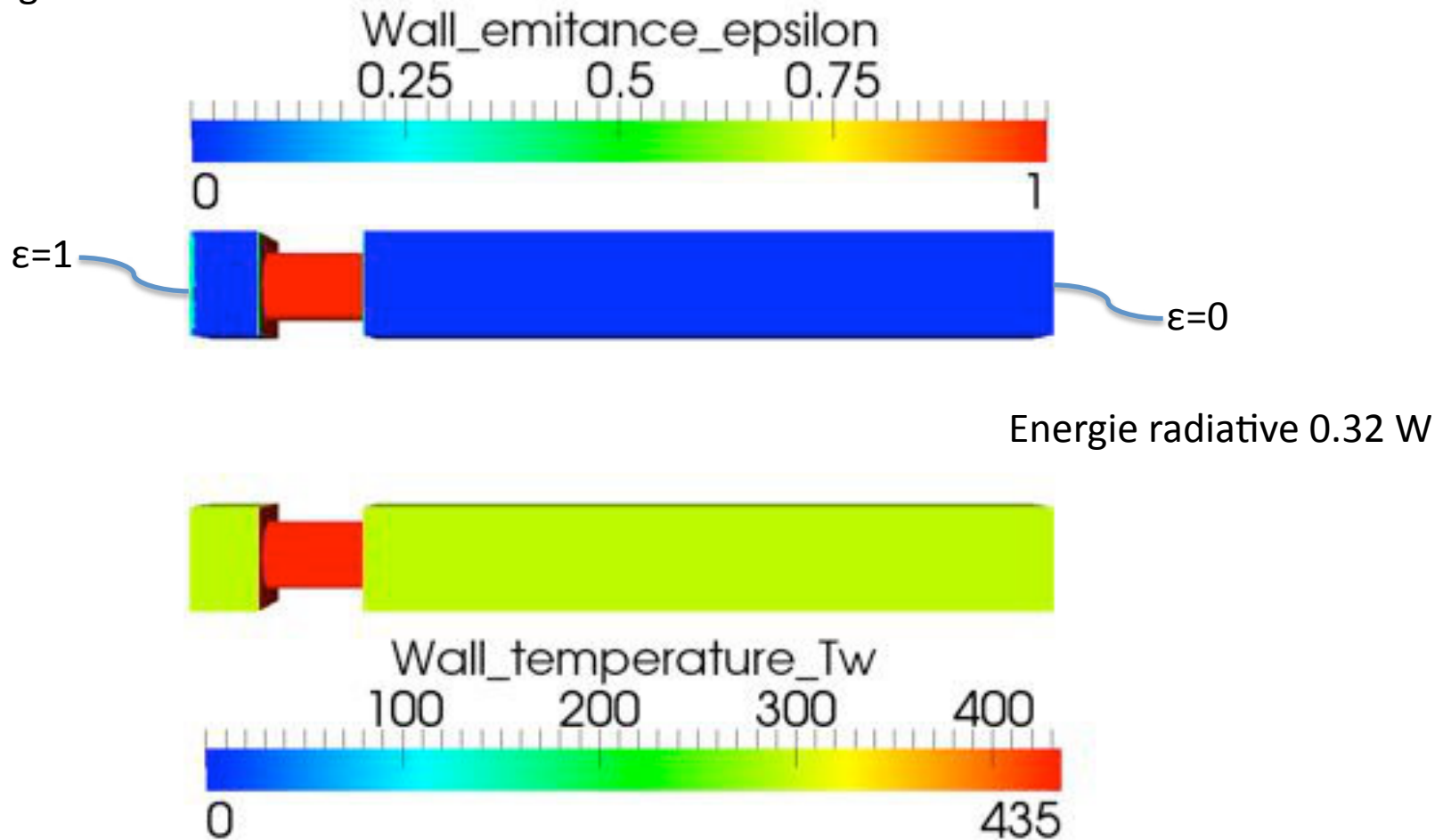


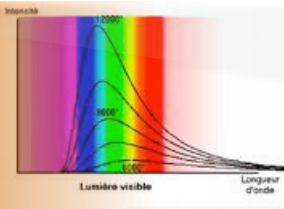


# Cas test 2 solution AVBP

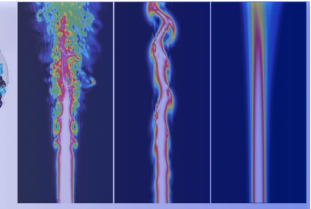


- Maillage & Solution AVBP

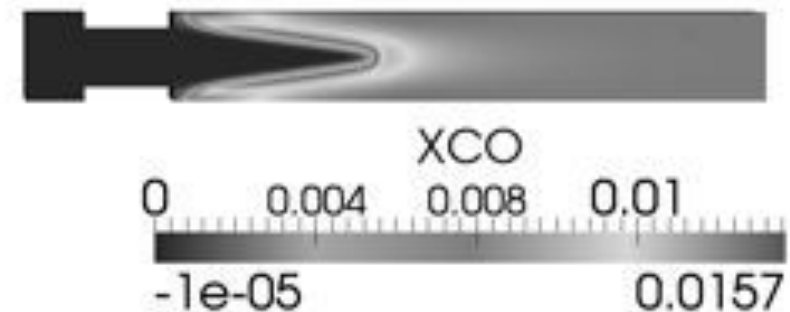
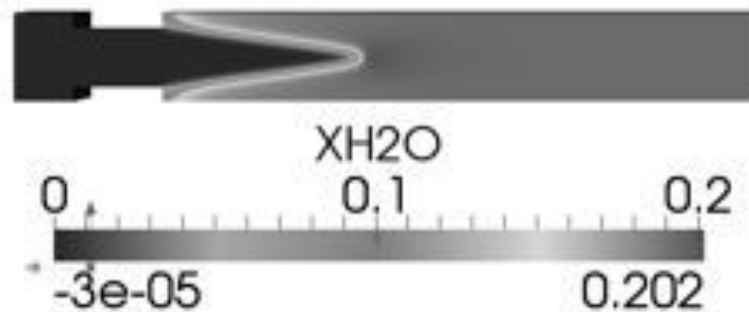
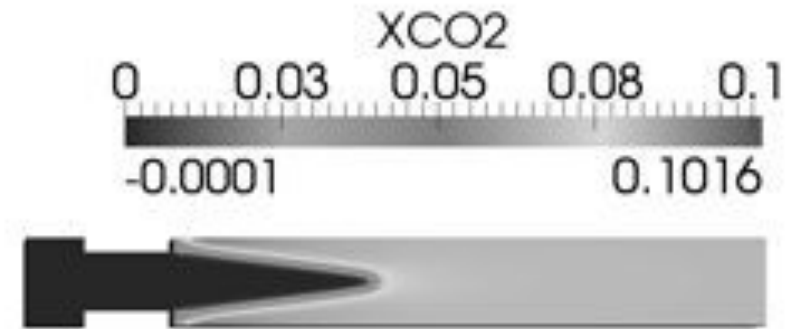
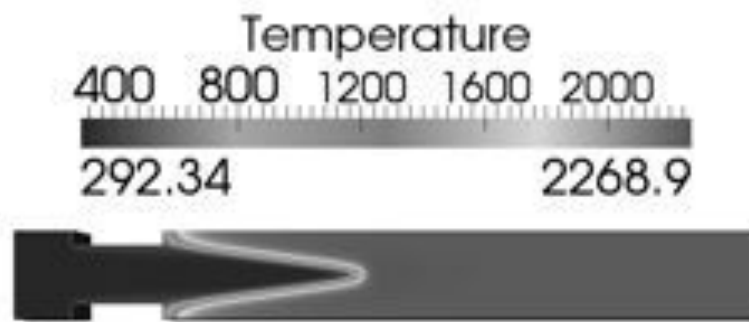




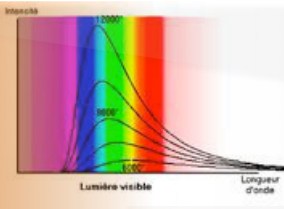
# Cas test 2 solution AVBP



- Maillage & Solution AVBP

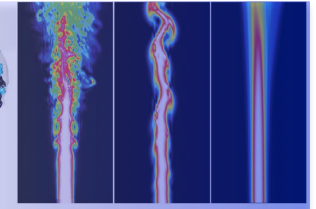




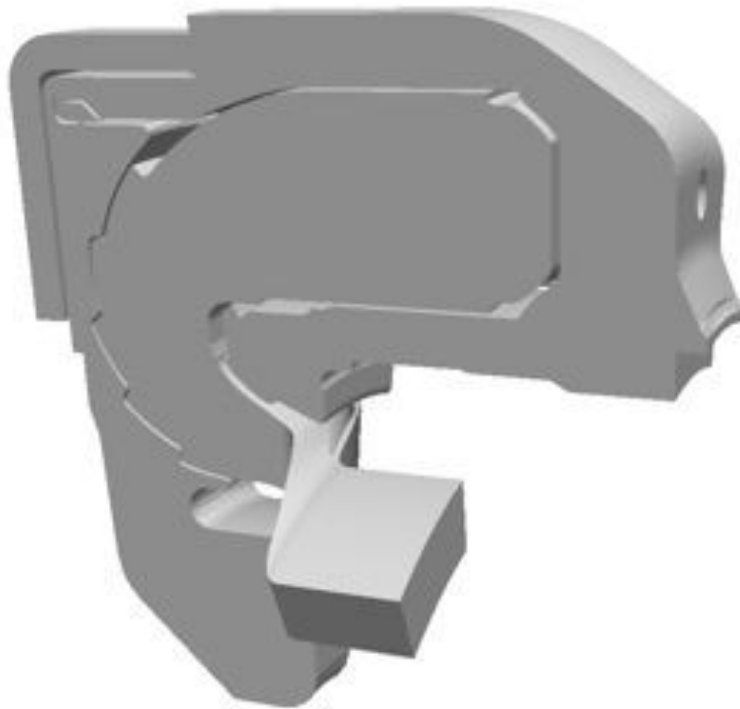


# Cas test 3

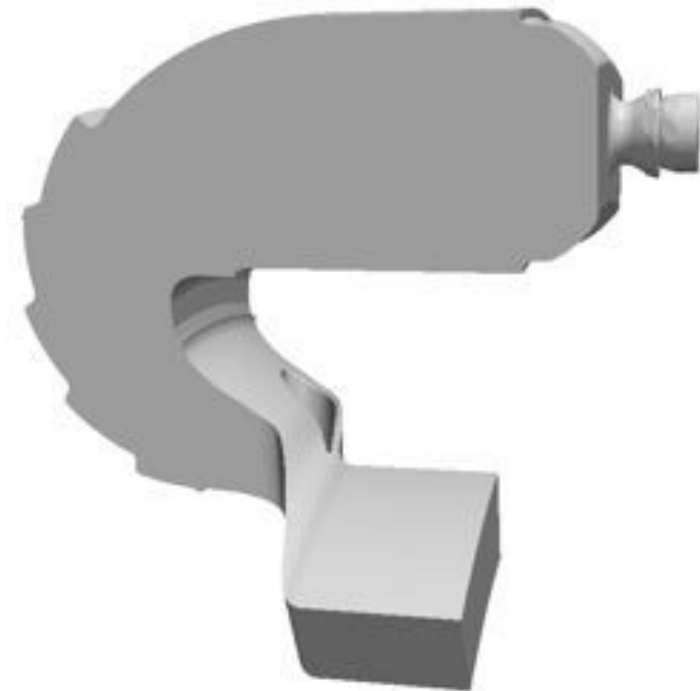
## Ardiden 3



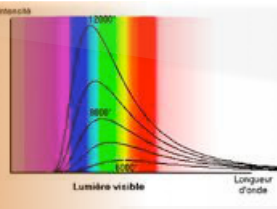
- Maillage réduit & Solution interpolée AVBP



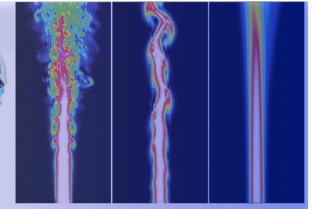
Maillage AVBP : Chambre + contournement  
11M de cellules



Maillage PRISSMA : Chambre seulement  
2,6M cellules



# Cas test 3 Ardiden 3



- Maillage réduit & Solution interpolée AVBP

Temperature

2628.157

2400

2000

1600

1200

800

578.3696

XH2O

0.159471

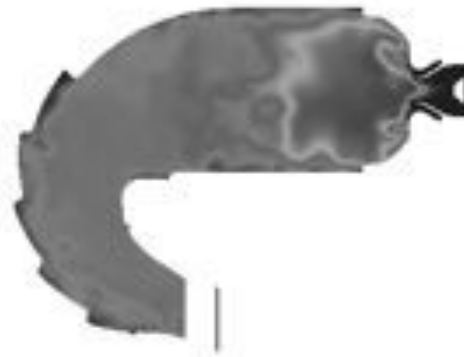
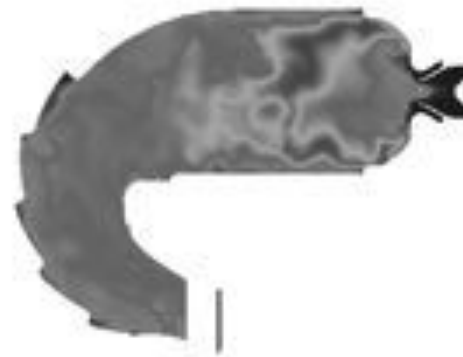
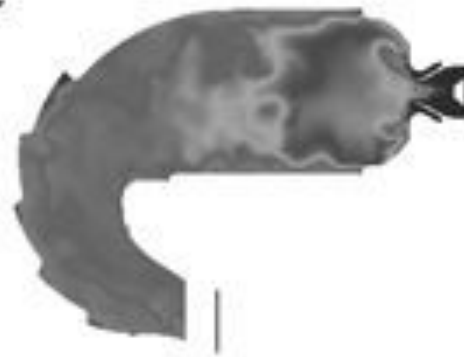
0.12

0.08

0.04

0

-0.000653



XCO2

0.112199

0.1

0.075

0.05

0.025

0

-0.000197

XCO

0.121398

0.1

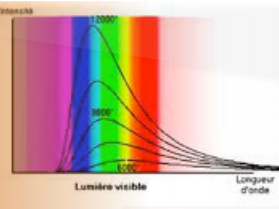
0.075

0.05

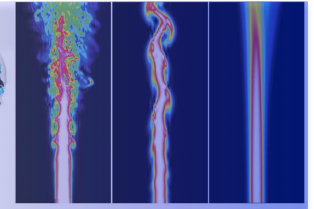
0.025

0

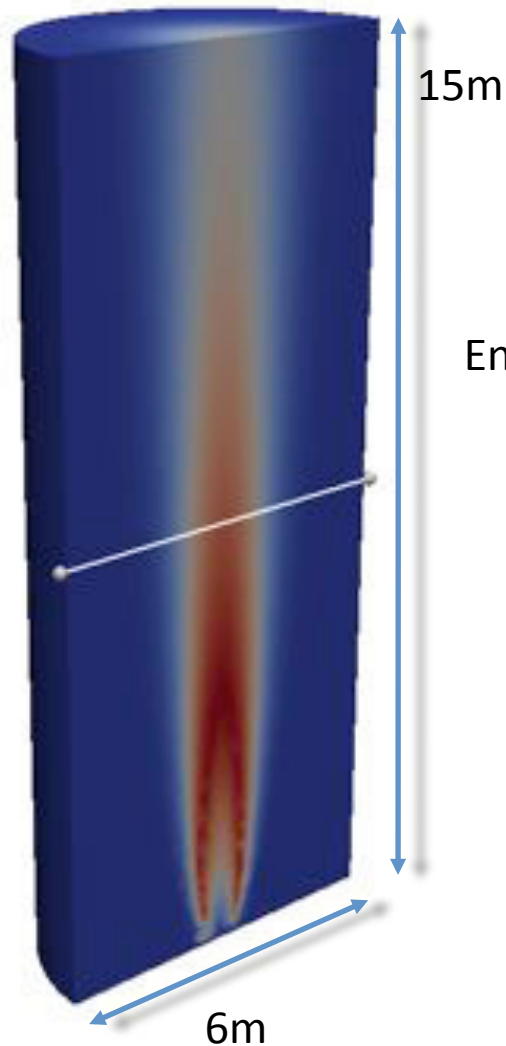
-0.000763



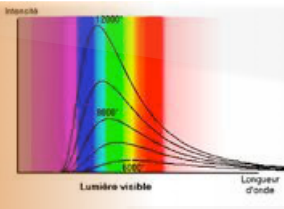
# Cas test 4 Four



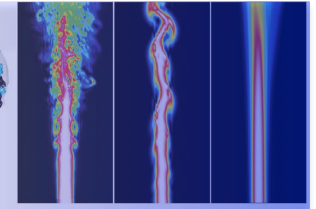
- Maillage AVBP
- Solution CANDLE



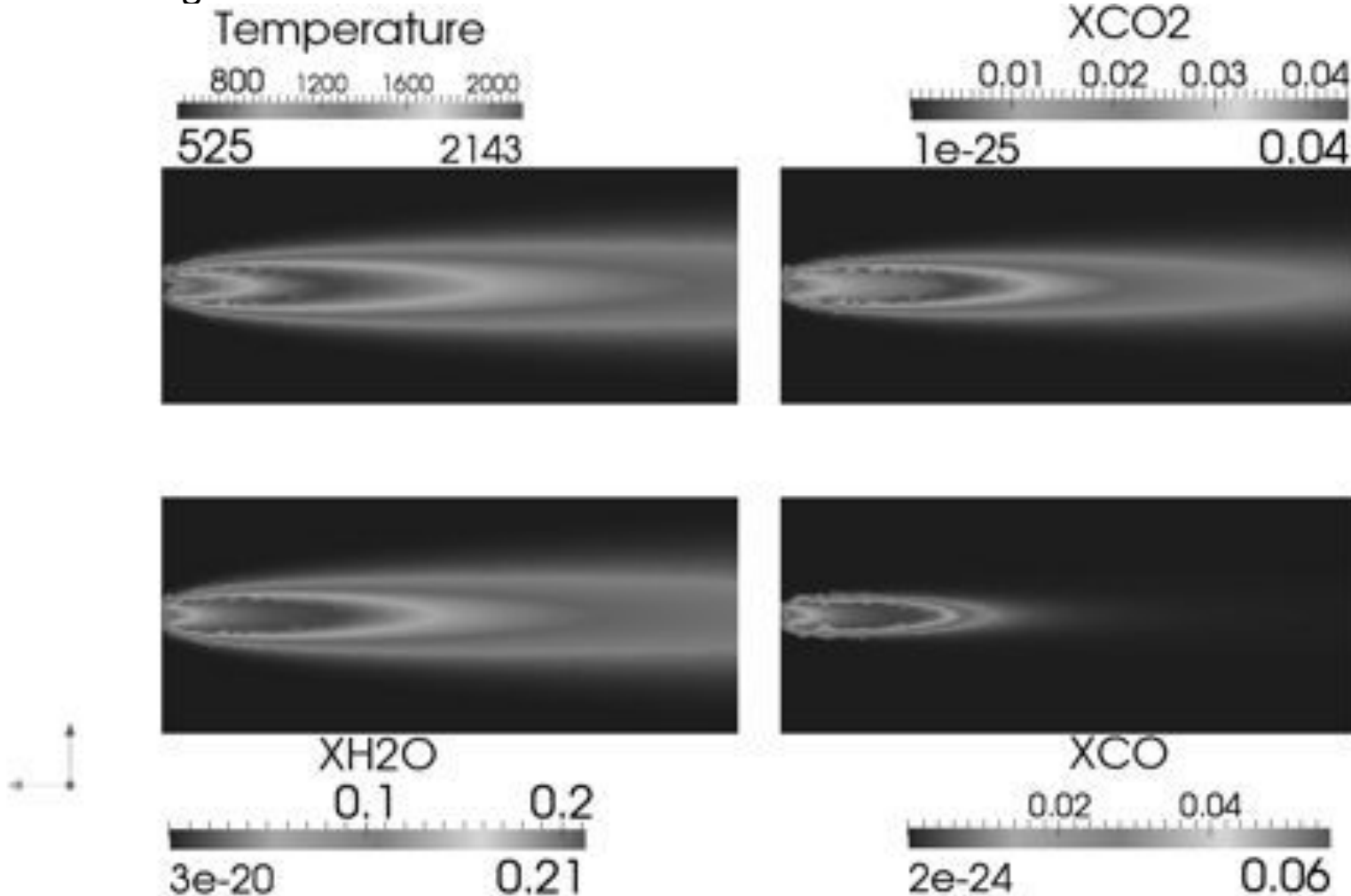
Energie radiative : 1508,33 kW

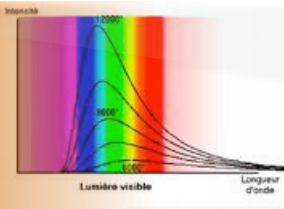


# Cas test 4 Four

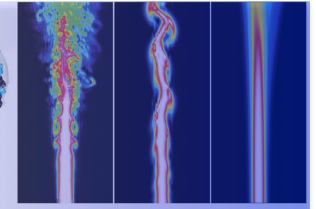


- Maillage AVBP & Solution CANDLE



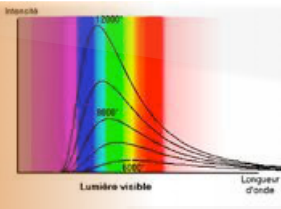


# Programme

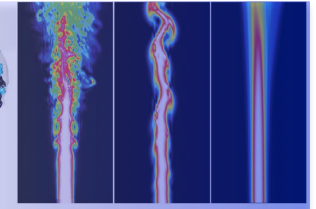


1. Contexte et théorie
2. Le code PRISSMA
- 3. Parallélisme**
4. Modèles spectraux
5. Vers le couplage...

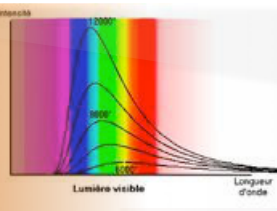




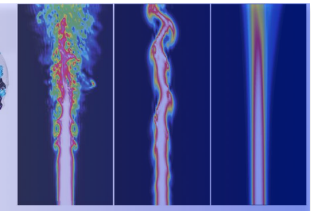
# Parallélismes



- Sur les tâches : MPI/OpenMP
  - Calcul spectral : blocs (MPI ou OpenMp)
  - Calcul angulaire :
    - direction (MPI ou OpenMP),
    - quadrature spectrale/fréquence (MPI)
- Sur les données : Sous-domaines, MPI

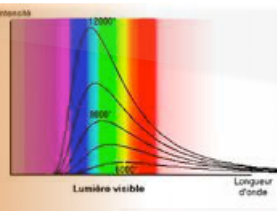


# Parallélismes

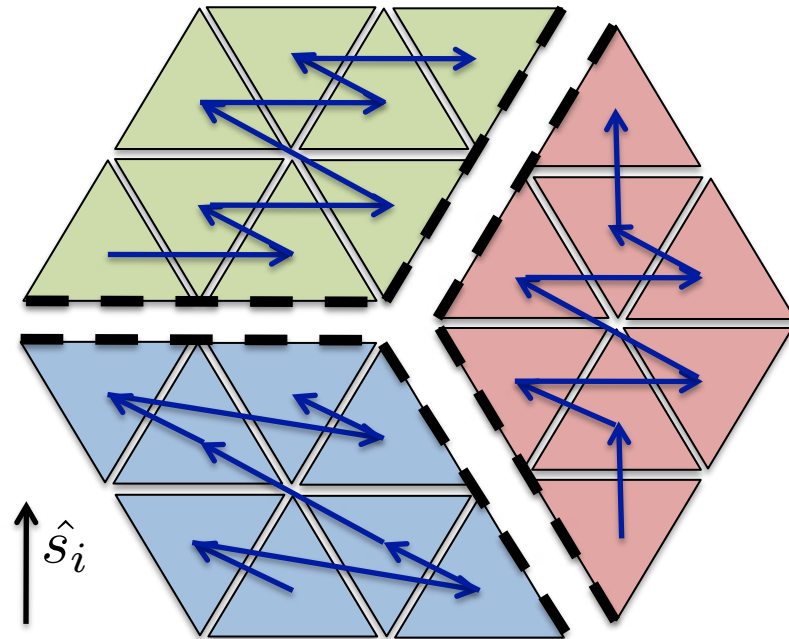
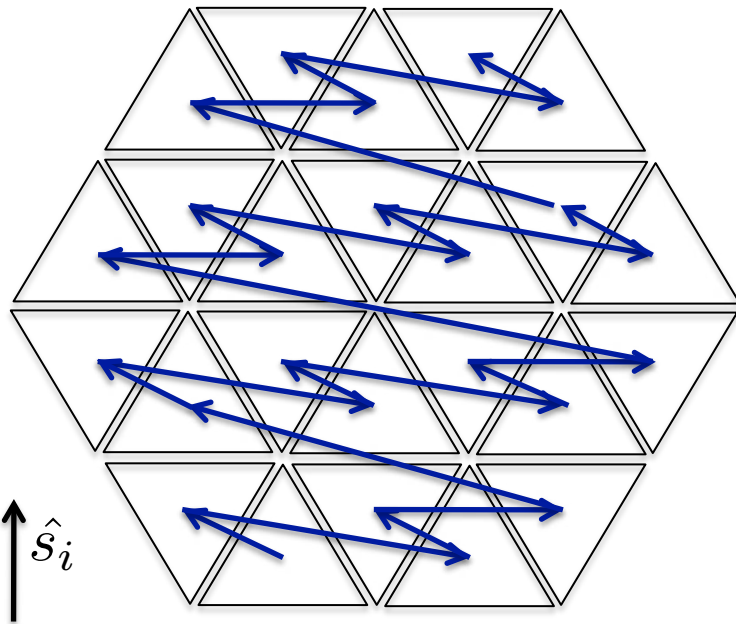
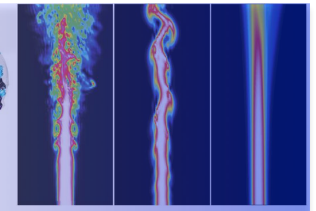


	Avantages	Inconvénients
Taches	Calcul radiatif adapté -> Directions et fréquences indépendantes	Scalabilité limitée $N_{dir} * N_{quad}$  Utilisation mémoire : - Très importante avec MP (duplication) - Constante avec OpenMP
Sous-domaines	Scalabilité : pas de limite théorique Utilisation mémoire réduite par domaine	Coût CPU plus important, itérations pour tenir compte des échanges à distance

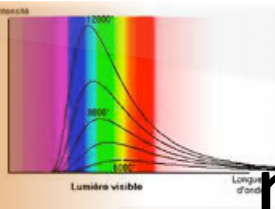
=> Parallélisation hybride pour combiner l'avantage de chaque parallélisme



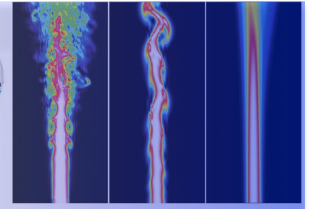
# Reordonnement et sous-domaines



1. Chaque sous domaine balaye ses cellules
2. La luminance est échangée uniquement aux frontières des sous-domaines  
=> Itérations de calcul tant que que la luminances aux frontières n'est pas convergée



# Parallélisme modèle bande étroite (CK)

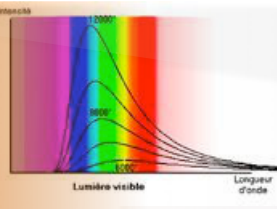


```

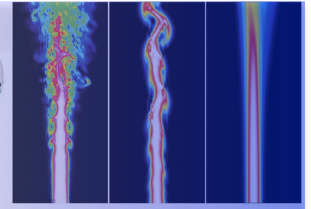
Do i_band = 1, N_bands
  Do i_quad = 1, N_quad
    WHILE CONVERGENCE > 1% Do
      Do i_dir = 1, N_dir
        Do i_cell = 1, N_cell(domain)
          X = pathway (i_cell, i_dir)
          
$$S_r(\mathbf{x}) \simeq \sum_{j=1}^{N_q} \sum_{j=1}^{N_q} \omega_j \kappa_{i,j} \left( 4\pi\sigma L_{i,j}^0(\mathbf{x}) - \sum_{k=1}^{N_{dir}} \omega_k^a L_{i,j}(\mathbf{x}, \mathbf{u}_k) \right)$$

          Update H and L_virt(i_dir, i_quad, i_band)
        EndDo
      EndDo
      MPI_REDUCTIONS:   H (local subdomain),
                       L_virt(all domains)
      TEST CONVERGENCE = max(REFLECTION, SUBDOMAINS)
    END WHILE
  EndDo
EndDo

```



# Parallélisme Modèles Globaux (FSK, FSCK, WSGG)



WHILE CONVERGENCE > 1% Do

Do  $i_{quad} = 1, N_{quad}$

Do  $i_{dir} = 1, N_{dir}$

Do  $i_{cell} = 1, N_{cell}(\text{domain})$

X = pathway ( $i_{cell}, i_{dir}$ )

$$S_r(\mathbf{x}) \simeq \sum_{j=1}^{N_q} \omega_j \kappa_i \left( 4\pi\sigma T^4(\mathbf{x}) - \sum_{k=1}^{N_{dir}} \omega_k^a L_j(\mathbf{x}, \mathbf{u}_k) \right)$$

UPDATE H and  $L_{virt}(i_{dir}, i_{quad}, i_{band})$

EndDo

EndDo

EndDo

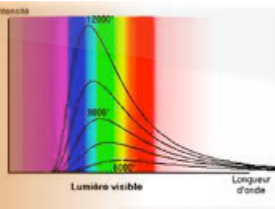
MPI\_REDUCTIONS: H (local subdomain),

$L_{virt}$ (all domains)

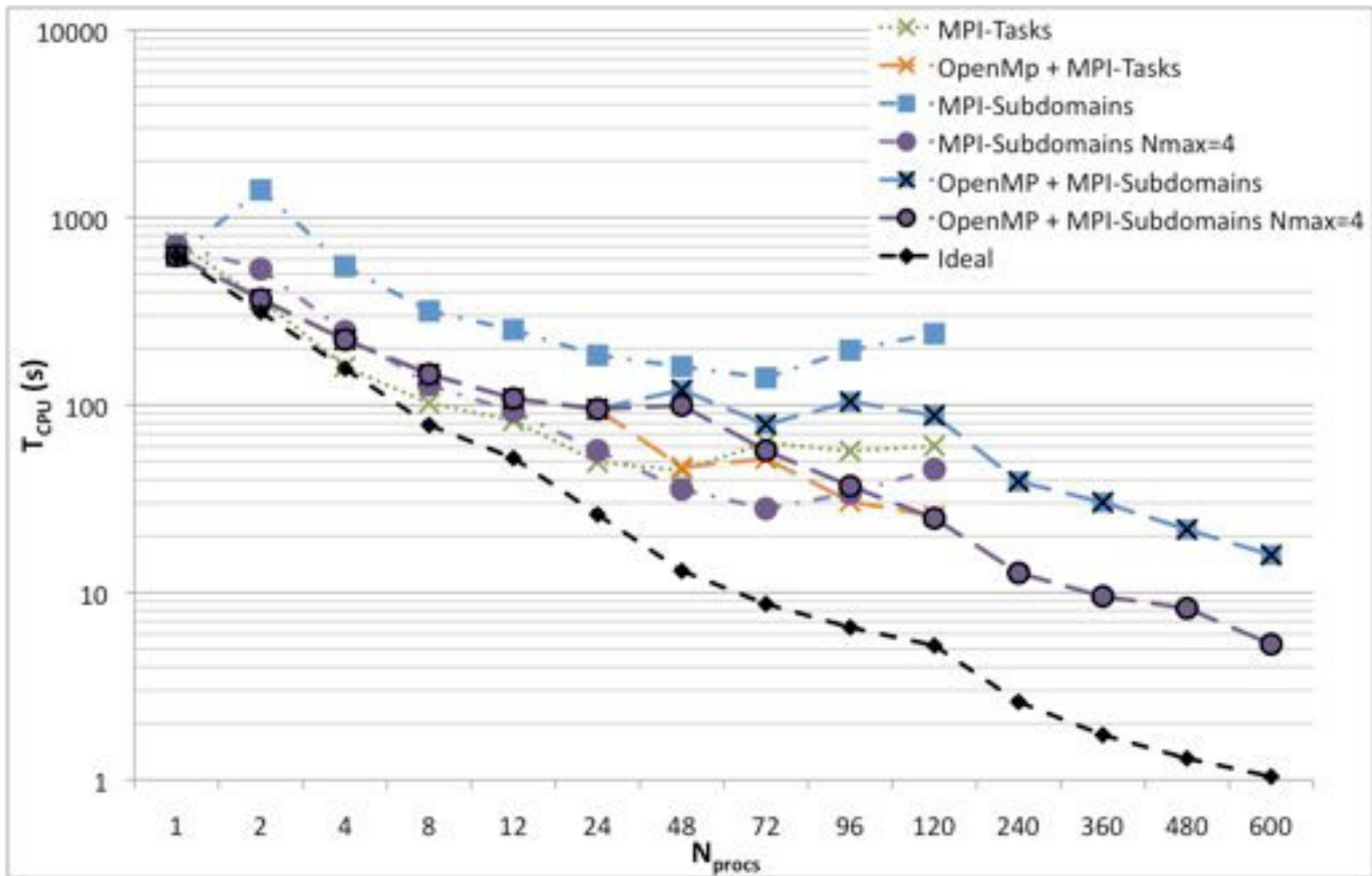
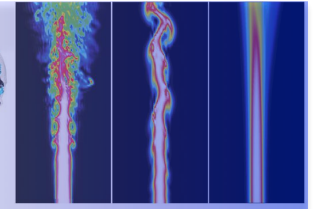
TEST CONVERGENCE = max(REFLECTION, SUBDOMAINS)

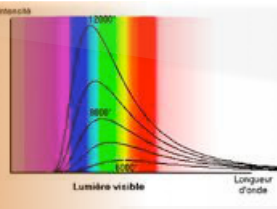
END WHILE



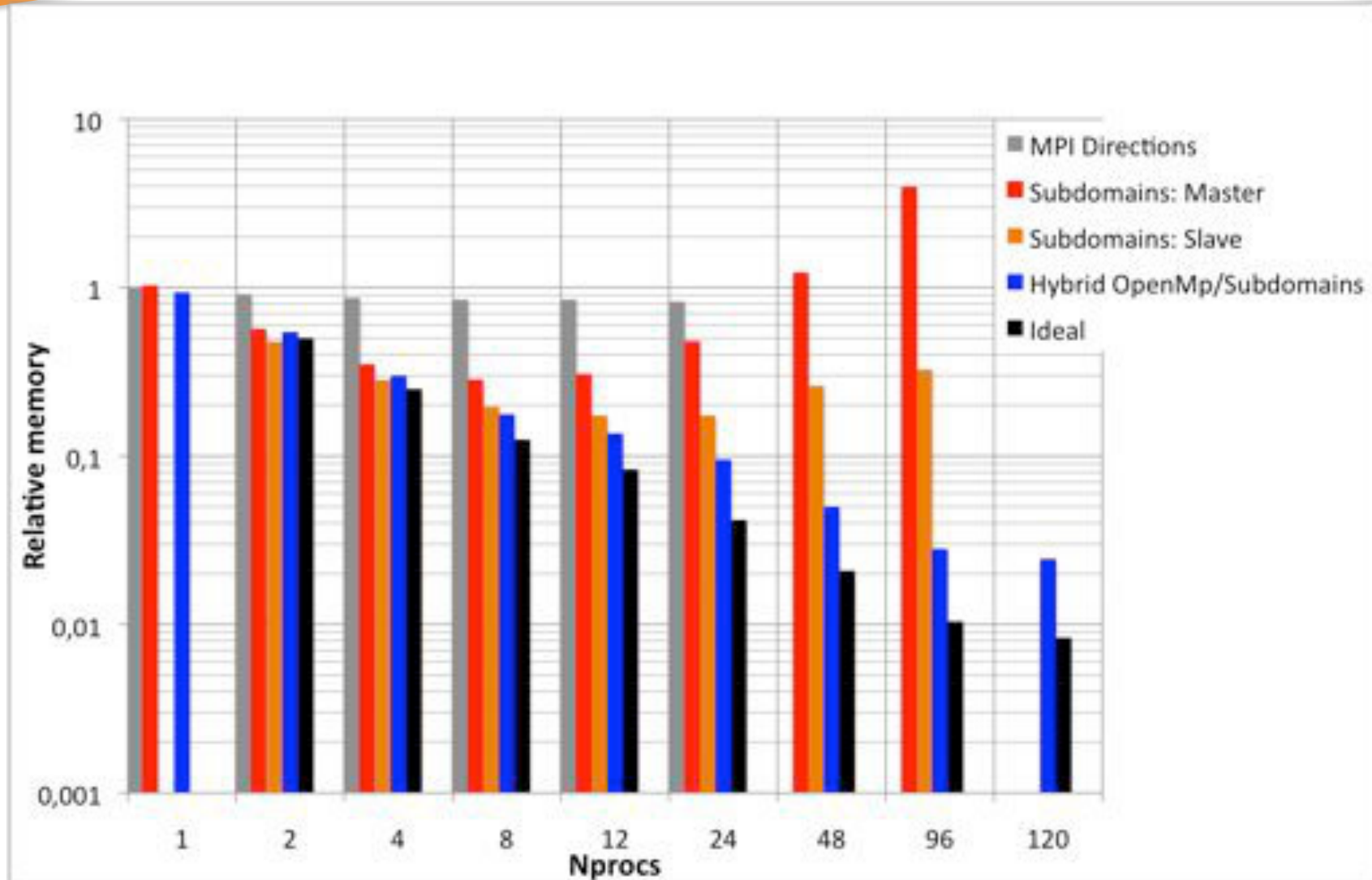
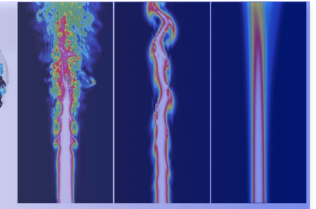


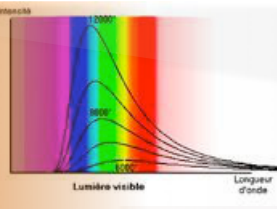
# Speed-up fort



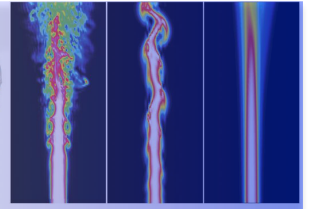


# Parallélisme et mémoire





# Parallélisme : 3 paramètres



- mpirun -np **P1** ./mpiprissima\_V2.X.e
- Prissima.choices

1

```

'./INFILES' | Path to *.in files
'./SPECTRAL' | Path to spectral data
'./OUTFILES' | Output path
DMFS | Spatial discrization [ DMFS | SMFS | EXPON ]
SNB | Narrow band data base [ SNB | NBKM ]
CK | Spectral model [ CK | (T)FSCK | (T)FSK | MSGG | GRAY ]
5 | Spectral quadrature points (CK:5, FS(C)K:5->15)
1.e-2 | Convergence criterion (Reflection and subdomains)
NO | Homogeneous system [ NO | YES ]
P2 | Print directions [ 1 | 0 ]
P3 | Number of subdomains (Ndomains < Nprocs)
1 | Number of threads (Nthreads < Ndirs )

```

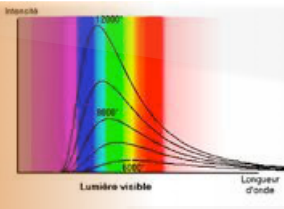
2

3

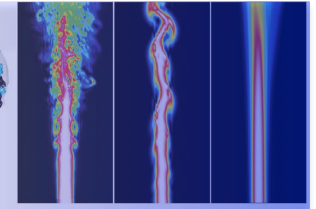
Parallélisation OpenMP = P3-> nombre de proc/nœud de calcul & <Ndirs  
*corail 24 procs/nœud!*

Nprocs total = P1 x P3

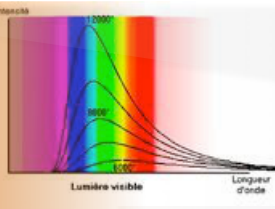
Parallélisation par tâches MPI (direction ou fréquence) automatique si P2<P1,  
Ntaches=P1/P2



# Programme

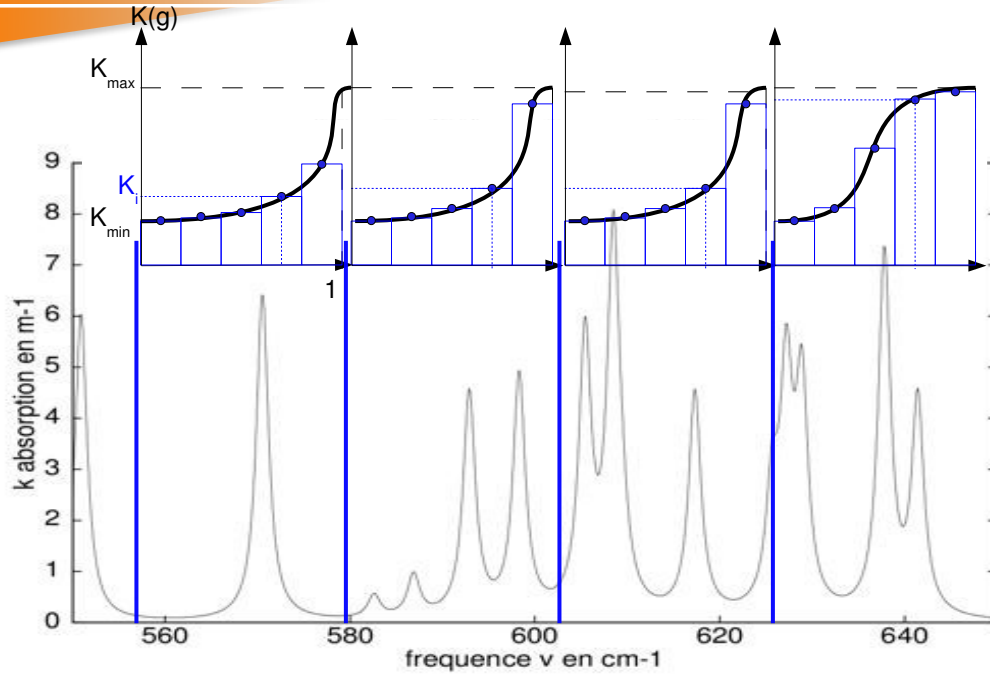
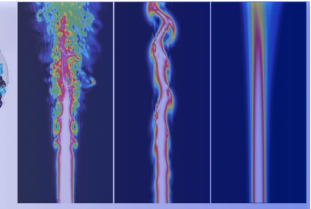


1. Contexte et théorie
2. Le code PRISSMA
3. Parallélisme
4. Modèles spectraux
5. Vers le couplage...



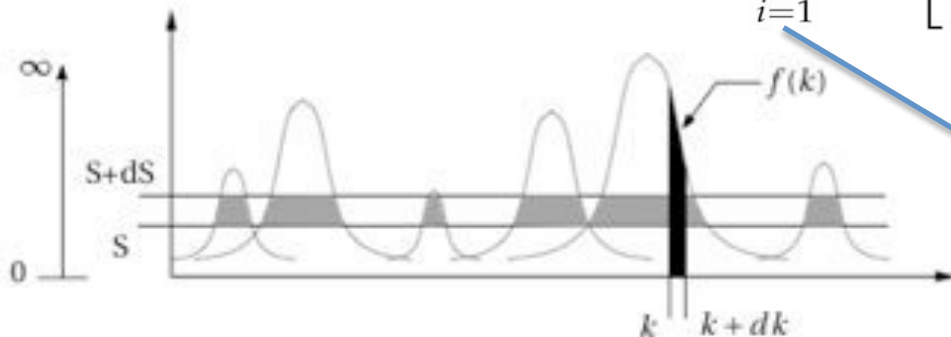
# Modèles spectraux

## Bandes étroites



**371\*5 intégrations par direction**

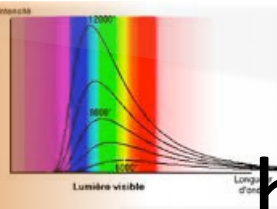
$$S_r(\mathbf{x}) \simeq \sum_{i=1}^{N_{band}} \Delta\nu_i \left[ \sum_{j=1}^{N_{quad}} \omega_j \kappa_{ij} \left( 4\pi \overline{L_{\Delta\nu_i}^0(\mathbf{x})} - \sum_{k=1}^{N_{dir}} \omega_k^a L_{i,j}(\mathbf{x}, \mathbf{u}_k) \right) \right]$$



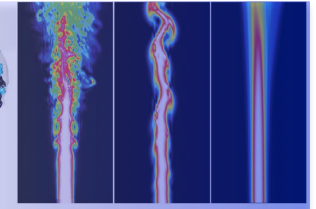
Nquadrature gi

Numéro de bande étroite





# Modèle à bandes étroites SNBck



- Paramètres CK calculés pour un mélange à partir de la base SNB de Taine et Soufiani (1997) suivant le modèle de Liu (2001) :

$$\langle \kappa_{mix} \rangle_{\Delta\nu} = \sum_{k=1}^{N_g} \bar{\kappa}_k \quad \text{①}$$

$$\frac{\langle \kappa_{mix}^2 \rangle_{\Delta\nu}}{\Phi_{\Delta\nu, mix}} = \sum_{k=1}^{N_g} \frac{\bar{\kappa}_k^2}{\Phi_{\Delta\nu, k}}$$

- Modèle de Malkmus :  $\bar{T}_{\Delta\nu} = \exp \left[ \Phi \left( 1 - \left( 1 + \frac{2\bar{\kappa}}{\Phi} \right)^{1/2} \right) \right] \quad \text{②}$

- Le spectre de la bande étroite est réordonné suivant les valeurs probables du coefficient d'absorption.

Transformée de laplace inverse de  $\bar{T}_{\Delta\nu} \rightarrow$  pdf  $f(k) \rightarrow$  calcul de la cumulée  $g(k)$  ③

- Inversion de  $g(k)$  sur les point d'une quadrature (Gauss-Legendre)  $k_j(g)$  pour la bande  $i$  ④

1+2 : SNB ; 3+4 : cK



# Modèle à bandes étroites SNBCK

- Hypothèses : Profils de raie de Lorentz, fonction de Planck cst. par bande, Inhomogénéités (mélange + hypothèse de corrélation).

- **Hypothèse de corrélation :**

=> Les spectres d'absorption sur le chemin optique sont réordonnés de la même manière

-> Exact en homogène;

-> En inhomogène : On suppose que les échanges ne sont pas sensibles à la position exacte des raies.

$L_u \rightarrow L_{i,j}$  échanges monochromatiques à la fréq.  $\nu$  remplacés dans l'espace réordonné en  $g$

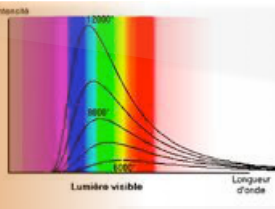
**Solutions de réf.** dans les problèmes de combustion :

-> sauf pour gradients de température importants dans les gaz absorbants (signature IR),

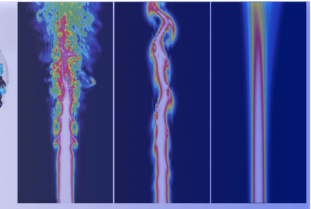
-> dans les **chambre de combustion** les produits sont corrélés à la température :

**assez homogène pour le rayonnement.**

-> temps CPU important en DOM pour couplage instationnaire.



# Modèles Globaux : WSGG

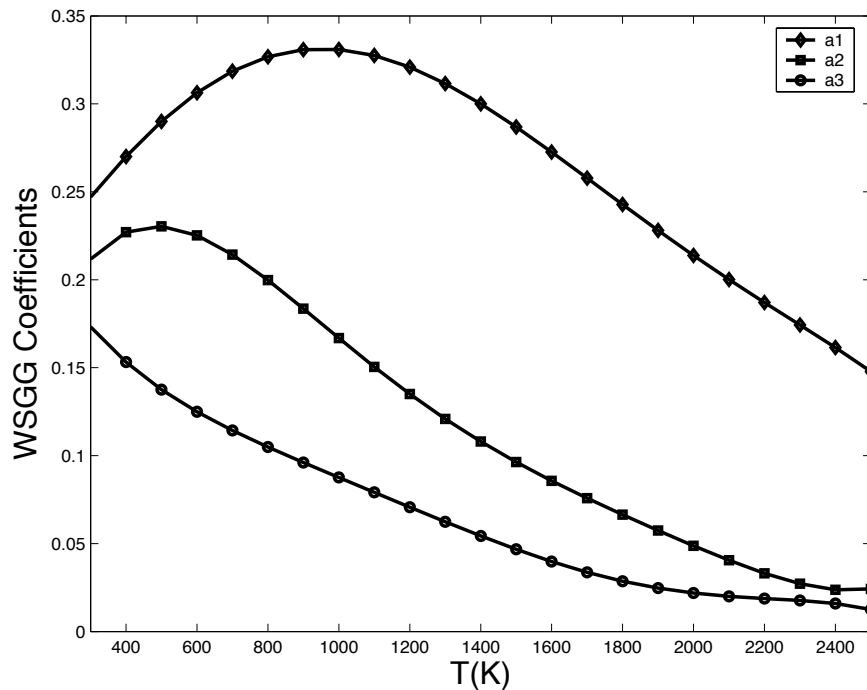


$$I = \sum_{k=1}^n I^k$$

$$\frac{dI^k}{ds} = \kappa_k p_a (a_k I_b - I^k)$$

$$\text{Condition limite } s = 0 : I_k = [a_k I_b](T_w)$$

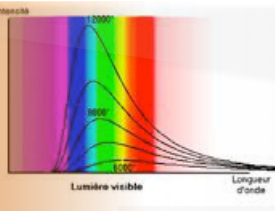
$$\epsilon_T(T, l, p_a) = \sum_{k=1}^n a_k(T) [1 - \exp(-\kappa_k p_a l)]$$



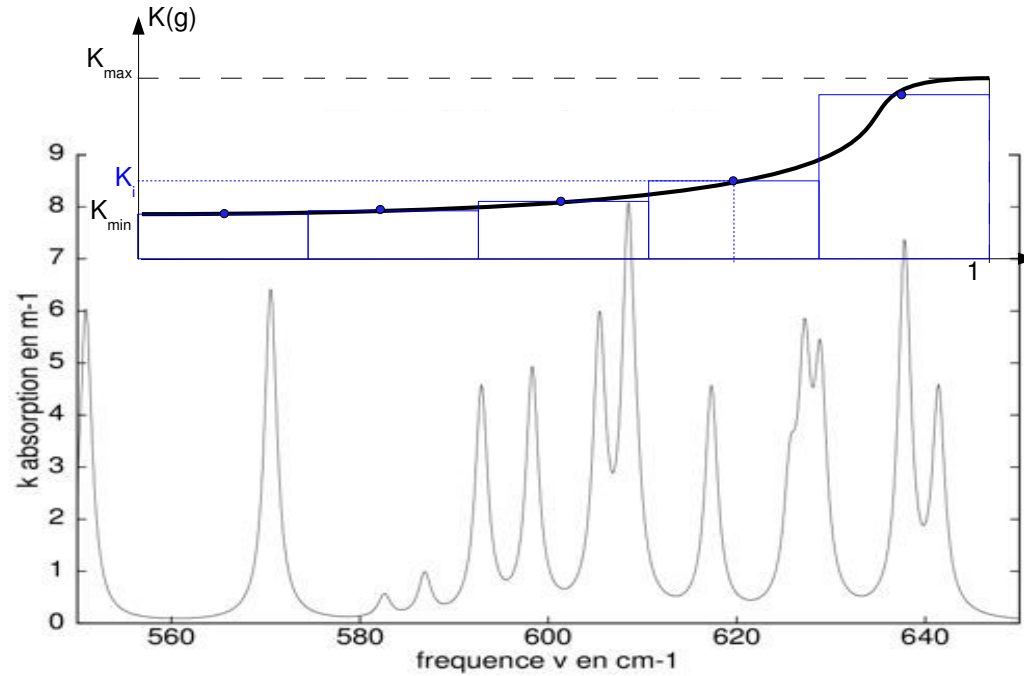
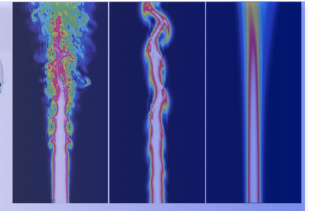
Forme polynomiale simple pour  $a_k(T)$  :

- **Temps de calcul très réduits**,
- **Précision limitée** : rapport de CO2/H2O constant, Inhomogénéités, cas de référence utilisé pour Construction, ...

**3 intégrations par direction**

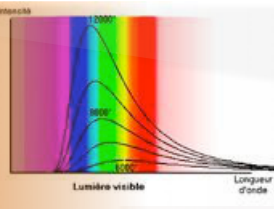


# Modèles globaux : SNB-FSK

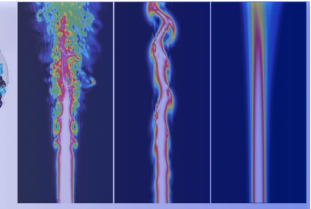


$$S_r(\mathbf{x}) \simeq \sum_{j=1}^{N_q} \omega_j k_j \left( 4\pi\sigma T^4(\mathbf{x}) - \sum_{k=1}^{N_{dir}} \omega_k^a L_j(\mathbf{x}, \mathbf{u}_k) \right)$$

**5-15 intégrations par direction**



# Modèles globaux : SNB-FSK



- Étapes 1 à 3 du modèle SNBCK ->  $g_i(\mathbf{k})$  sur chaque bande  $i$

1

- Cumulée sur l'ensemble du spectre :  
Avec  $T_p = T_{\text{gaz}}$

$$g_{FS}(\kappa) = \frac{1}{\sigma T_p^4} \sum_{i=1}^{371} I_{b\nu,i} g_i(\kappa) \Delta\nu_i$$

2

- ETR résolue :

$$S_r(\mathbf{x}) \simeq \sum_{j=1}^{N_q} \omega_j \kappa_j \left( 4\pi\sigma T^4(\mathbf{x}) - \sum_{k=1}^{N_{dir}} \omega_k^a L_j(\mathbf{x}, \mathbf{u}_k) \right)$$

-> Exacte seulement **en milieu homogène**

Hypothèse de corrélation appliquée à tout le spectre : impact fort si milieu anisotherme  
⇒ ÉCHANGES ENTRE POINTS À DES FRÉQUENCES/TEMPÉRATURE DIFFÉRENTES !!

-> dans les **chambre de combustion** les produits sont corrélés à la température :  
**assez homogène pour le rayonnement.**

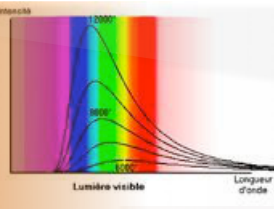
Gain par rapport au SNBCK sur le nombre d'intégration de l'ETR : 1800 -> 15 / direction



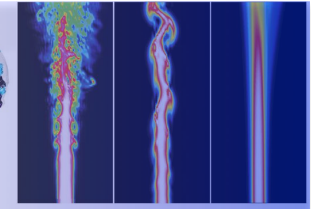


# Modèles globaux : SNB-FSCK

- Notion d'**état de référence**  $\Phi_0$  avec  $\Phi = (T_{\text{gaz}}, X_{\text{H}_2\text{O}}, X_{\text{CO}_2}, X_{\text{CO}})$ : fixée comme l'état « moyen » du système :
  - **Paramètre 1** : Moyenne volumique du système, point le plus chaud,...
- Étapes 1 à 3 du modèle SNBCK ->  $g_i(\mathbf{k})$  sur chaque bande  $i$
- Calcul de la de cumulée  $g_{\text{FS}}$  comme en FSK Température de **pondération de Planck**  $T_p$  ( $\neq T_{\text{gaz}}$ ) => **Paramètre 2**
- Calcul de la corrélation par rapport à l'état de référence : **Prise en compte des inhomogénéités.**
- Même ordre de temps CPU que FSK : 5-15 intégrations/direction.



# Modèles globaux : SNB-FSCK



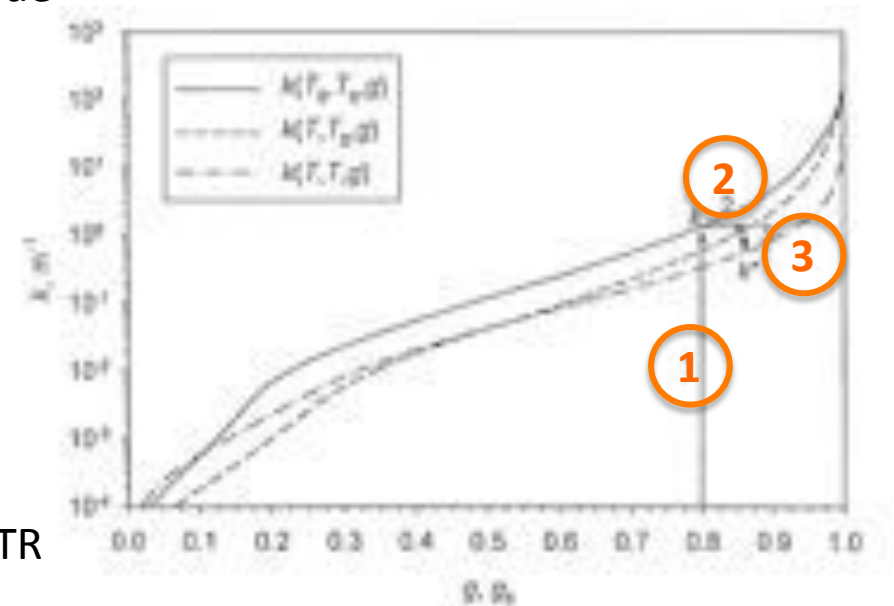
- ETR résolue :

$$\frac{I^g}{ds} = k^*(T_0, \phi, g_0)[a(T, T_0, g_0)I_b(T) - I^g]$$

Condition limite  $s = 0 : I^g = [a_k I_b](T_w)$

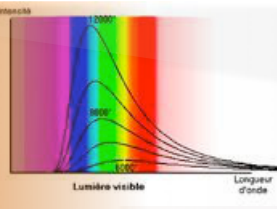
- Mise en œuvre :

1. Calcul de  $g_{FS}(T_p = T_0, \Phi_0, k) \rightarrow$  inversion au pt de quadrature  $g_i : k_0$
2. Cumulé à la température  $T_{gaz}$  :  
 $g_{FS}(T_p, \Phi_0, k_0)$
3. **Hypothèse de corrélation** pour le calcul de l'état  $\Phi$  en chaque point :  
 $g_{FS}(T_p, \Phi_0, k) = g_{FS}(T_p, \Phi, k^*)$

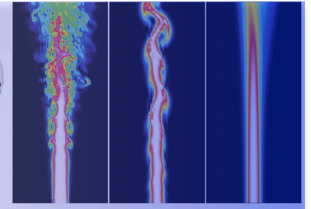


Inversion terme de droite  $\rightarrow k^*$  utilisé dans l'ETR

4. Calcul de la fraction de corps noir :  $a(T, T_0, g_0) = \frac{f(T, \phi_0, k)}{f(T_0, \phi_0, k)}$



# Modèles globaux : Tabulation



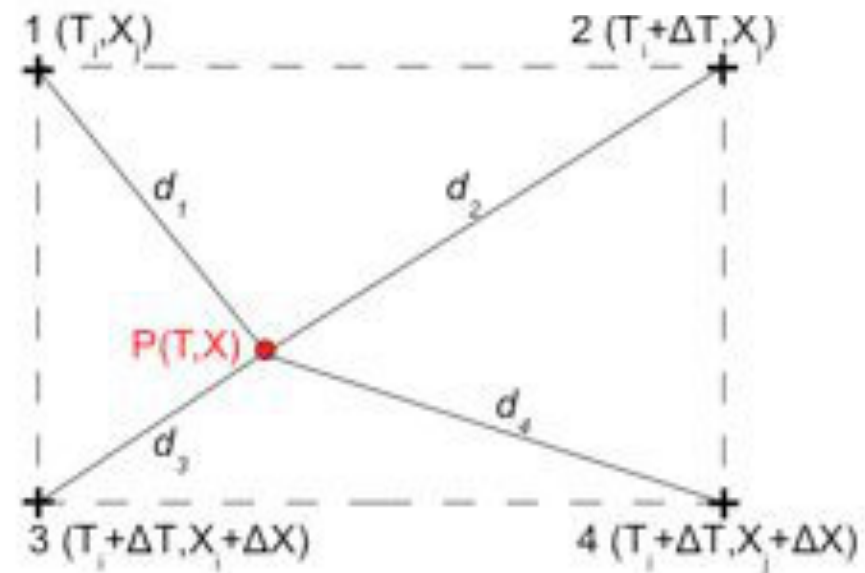
- Calcul et inversion de la cumulée  $g_{FS}$  pour SNB-FSK et SNB-FSCK coûteux.

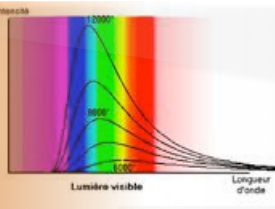
⇒ Tabulation des coefficients d'absorption en fonction des valeurs locales

$$\Phi = (T, p, X_{H_2O}, X_{CO_2}, X_{CO})$$

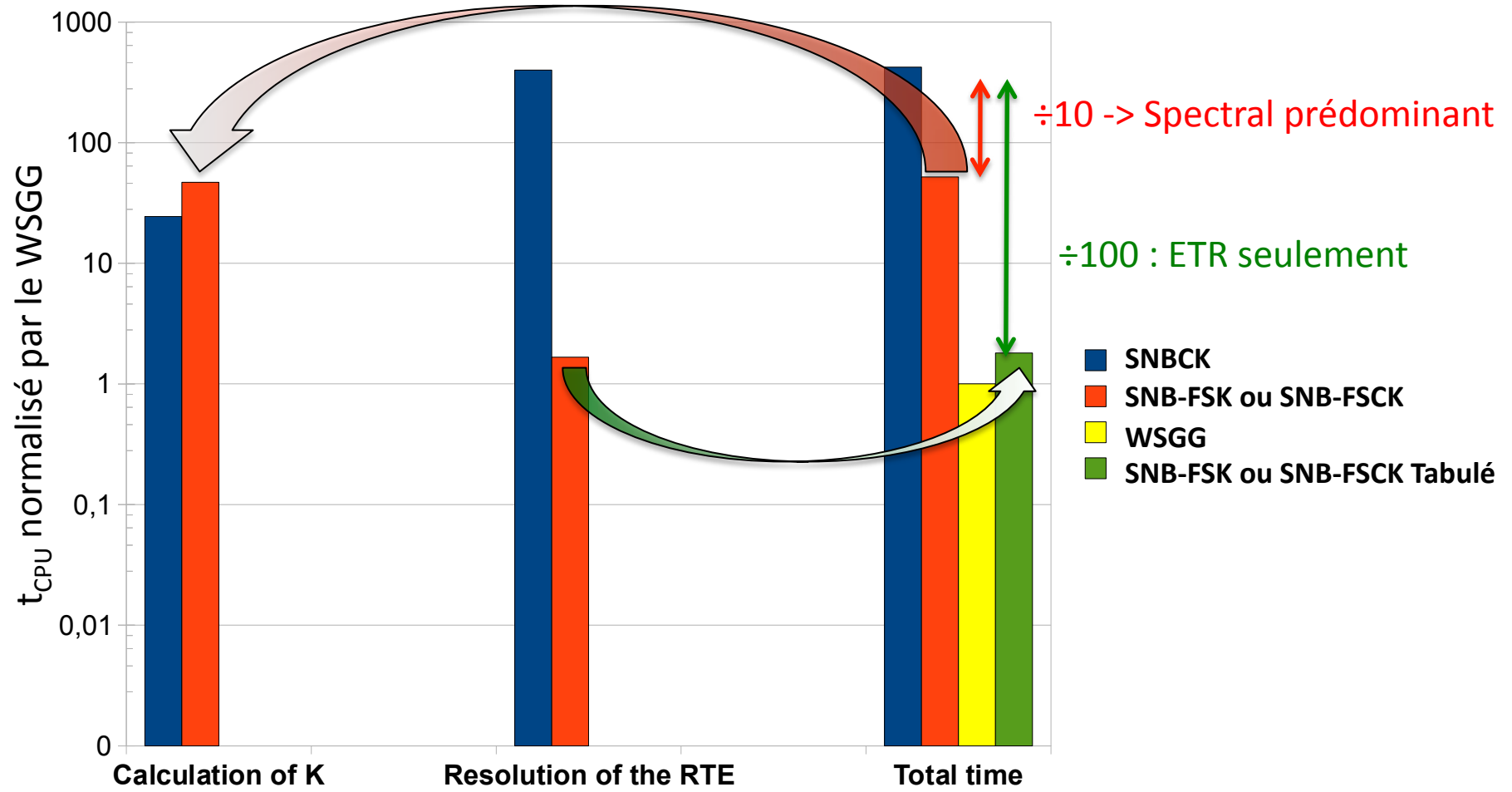
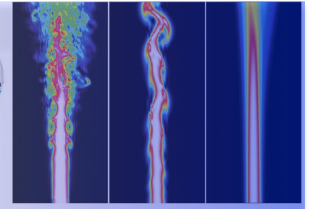
Hyp.  $P = \text{cst}$  → Interpolation linéaire sur 4 paramètres  $\kappa(T, X_i) = \left( \sum_{k=1}^{16} \frac{1}{d_k} \right)^{-1} \sum_{j=1}^{16} \frac{1}{d_j} \kappa_j$

- Pas constants
- $\Delta T$  : 10K → 100K
- $\Delta X_i$  : 0,5% → 10%



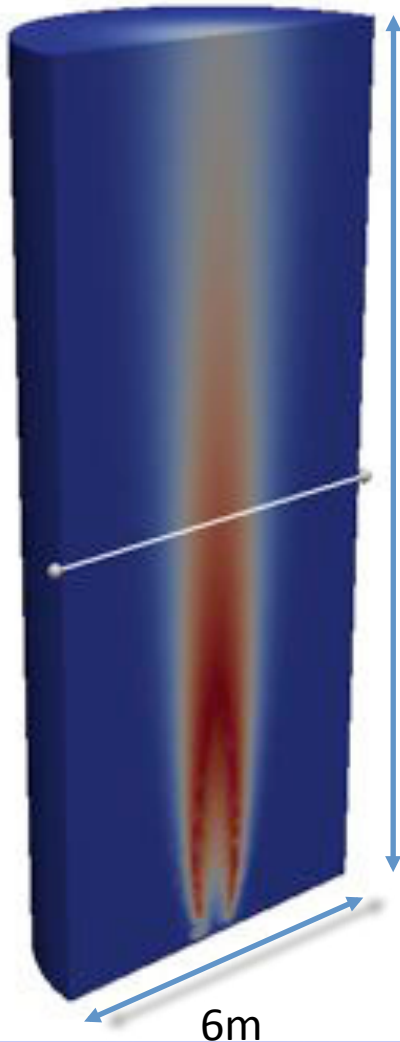
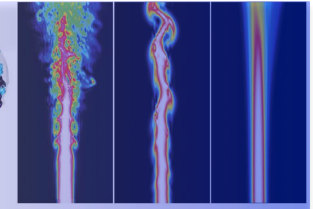
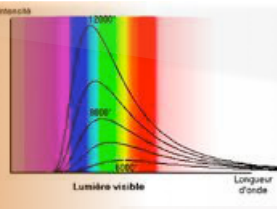


# Modèles Globaux : Temps de calcul



**FSK/FSCK + tabulation gain CPU : 2 ordres de grandeur (cf 371 bandes)**

# Cas test 4 : optiquement épais

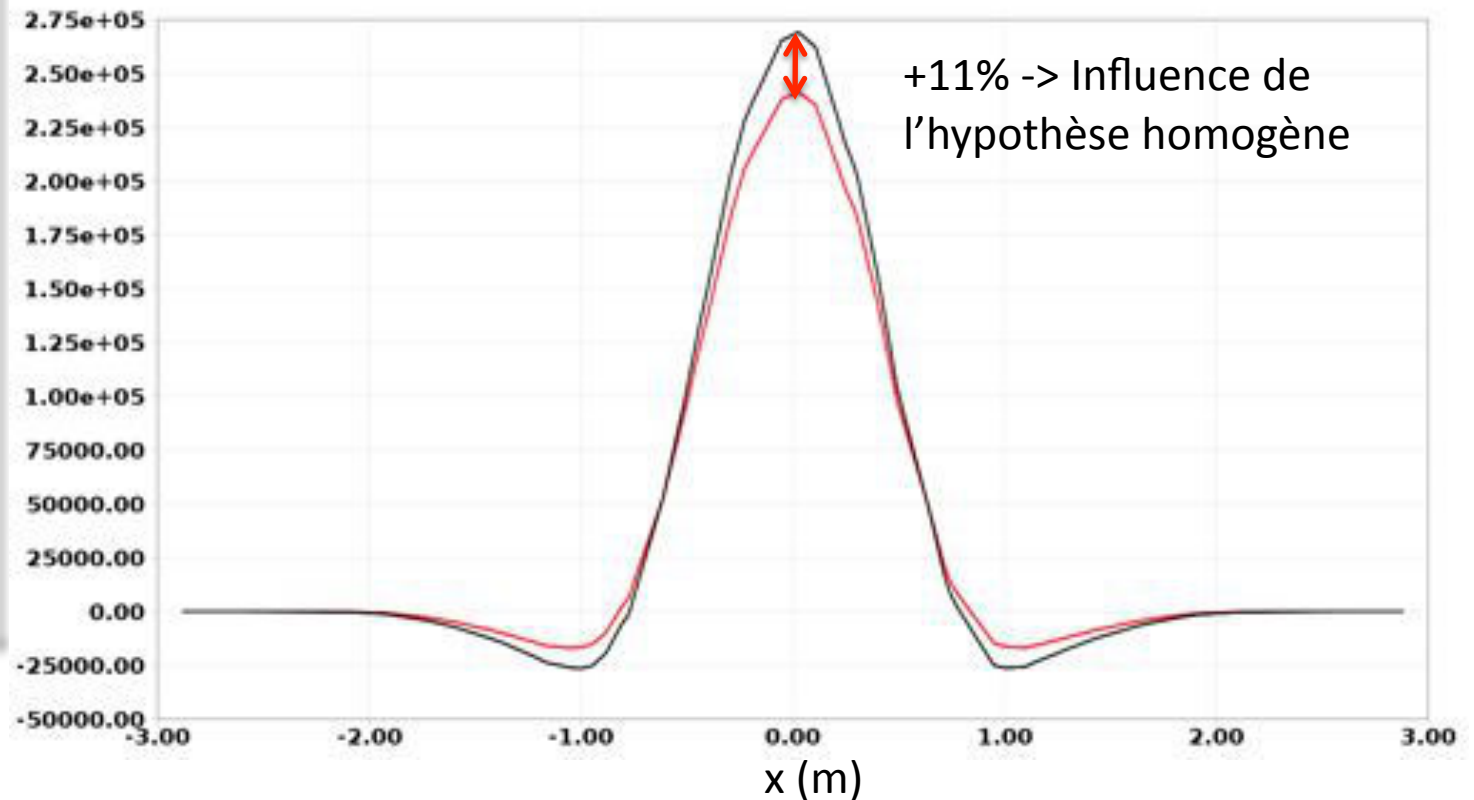


15m

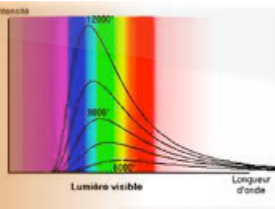
SNBCK

SNB-FSK  $N_q=15$

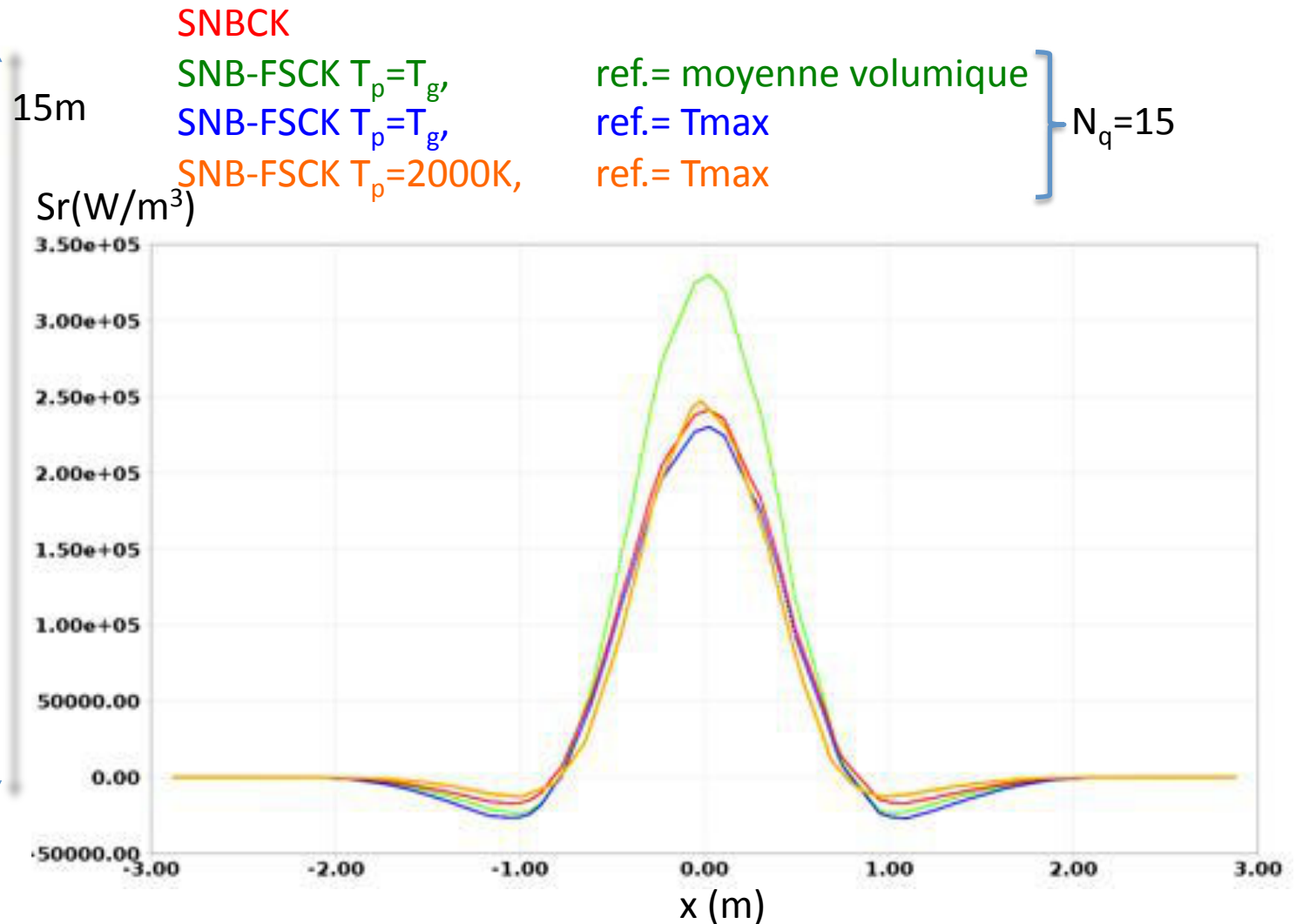
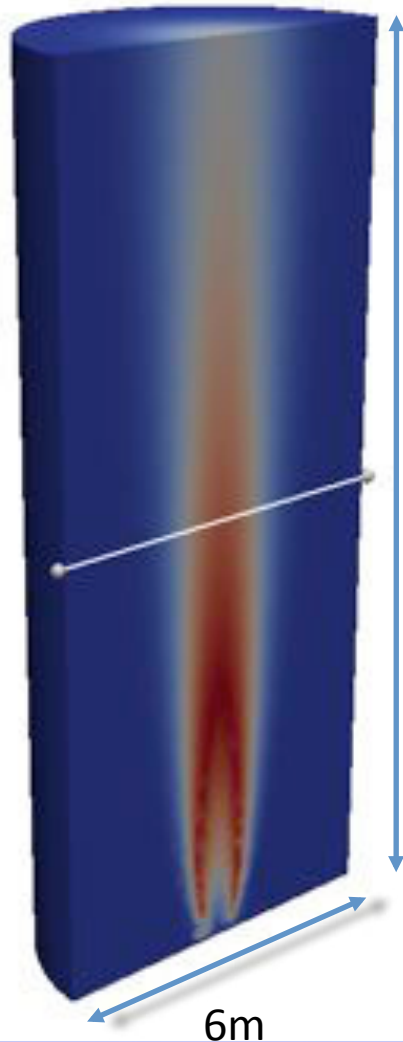
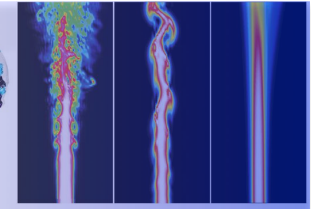
$S_r(W/m^3)$

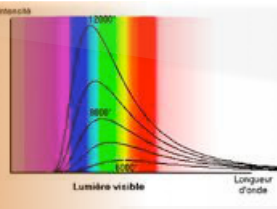




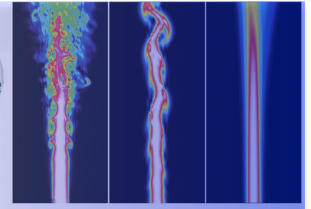


# Cas test 4 : optiquement épais





# Exemple de calcul



- Prisma.choices

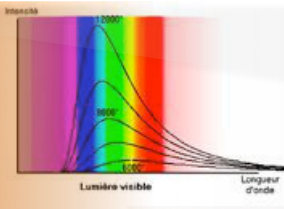
```

./INFILES' | Path to *.in files
./SPECTRAL' | Path to spectral data
./OUTFILES' | Output path
DMFS | Spatial discretization [ DMFS | SMFS | EXPON ]
SNB | Narrow band data base [ SNB | NBKM ]
FSCK 2 2000.d0 | Spectral model [ CK | (T)FSCK | (T)FSK | WSGG | GRAY ]
5 | Spectral quadrature points (CK:5, FS(C)K:5->15)
1.e-2 | Convergence criterion (Reflection and subdomains)
NO | Homogeneous system [ NO | YES ]
0 | Print directions [ 1 | 0 ]
2 | Number of subdomains (Ndomains < Nprocs)
1 | Number of threads (Nthreads < Ndirs )

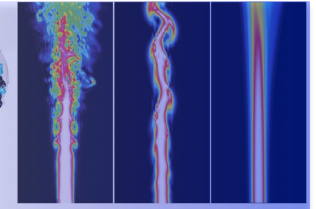
```

Paramètres optionnels pour FSCK/TFSCK et SLMB

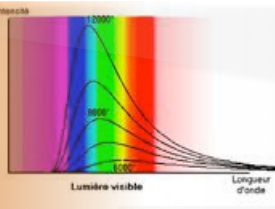
1.  $i_{ref} = 0$  : état de réf. Lu dans input\_fsck.dat  
    1 (défaut) : " Moyenne volumique  
    2 : " Point le plus chaud ( $T_{max}$ )  
    3 : " Point fraction molaire max  
       ( $H_2O$ ,  $CO_2$  ou  $CO$ )
2.  $T_p = 0$  (défaut) :  $T_p = T_g$   
    X.d0 :  $T_p = X.d0$



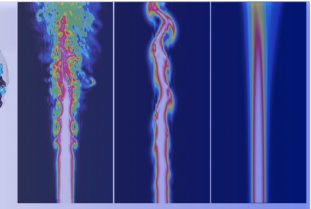
# Programme



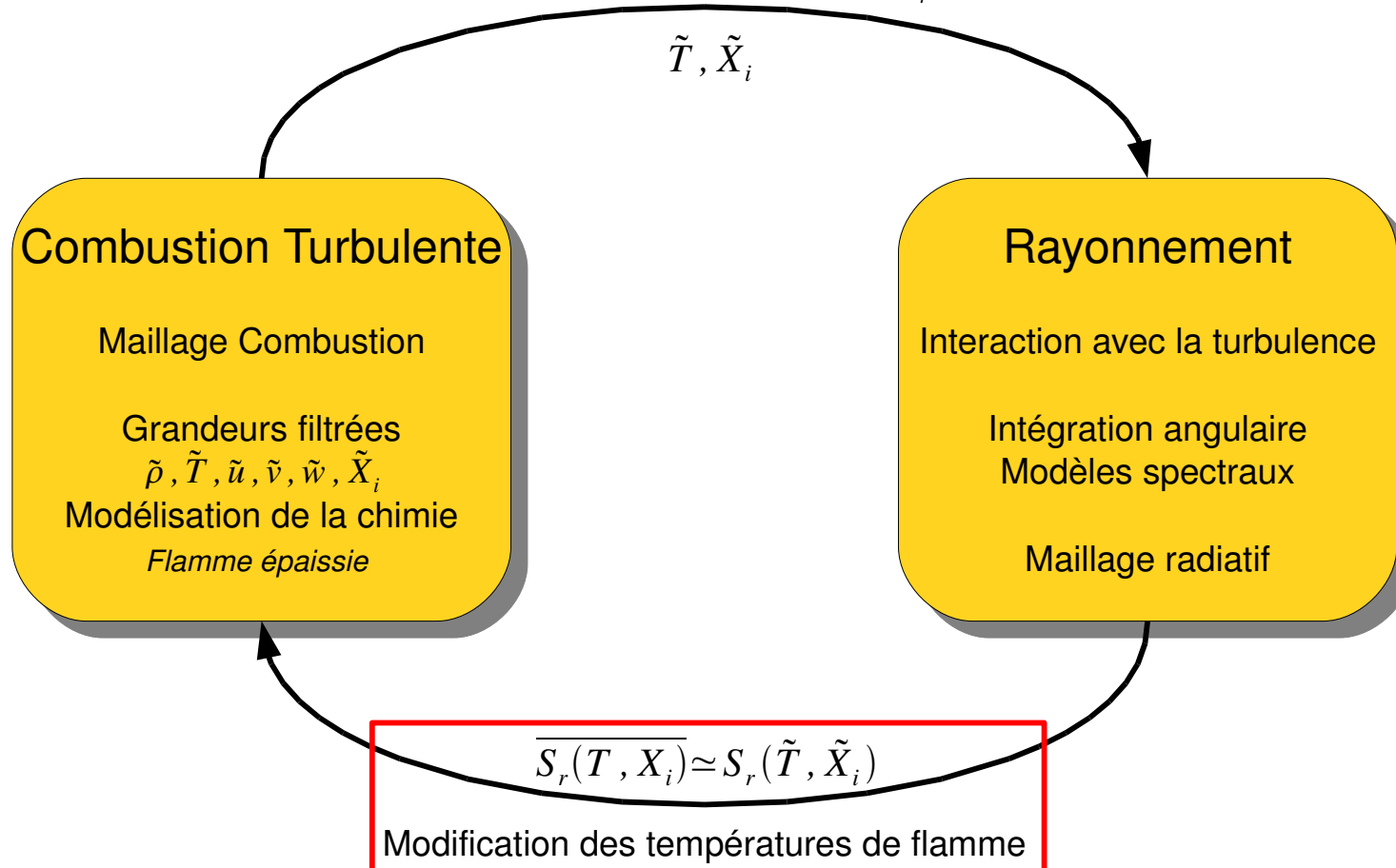
1. Contexte et théorie
2. Le code PRISSMA
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# Couplage LES/DOM

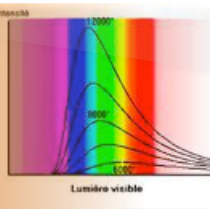


Impact des fluctuations  $T', X_i'$

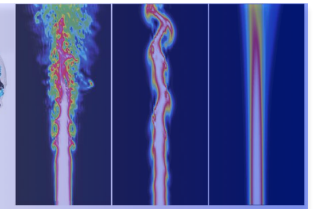
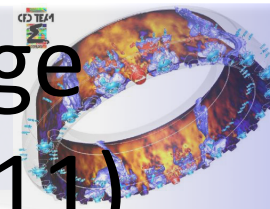


Pas de modèle sous maille Poitou et al. 2007

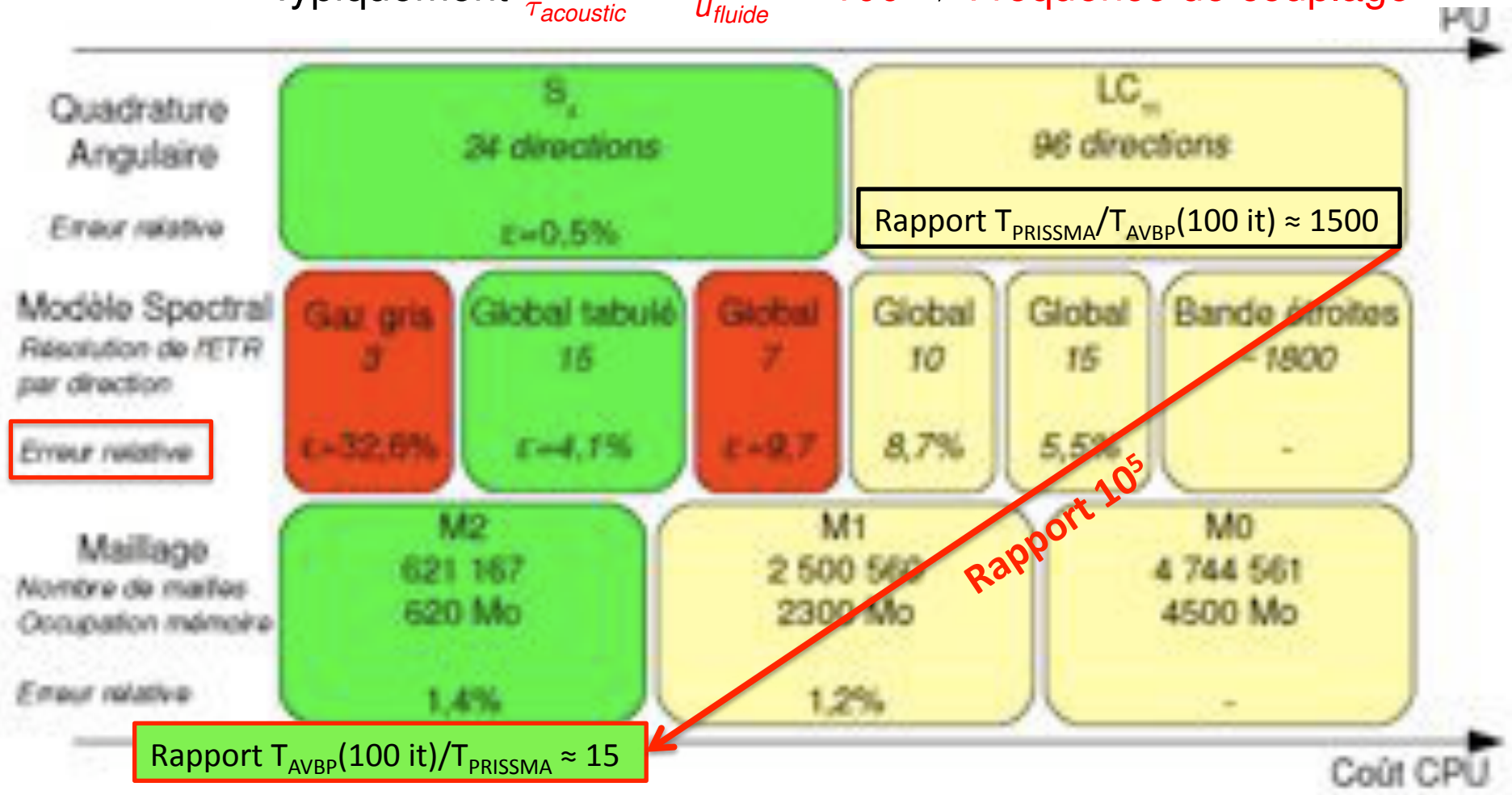
Loi de parois non modifiée Amaya et al. 2009



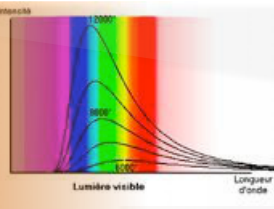
# Stratégie de couplage (Poitou et al. JHT, 2011)



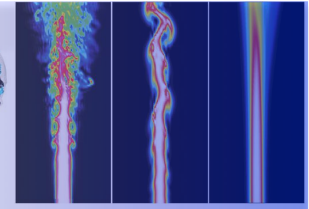
- Typiquement  $\frac{\tau_{rad}}{\tau_{acoustic}} \approx \frac{\bar{u}_c}{\bar{u}_{fluide}} \sim 100 \Rightarrow$  Fréquence de couplage



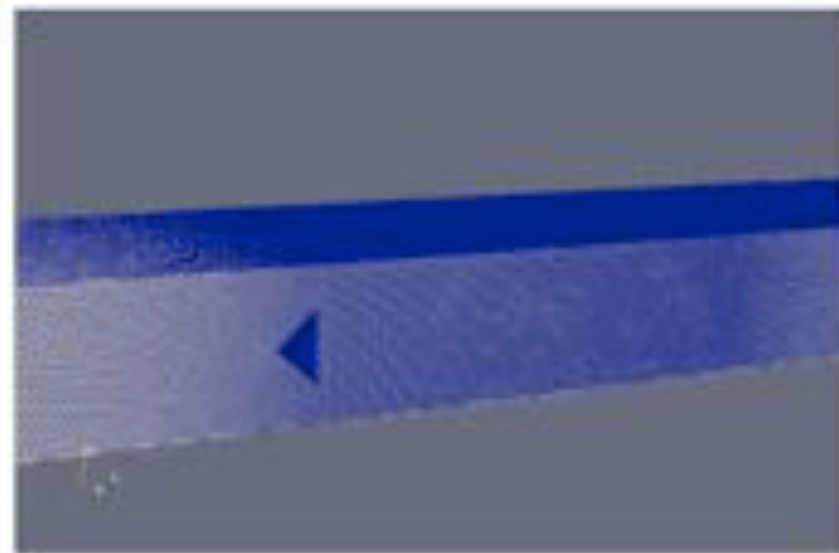
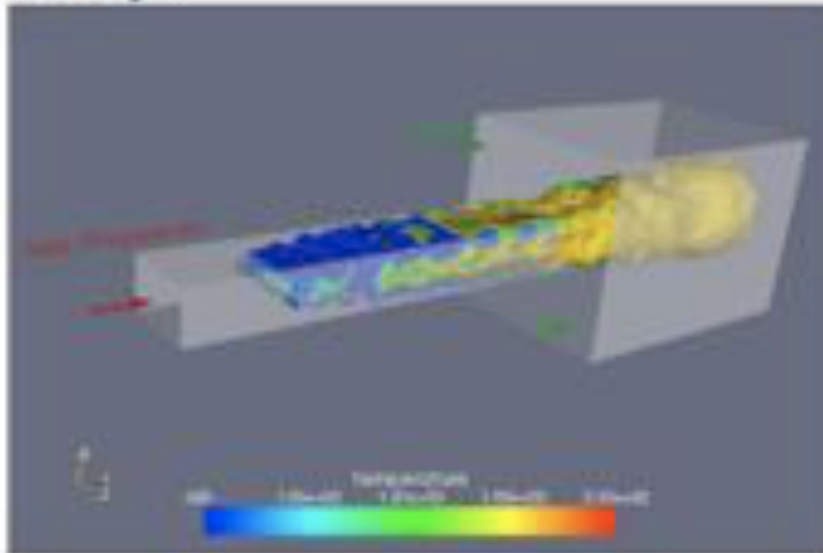




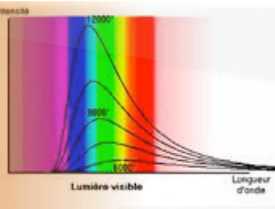
# Configuration étudiée



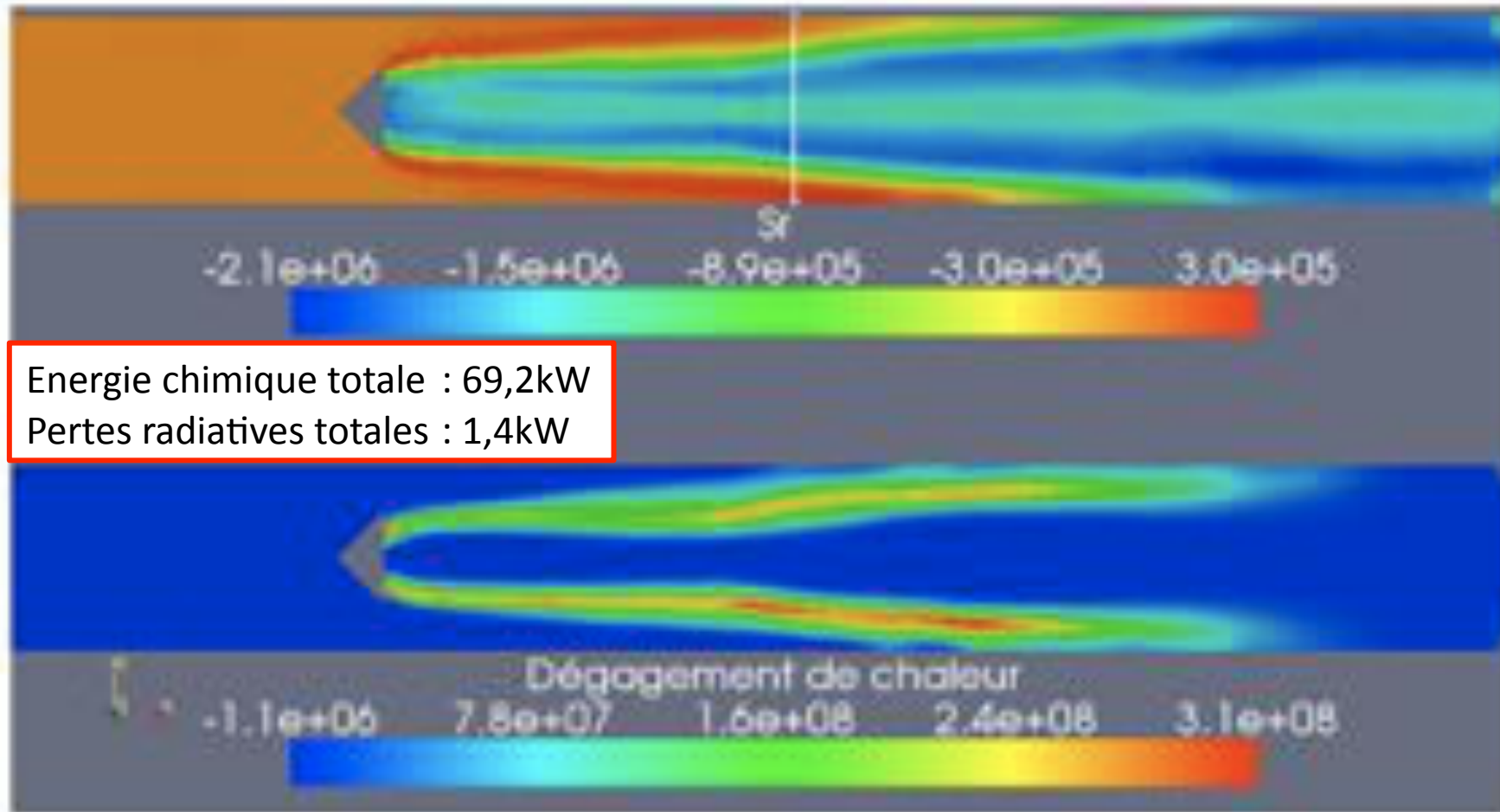
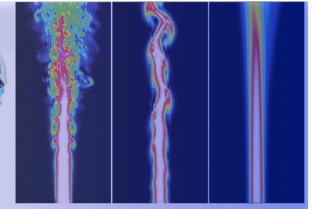
Impact du rayonnement sur la combustion → flamme de laboratoire **turbulente** comparable à une **configuration industrielle** [Knikker et al. 2000]:



- Flamme prémélangée  $C_3H_8/Air$  ( $\Phi = 1$ ),  
4,7 M de cellules ( $\Delta x \sim 1 \text{ mm}$ ), chimie à 2 étapes
  - Dimensions :  $L_x = 40 \text{ cm}$ ,  $L_y = 8 \text{ cm}$ ,  $L_z = 5 \text{ cm}$ ,
- ⇒ Calcul radiatif **couplé**, **parois réfléchissantes**,  $T_w = 300 \text{ K}$ .

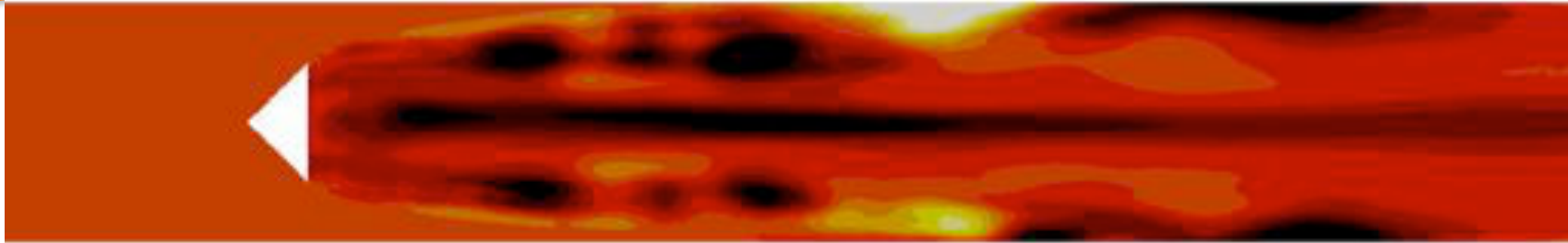
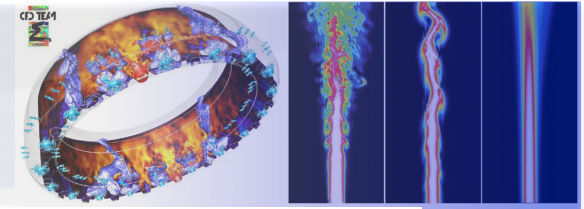
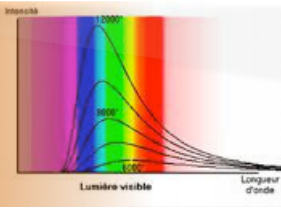


# Termes sources radiatif et chimique



Energie chimique totale : 69,2kW  
Pertes radiatives totales : 1,4kW

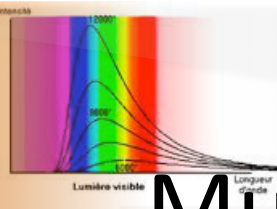
# Impact du rayonnement



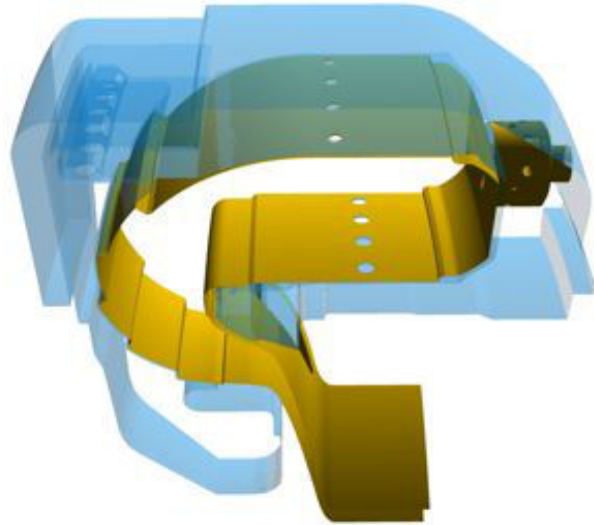
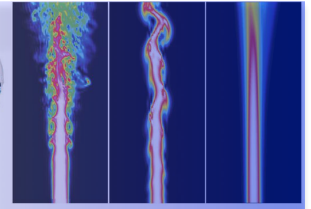
⇒ Prise en compte du rayonnement dans la combustion turbulente instationnaire d'une flamme de laboratoire :

- Modification des pics de température  $\sim 100\text{ K}$ , jusqu'à +60% sur  $T_{\text{RMS}}$ ,
- Impact important sur les espèces mineures, diminution de 20% pour le CO ,
- Impact faible sur la dynamique moyenne,
- Modification des fréquences instationnaires.



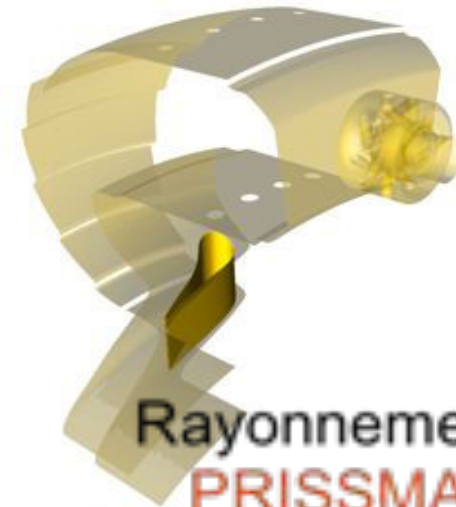


# Ardiden DHP + Pale: Multi-physiques (J. Amaya)

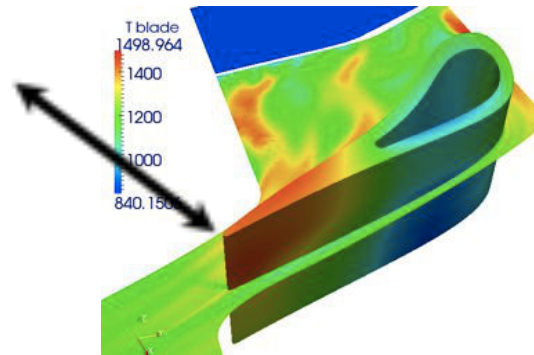


Combustion LES  
AVBP

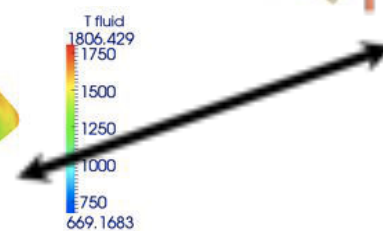
PALM



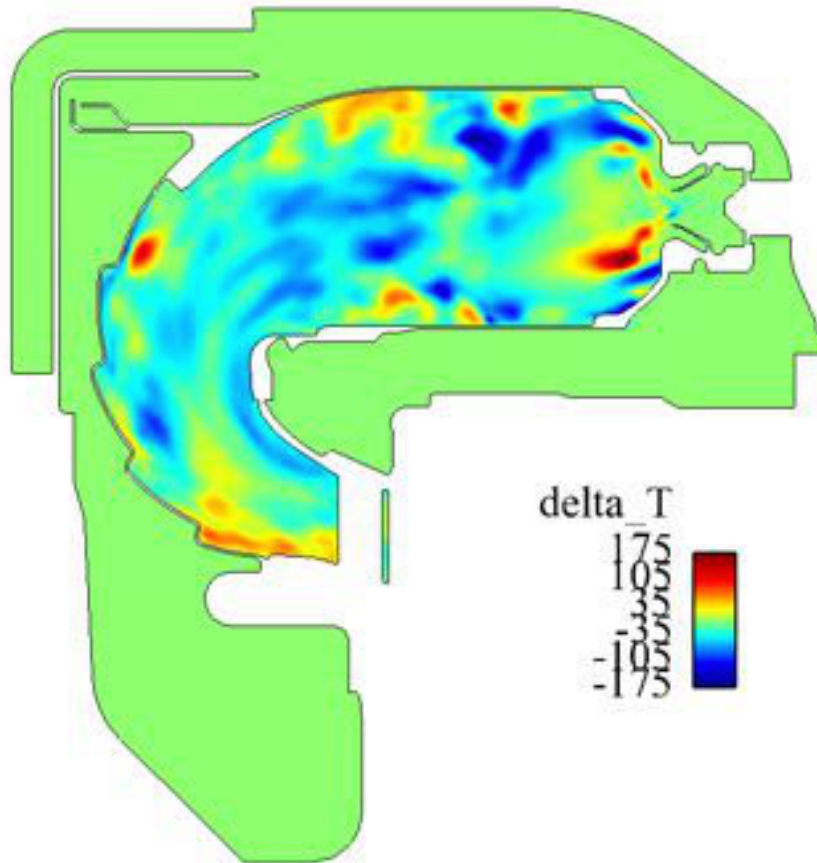
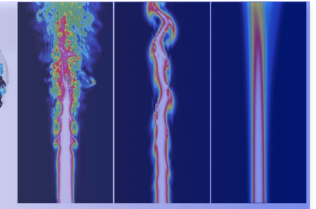
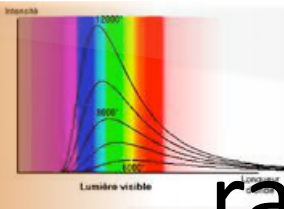
Rayonnement  
PRISSMA



Heat Conduction  
AVTP



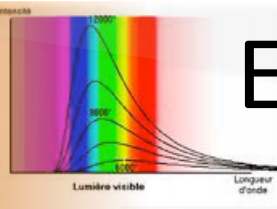
# Inclusion du rayonnement (J. Amaya)



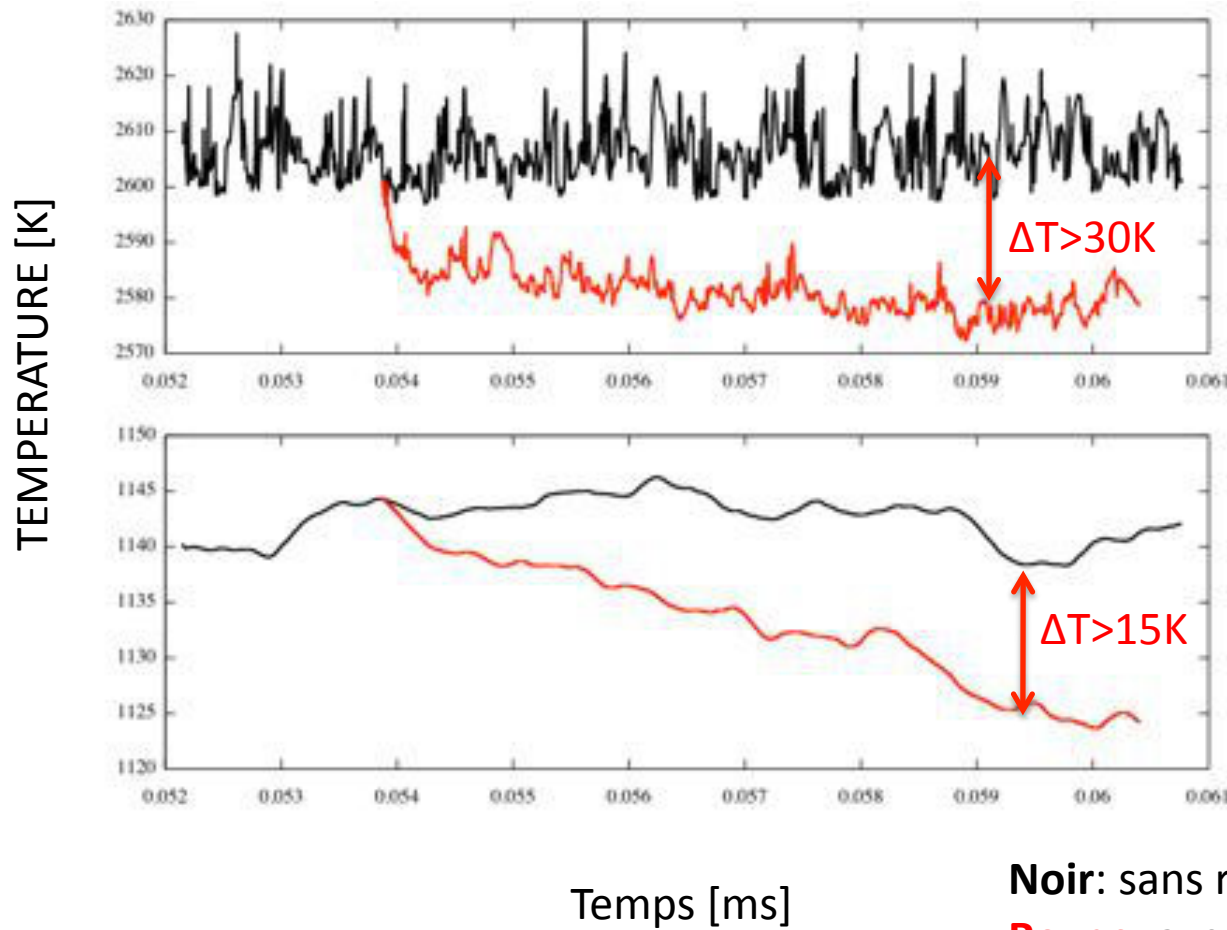
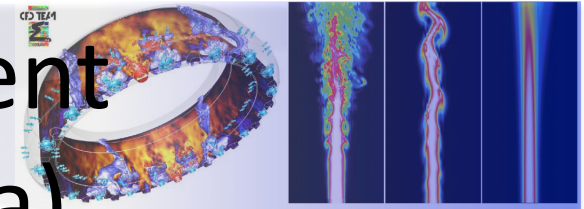
Gain de température dans les zones froides, autour des multiperf et des jets de dilution, et près des films de refroidissement.

Perte de température dans les gaz chauds au centre du domaine



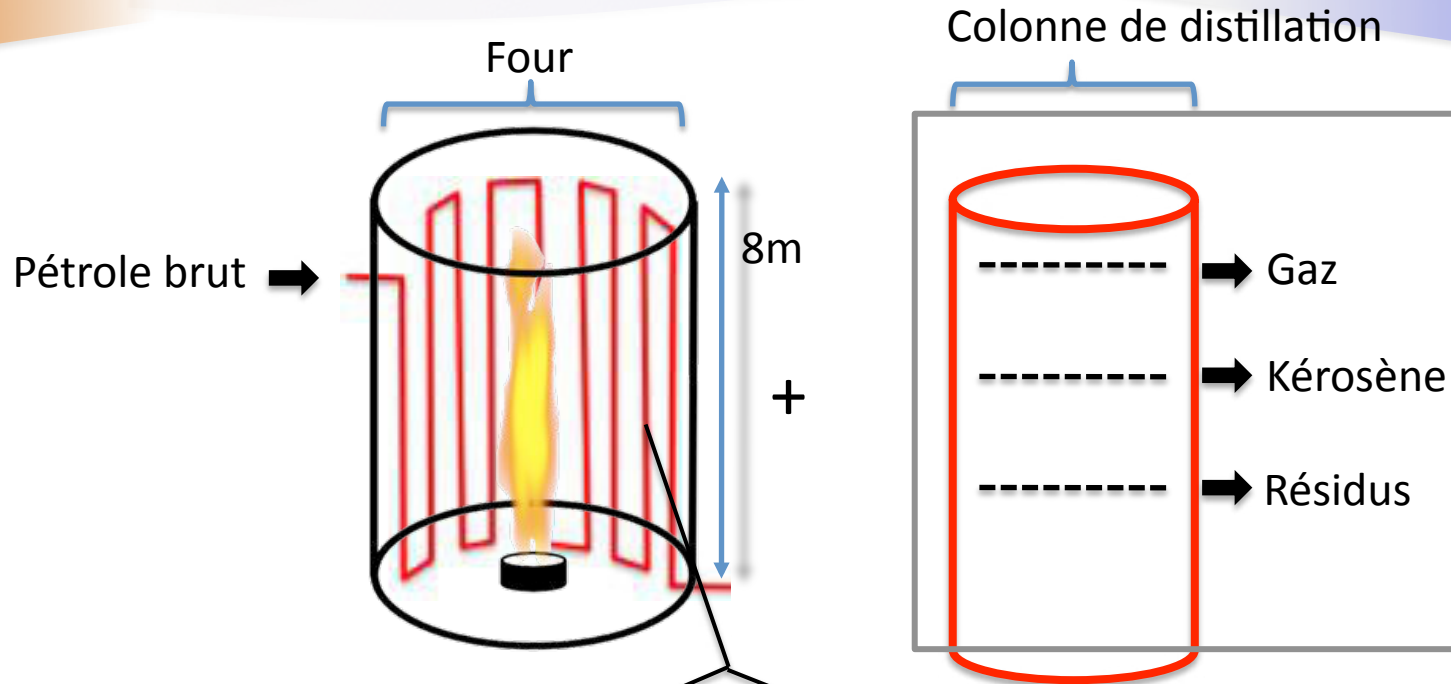


# Effets du rayonnement sur la LES (J. Amaya)



**Noir:** sans rayonnement  
**Rouge:** avec rayonnement

# Formation de coke dans un four de raffinerie (Thèse T. Pedot)



**Formation de coke**

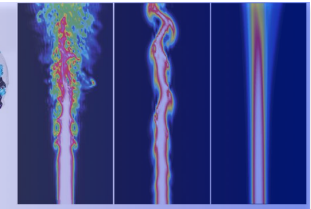
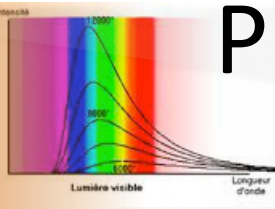



**Corrosion**





Impose des cycles de nettoyage des tubes  
Diminue la durée de vie des tubes dans les fours industriels


# Phénomènes physiques en jeu (T. Pedot)




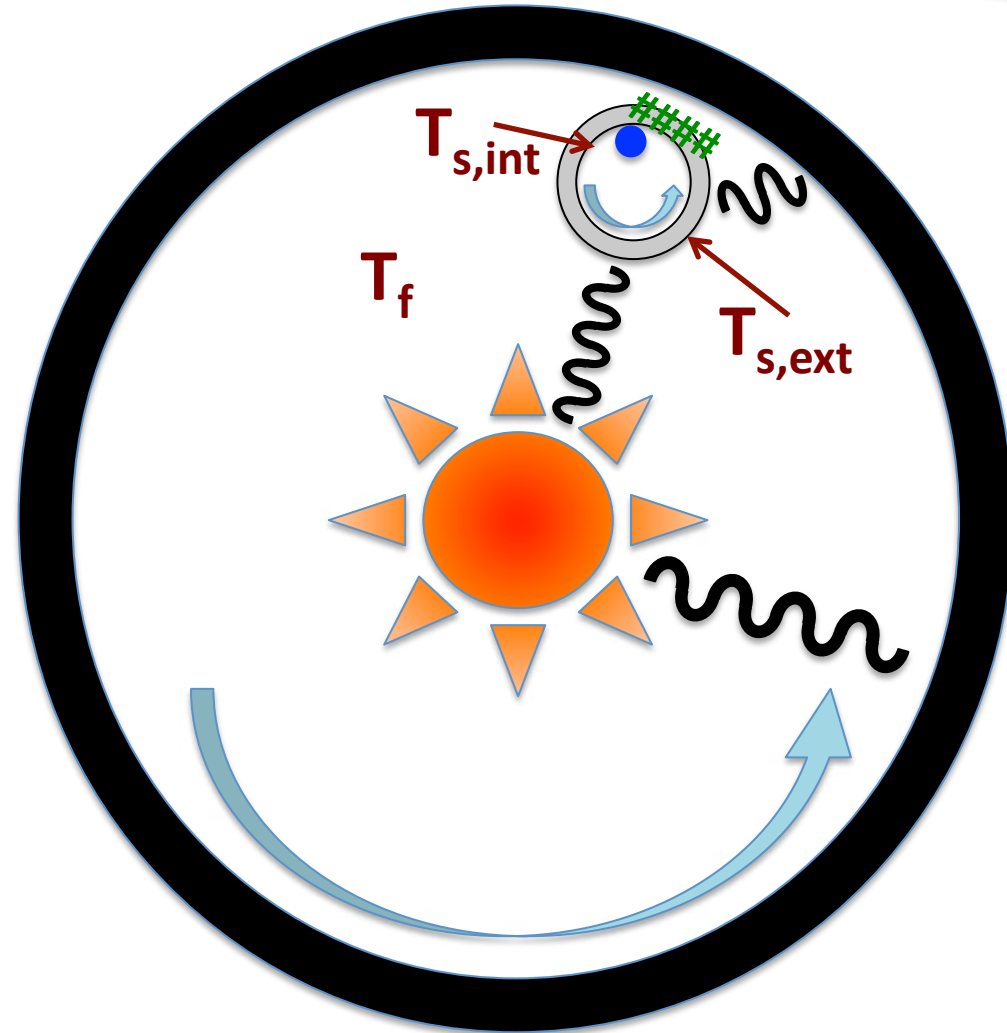
 **Combustion**

 **Ecoulement**  
- dans le four  
- dans les tubes

 **Rayonnement**  
- flamme-tubes  
- flamme-parois  
- tubes-parois

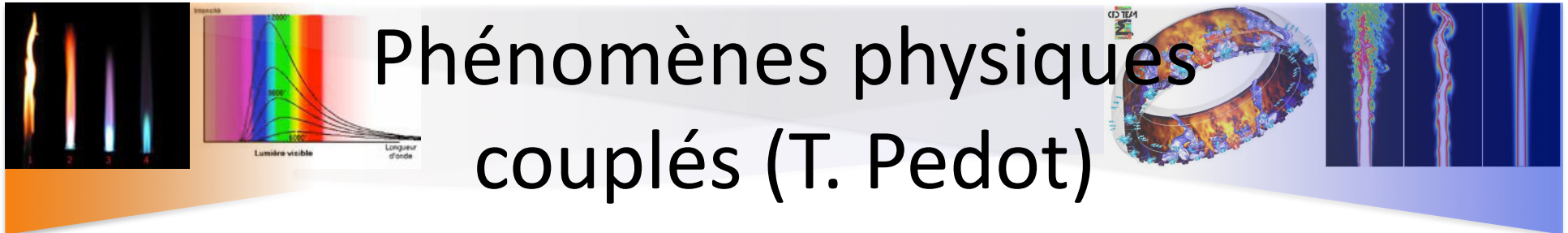
 **Thermique dans les parois solides**

 **Chimie de dépôt**

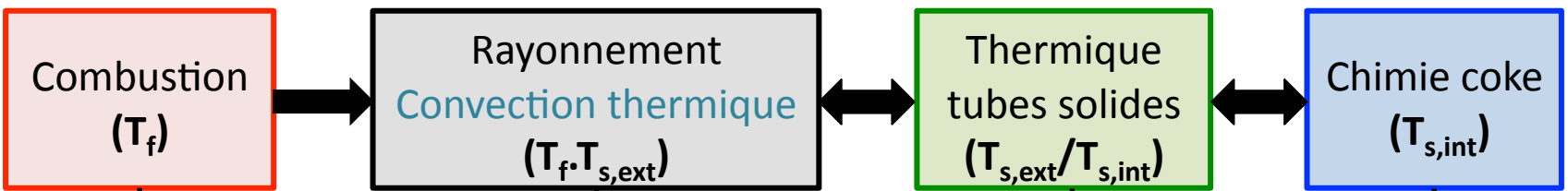


$T_f$     Température fluide  
 $T_{s,ext}$     Température solide externe  
 $T_{s,int}$     Température solide interne

# Phénomènes physiques couplés (T. Pedot)



Phénomènes



Codes



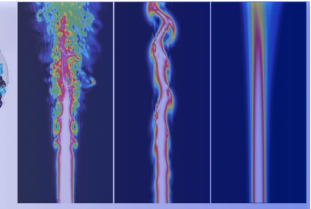
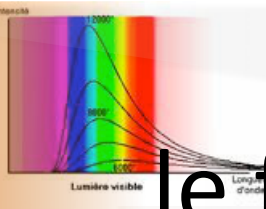
Méthodes

<p>Solution analytique axisymétrique de flamme de diffusion avec chimie réelle</p>	<p>Méthodes aux Ordonnées Discrètes (DOM) avec schéma spectral semi-détaillé + Corrélations pour les coefficients de transfert convectif<sup>4</sup></p>	<p>Equations de conduction de la chaleur dans les solides en géométrie complexe</p>	<p>Cinétique chimique simplifiée<sup>6</sup> + Résistance thermique équivalente</p>
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## 1. Bilan thermique four Feyzin

<sup>1</sup> T. Pedot. *Rapport de 1<sup>ère</sup> année de thèse*, 2010.  
<sup>2</sup> D. Joseph et al. *Int. J. of Therm. Sci.*, 2005.  
<sup>3</sup> J. Amaya et al. *J. of Quantitative Spectroscopy and Radiative Transfer*, 2010.  
<sup>4</sup> A. Bejan, *Convection Heat Transfer*, 1995.  
<sup>5</sup> F. Duchaine et al. *Int. J. of Heat and Fluid Flow*, 2009.  
<sup>6</sup> AP. Watkinson & N. Epstein, *Proc. of 4th Int. Heat Transfer Conference*, 1970.

# Bilan thermique dans le four de Feyzin (T. Pedot)



$\phi_{\text{rad, inc, comb}}$	13,1 MW
$\phi_{\text{rad, émis, tube}}$	3,1 MW
$\phi_{\text{conv, ext}}$	0,385 MW
$\phi_{\text{rad, inc, comb}} - \phi_{\text{rad, émis, tube}} + \phi_{\text{conv, ext}}$	10,31 MW
$\phi_L = \dot{m}C_p\Delta T$	10,86 MW

- Bon ordre de grandeur du bilan thermique
- Forte influence de :
  - La température des parois du four
  - L'écoulement autour de la flamme