Eulerian Monte Carlo Method for solving joint velocity-scalar PDF: numerical aspects and validation

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Velocity-scalar PDF

Reactive Navier-Stokes equations

- Navier-Stokes equations for the velocity $\boldsymbol{U}$, the density ρ, and a turbulent reactive scalar c :

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho U_j\right) = 0 \\
&\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \nabla^2 U_i \\
&\frac{\partial c}{\partial t} + U_j \frac{\partial c}{\partial x_j} = -\frac{1}{\rho}\frac{\partial J_j}{\partial x_j} + S
\end{aligned}
$$

  with P: pressure, ν: cinematic diffusion coefficient,
  $-\frac{1}{\rho}\frac{\partial J_j}{\partial x_j}$: scalar diffusion term and S: chemical source terms.

- Low Mach number assumption:

$$\rho = \rho(c) \text{ and } S = S(c, \rho(c)) = S(c)$$

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Density weighted statistics

- For variable density flows, it is usual to work with density-weighted statistics:

$$p_{Uc}(\boldsymbol{U}, c) = \langle \delta(c(x,t) - c)\delta(\boldsymbol{U}(x,t) - \boldsymbol{U}) \rangle$$

$$\widetilde{f}_{Uc}(\boldsymbol{U}, c) = \frac{\langle \rho | \, \boldsymbol{U}, c \rangle}{\langle \rho \rangle} p_{Uc}(\boldsymbol{U}, c)$$

$$= \frac{\rho(c)}{\langle \rho \rangle} p_{Uc}(\boldsymbol{U}, c) \quad \text{(Low Mach assumption)}$$

- Favre averages are noted $\widetilde{Q}$:

$$\widetilde{Q} = \frac{\langle \rho Q \rangle}{\langle \rho \rangle}$$

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Modeled velocity-composition PDF equation

- Modeled transport equation for the Favre PDF $\widetilde{f}_{Uc}$:

$$\frac{\partial}{\partial t}\left(\langle\rho\rangle\,\widetilde{f}_{Uc}\right)+\frac{\partial}{\partial x_j}\left(\langle\rho\rangle\,U_j\widetilde{f}_{Uc}\right)=$$
$$-\frac{\partial}{\partial U_j}\left(\langle\rho\rangle\left[-\frac{1}{\langle\rho\rangle}\frac{\partial\langle P\rangle}{\partial x_j}-G_{jk}(U_k-\widetilde{U}_k)\right]\widetilde{f}_{Uc}\right)+\frac{1}{2}\langle\rho\rangle\,C_0\,\langle\epsilon\rangle\,\frac{\partial^2\widetilde{f}_{Uc}}{\partial U_j\partial U_j}$$
$$+\frac{\partial}{\partial c}\left(\langle\rho\rangle\,\langle\omega_c\rangle\,(c-\widetilde{c})\,\widetilde{f}_{Uc}\right)-\frac{\partial}{\partial c}\left(\langle\rho\rangle\,S(c)\widetilde{f}_{Uc}\right) \qquad (1)$$

- with:
  - → First line: transport in physical space, treated exactly
  - → Second line: pressure fluctuations and molecular diffusion modelled by the Generalized Langevin model. ϵ is the turbulent dissipation
  - → Third line: Scalar mixing is modeled by the IEM model. Chemistry is treated exactly
- Equation (1) is a Fokker-Planck equation

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Solving PDF equation (1)

- PDF equation (1) has $N_d = N + 7$ dimensions
  where N is the number of scalars = large in practical applications

- Finite volume/element/difference methods:
  → CPU cost increases exponentially with $N_d \Rightarrow$ Not suitable

- Monte Carlo methods:
  → CPU cost increases linearly with $N_d \Rightarrow$ OK
  → Two options:
    ☞ Lagrangian (Particle) Monte Carlo (LMC) methods
    ☞ Eulerian Monte Carlo (EMC) methods

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Lagrangian Monte Carlo methods (1/2)

- PDF is represented by a set of N_p stochastic particles
  - → Each particle is a sample of the physical properties of the system

$$\mathcal{F}_{N_p} = \sum_{n=1}^{N_p} w^{(n)} \delta(c - c^{(n)}) \delta(\boldsymbol{U} - \boldsymbol{U}^{(n)}) \delta(x - x^{(n)}) \quad ; \quad \langle \rho \rangle \, \widetilde{f}_{\boldsymbol{U}\,c} = \left\langle \mathcal{F}_{N_p} \right\rangle$$

$w^{(n)}$, $c^{(n)}$, $\boldsymbol{U}^{(n)}$, $x^{(n)}$: mass, concentration, velocity, position of particle (n)

- Particles evolve according to Ito stochastics ODEs (SODEs) (Pope, 1985):

$$dc^{(n)} = - \langle \omega_c \rangle \left(c^{(n)} - \widetilde{c} \right) dt + S(c^{(n)}) dt \tag{2}$$

$$dU_j^{(n)} = - \frac{1}{\langle \rho \rangle} \frac{\partial \langle P \rangle}{\partial x_j} dt - G_{jk}(U_k^{(n)} - \widetilde{U}_k) dt + \sqrt{C_0 \langle \epsilon \rangle} dW_j^{(n)}(t) \tag{3}$$

$$dx_j^{(n)} = U_j^{(n)} dt \tag{4}$$

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Lagrangian Monte Carlo methods (2/2)

- $W_j^{(n)}$ are independent Gaussian white (Brownian) noises :
  $\left\langle dW_j^{(n)} dW_k^{(m)} \right\rangle = \delta_{nm}\delta_{ij}dt$
- The absence of symbol in the stochastic product (multiplicative noise) in eq. (3) denotes the Ito interpretation (no-correlation property)
- Numerous publications document the convergence and accuracy of LMC methods
  - → LMC used in many complex calculations (including LES)
  - → LMC implemented in commercial CFD codes

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Eulerian Monte Carlo methods

- Principle → PDF represented by stochastic Eulerian fields
  - → Each field is a sample of the physical properties of the system
  - → Each field evolves according to a stochastic PDE (SPDE)
- Development of EMC methods is useful and stimulating
  - → LMC/EMC competition could push both approaches forward
- EMC methods already designed for joint scalar PDFs
  - → Theoretical works : Valiño (98), Sabel'nikov & Soulard (05)
  - → Calculations : Naud et al (04), Sabel'nikov & Soulard (06), Mustata et al. (06)

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Derivation of SPDEs for solving velocity-scalar PDFs

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Objectives and Method

- The question is :

> How can we derive SPDEs for
>
> → a stochastic velocity field $\mathcal{U}$
>
> → a stochastic scalar field θ
>
> so that their statistics yield the Favre PDF ?

- To answer this question :
  we transpose existing LMC models to a Eulerian framework $\Rightarrow$ 3 steps
  1. We introduce the stochastic density (necessary to convert Lagrangian statistics into Eulerian ones)
  2. We use the notion of stochastic characteristics to convert Lagrangian equations (SODEs) into Eulerian ones (SPDEs)
  3. We show that Eulerian PDF (of $\mathcal{U}$ and θ) weighted by the stochastic density is identical to Favre PDF $\widetilde{f}_{Uc}$:

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Stochastic density (1/2)

- The following Ito SODEs are used in LMC methods (Pope (1985))

$$d\theta = -\langle \omega_c \rangle \left(\theta - \widetilde{\theta}\right) dt + S(\theta) dt \quad (5)$$

$$d\mathcal{U}_j = -\frac{1}{\langle \rho \rangle} \frac{\partial \langle P \rangle}{\partial x_j} dt - G_{jk}(\mathcal{U}_k - \widetilde{\mathcal{U}}_k) dt + \sqrt{C_0 \langle \epsilon \rangle} dW_j(t) \quad (6)$$

$$dx_j = \mathcal{U}_j dt \quad (7)$$

Important:

- SODEs (5)-(7) not only define a stochastic velocity $\boldsymbol{\mathcal{U}}$ and a stochastic scalar θ, but also a stochastic density, noted $\mathtt{r}$

- In a Lagrangian framework, the continuity equation is given by :

$$\mathtt{r} = \frac{\mathtt{r}_0}{j} \quad ; \quad j = Det\left[j_{ik}\right], \text{ with } j_{ik} = \frac{\partial x_i}{\partial x_{0_k}}$$

→ j is the Jacobian and $\mathtt{r}_0$ is the initial stochastic density

→ j defines the transformation from intial position $\boldsymbol{x}_0$ to current one $\boldsymbol{x}$

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Stochastic density (2/2)

- The stochastic density $\mathtt{r}$ is different from the physical density ρ
- The evolution of $\mathtt{r}$ is given by:

$$d\mathtt{r} = -\mathtt{r} \;\; div\,(\mathcal{U})\,dt \qquad (8)$$

- For instance, in the case of a constant density $\rho = const$, but $\mathtt{r} \neq const$ because $div(\mathcal{U}) \neq 0$:

$$\frac{d}{dt}\,(div(\mathcal{U})) = -\,\frac{\partial \mathcal{U}_i}{\partial x_j}\frac{\partial \mathcal{U}_j}{\partial x_i} - \frac{1}{\rho}\frac{\partial^2 \langle P \rangle}{\partial x_i \partial x_i} + \frac{\partial}{\partial x_i}\,(G_{ij}(\mathcal{U}_j - \langle \boldsymbol{U}_j \rangle)) + \frac{1}{2}\sqrt{\frac{C_0}{\langle \epsilon \rangle}}\,\frac{\partial \langle \epsilon \rangle}{\partial x_i}\,\dot{W}_i \qquad (9)$$

- This property is a consequence of the closure assumption used in the Langevin model, which only imposes a continuity constraint on the mean velocity field, but not on its instantaneous value

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Lagrangian - Eulerian transposition

- SODEs (5) - (8) are the stochastic characteristics of the following hyperbolic Ito SPDEs :

$$\frac{\partial \mathrm{r}}{\partial t} + \mathcal{U}_j \frac{\partial \mathrm{r}}{\partial x_j} = -\mathrm{r} \frac{\partial}{\partial x_j} (\mathcal{U}_j) \tag{10}$$

$$\frac{\partial \theta}{\partial t} + \mathcal{U}_j \frac{\partial \theta}{\partial x_j} = -\langle \omega_c \rangle (\theta - \widetilde{\theta}) + S(\theta) \tag{11}$$

$$\frac{\partial \mathcal{U}_i}{\partial t} + \mathcal{U}_j \frac{\partial \mathcal{U}_i}{\partial x_j} = -\frac{1}{\langle \rho \rangle} \frac{\partial \langle P \rangle}{\partial x_i} - G_{ij}(\mathcal{U}_j - \widetilde{\mathcal{U}_j}) + \sqrt{C_0 \langle \epsilon \rangle} \dot{W}_i \tag{12}$$

- These hyperbolic equations can be rewritten also in conservative form:

$$\frac{\partial \mathrm{r}}{\partial t} + \frac{\partial}{\partial x_j} (\mathrm{r}\mathcal{U}_j) = 0 \tag{13}$$

$$\frac{\partial}{\partial t} (\mathrm{r}\theta) + \frac{\partial}{\partial x_j} (\mathrm{r}\mathcal{U}_j\theta) = -\mathrm{r} \langle \omega_c \rangle (\theta - \widetilde{\theta}) + \mathrm{r}S(\theta) \tag{14}$$

$$\frac{\partial}{\partial t} (\mathrm{r}\mathcal{U}_i) + \frac{\partial}{\partial x_j} (\mathrm{r}\mathcal{U}_j\mathcal{U}_i) = -\frac{\mathrm{r}}{\langle \rho \rangle} \frac{\partial \langle P \rangle}{\partial x_i} + \mathrm{r}G_{ij} (\mathcal{U}_j - \langle U_j \rangle) + \mathrm{r}\sqrt{C_0 \langle \epsilon \rangle} \dot{W}_j \tag{15}$$

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Eulerian PDF

- The Eulerian PDF of $\boldsymbol{\mathcal{U}}$ and θ is defined by :

$$f_{\mathcal{U}\theta}(\boldsymbol{U},\Theta;\boldsymbol{x},t) = \langle \delta(\boldsymbol{U} - \boldsymbol{\mathcal{U}}(\boldsymbol{x},t))\delta(\Theta - \theta(\boldsymbol{x},t))\rangle \tag{16}$$

- $\mathtt{r}$ varies $\Rightarrow$ we introduce statistics weighted by the stochastic density $\mathtt{r}$

$$f_{\mathcal{U}\theta:\mathtt{r}}(\boldsymbol{U},\Theta;\boldsymbol{x},t) = \frac{\langle \mathtt{r} | \boldsymbol{U},\Theta\rangle}{\langle \mathtt{r}\rangle} f_{\mathcal{U}\Theta}(\boldsymbol{U},\Theta;x,t) \tag{17}$$

- By standard techniques, one can show that weighted PDF is identical to Favre PDF $\widetilde{f}_{\boldsymbol{U}c}$:

$$f_{\mathcal{U}\theta:\mathtt{r}} = \widetilde{f}_{\boldsymbol{U}c}$$

provided that

$$\langle \mathtt{r}\rangle = \langle \rho \rangle$$

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Implications for scalar PDF methods

Implications for scalar PDF methods (1/3)

- EMC method has been devised for the full velocity-composition PDF
- How do the previous results apply to the computation of the following scalar PDF equation ?

$$\frac{\partial}{\partial t}\left(\langle\rho\rangle\,\widetilde{f}_c\right)+\frac{\partial}{\partial x_j}\left(\langle\rho\rangle\,\widetilde{U}_j\widetilde{f}_c\right)=\frac{\partial}{\partial x_j}\left(\langle\rho\rangle\,\Gamma_T\frac{\partial\widetilde{f}_c}{\partial x_j}\right)$$
$$+\frac{\partial}{\partial c}\left(\langle\rho\rangle\,\langle\omega_c\rangle\,(c-\tilde{c})\widetilde{f}_c\right)-\frac{\partial}{\partial c}\left(\langle\rho\rangle\,S(c)\widetilde{f}_c\right) \qquad (18)$$

→ scalar turbulent advection is now directly modelled by a gradient diffusion assumption

→ $\Gamma_T=C_\mu\widetilde{k}^2/\widetilde{\epsilon}$ is a turbulent diffusivity

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Implications for scalar PDF methods (2/3)

- Previous work by Sabel'nikov & Soulard (PRE 72, 016301, 2005):
  - → Velocity $\mathcal{U}$ is modeled by a gaussian decorrelated velocity
  - → An equation is sought for the stochastic scalar θ so that its unweighted statistics give immediately the Favre PDF: $p^*_\theta = \widetilde{f}_c$ (in particular $\langle \theta \rangle = \widetilde{c}$), and thus the introduction of stochastic density is not needed

- Sabel'nikov & Soulard obtained the following SPDE for the scalar θ:

$$\frac{\partial \theta}{\partial t} + \mathcal{U}_j \circ \frac{\partial \theta}{\partial x_j} = - \langle \omega_c \rangle \left(\theta - \langle \theta \rangle \right) + S(\theta)$$

$$\mathcal{U}_i = \widetilde{U}_i - \Gamma_T \frac{1}{\langle \rho \rangle} \frac{\partial \langle \rho \rangle}{\partial x_i} - \frac{1}{2} \frac{\partial \Gamma_T}{\partial x_i} + V_i \quad , V_i = \sqrt{2 \Gamma_T} \dot{W}_i \qquad (19)$$

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Implications for scalar PDF methods (3/3)

- The symbol $\circ$ denotes the Stratonovitch interpretation of the multiplicative noise - stochastic part of the convection term in (19). The mean value of $V_j \circ \frac{\partial \theta}{\partial x_j}$ is not zero and is equal to:
$\left\langle V_j \circ \frac{\partial \theta}{\partial x_j} \right\rangle_W = -\frac{\partial}{\partial x_j}\left(\Gamma_T \frac{\partial \langle \theta \rangle}{\partial x_j}\right) + \frac{1}{2}\frac{\partial \Gamma_T}{\partial x_j}\frac{\partial \langle \theta \rangle}{\partial x_j}$

- We remind that in Ito calculus this correlation is equal zero:
$\left\langle V_j \frac{\partial \theta}{\partial x_j} \right\rangle_W = 0$

- Stochastic convection and SPDE (19) can be rewritten in Ito form:

$$V_j \circ \frac{\partial \theta}{\partial x_j} = V_j \frac{\partial \theta}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\Gamma_T \frac{\partial \theta}{\partial x_j}\right) + \frac{1}{2}\frac{\partial \Gamma_T}{\partial x_j}\frac{\partial \theta}{\partial x_j}$$

$$\frac{\partial \langle \rho \rangle \theta}{\partial t} + \frac{\partial \langle \rho \rangle \widetilde{U_j \theta}}{\partial x_j} + \langle \rho \rangle V_j \frac{\partial \theta}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\langle \rho \rangle \Gamma_T \frac{\partial \theta}{\partial x_j}\right) - \langle \omega_c \rangle (\theta - \langle \theta \rangle) + S(\theta)$$

- Eq (19) is in non conservative form

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Zero-correlation time limit in (13)-(15)

- The same reasonings can be applied to system (13)-(15):
  - ➞ But equivalence is between weighted statistics $\widetilde{f}_\theta^* = \frac{\langle r|\theta\rangle^*}{\langle r\rangle^*} p_\theta^* = \widetilde{f}_c$
- To facilitate our derivation, we consider the Simplified Langevin model. The tensor G_{ij} reduces to :

$$G_{ij} = \frac{1}{\tau_{rel}}\delta_{ij}, \text{ where } \frac{1}{\tau_{rel}} = \left(\frac{1}{2} + \frac{3}{4}C_0\right)\frac{\widetilde{\epsilon}}{\widetilde{k}}$$

- We let $\tau_{rel} \to 0$ in (13)-(15) , but keep $\widetilde{\epsilon}\tau_{rel}^2$ finite :

$$\mathtt{r} \circ \mathcal{U}_j - \mathtt{r}\left\langle \mathcal{U}_j \right\rangle_{\mathtt{r}} + \mathtt{r}\sqrt{C_0\widetilde{\epsilon}\tau_{rel}^2}\dot{W}_j = 0 \qquad (20)$$

- A solution to (20) is

$$\mathcal{U}_i = \widetilde{U}_i + \Gamma_T \frac{1}{\langle\rho\rangle}\frac{\partial\langle\rho\rangle}{\partial x_i} + \frac{1}{2}\frac{\partial \Gamma_T}{\partial x_i} + \sqrt{2\Gamma_T}\dot{W}_i$$

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Final system of SPDEs

- The final system of hyperbolic SPDEs is :

$$\mathcal{U}_i = \widetilde{U}_i + \Gamma_T \frac{1}{\langle\rho\rangle}\frac{\partial\langle\rho\rangle}{\partial x_i} + \frac{1}{2}\frac{\partial\Gamma_T}{\partial x_i} + \sqrt{2\Gamma_T}\dot{W}_i \tag{21}$$

$$\frac{\partial \mathtt{r}}{\partial t} + \frac{\partial}{\partial x_j}\left(\mathtt{r}\circ\mathcal{U}_j\right) = 0 \tag{22}$$

$$\frac{\partial}{\partial t}\left(\mathtt{r}\theta\right) + \frac{\partial}{\partial x_j}\left(\left(\mathtt{r}\theta\right)\circ\mathcal{U}_j\right) = -\mathtt{r}\left\langle\omega_c\right\rangle\left(\theta - \left\langle\theta\right\rangle_{\mathtt{r}}\right) + \mathtt{r}S \tag{23}$$

- Eq. (21)-(23) are statistically equivalent to PDF equation (18)
  This remains true even in the case when τ_{rel} is not small
- These SPDEs are different from, but stochastically equivalent to those of Sabel'nikov & Soulard (PR 72, 016301, 2005)
  - → They are in conservative form $\Rightarrow$ may be easier to implement to CFD codes
  - → The fluctuating velocity has the property: $\widetilde{\mathcal{U}''} = 0$

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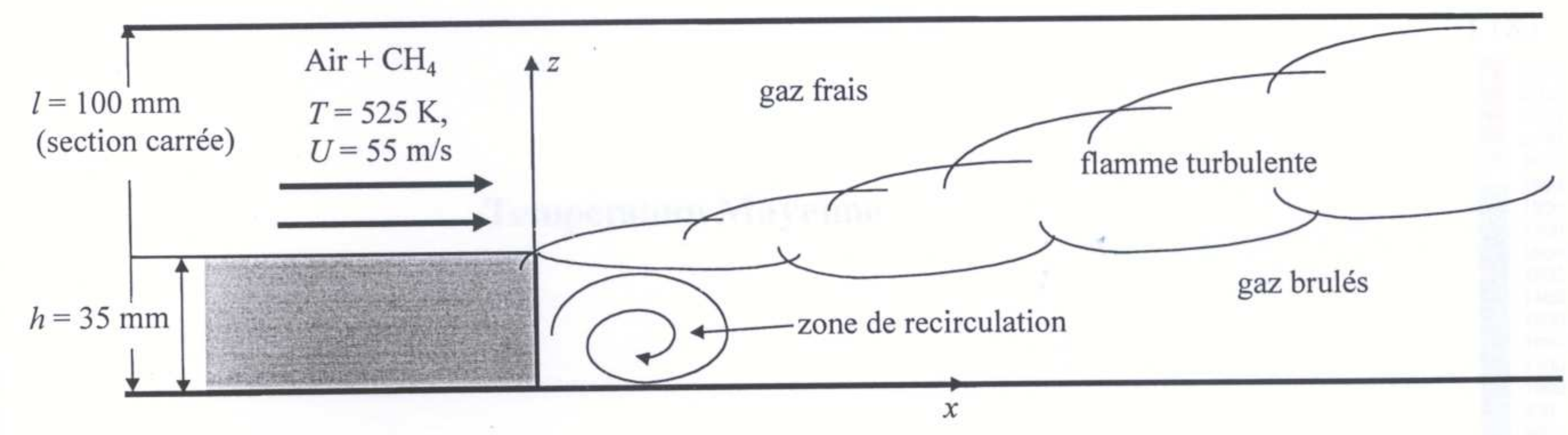
Simulation of a backward facing step with a RANS/EMC solver

Work done in collaboration with M. Ourliac (PhD student)

Configuration

- Stoichiometric premixed air/methane flame over a backward facing step:



Inlet velocity U_e	$55\ m/s$
Inlet temperature T_e	$525\ K$
Pressure P	$10^5\ Pa$
Equivalence ratio	1
Inlet t.k.e k_e	$40\ m^2/s^2$
Inlet turb. dissip. ϵ_e	$800\ m^2/s^3$

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RANS & EMC solver (1/2)

- RANS solver:

Continuity	$\frac{\partial \langle\rho\rangle}{\partial t} + \frac{\partial}{\partial x_j}\left(\langle\rho\rangle \tilde{U}_j\right) = 0$
Momentum	$\frac{\partial \langle\rho\rangle \tilde{U}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\langle\rho\rangle \tilde{U}_j \tilde{U}_i\right) = -\frac{\partial \langle P\rangle}{\partial x_j} + \frac{\partial \sigma_{ij}}{\partial x_j}$
Turbulent kinetic energy	$\frac{\partial \langle\rho\rangle k}{\partial t} + \frac{\partial}{\partial x_j}\left(\langle\rho\rangle \tilde{U}_j k\right) = \frac{\partial}{\partial x_j}\left(\langle\rho\rangle \frac{\nu_t}{Pr_k}\frac{\partial k}{\partial x_j}\right) + P_k - d_k$
Turbulent dissipation	$\frac{\partial \langle\rho\rangle \epsilon}{\partial t} + \frac{\partial}{\partial x_j}\left(\langle\rho\rangle \tilde{U}_j \epsilon\right) = \frac{\partial}{\partial x_j}\left(\langle\rho\rangle \frac{\nu_t}{Pr_\epsilon}\frac{\partial \epsilon}{\partial x_j}\right) + P_\epsilon - d_\epsilon$

- EMC solver:

Stoch. Vel.	$\mathcal{U}_i = \widetilde{U}_i + \Gamma_T \frac{1}{\langle\rho\rangle}\frac{\partial \langle\rho\rangle}{\partial x_i} + \frac{1}{2}\frac{\partial \Gamma_T}{\partial x_i} + \sqrt{2\Gamma_T}\dot{W}_i$
Stoch. Density	$\frac{\partial \mathtt{r}}{\partial t} + \frac{\partial}{\partial x_j}\left(\mathtt{r} \circ \mathcal{U}_j\right) = 0$
Mass fraction	$\frac{\partial}{\partial t}\left(\mathtt{r} Y_k\right) + \frac{\partial}{\partial x_j}\left(\left(\mathtt{r} Y_k\right) \circ \mathcal{U}_j\right) = -\mathtt{r}\widetilde{\omega_k}\left(Y_k - \widetilde{Y_k}\right) + \mathtt{r} S(Y, h_t)$
Total enthalpy	$\frac{\partial}{\partial t}\left(\mathtt{r} h_t\right) + \frac{\partial}{\partial x_j}\left(\left(\mathtt{r} h_t\right) \circ \mathcal{U}_j\right) = -\mathtt{r}\widetilde{\omega_h}\left(h_t - \widetilde{h_t}\right)$

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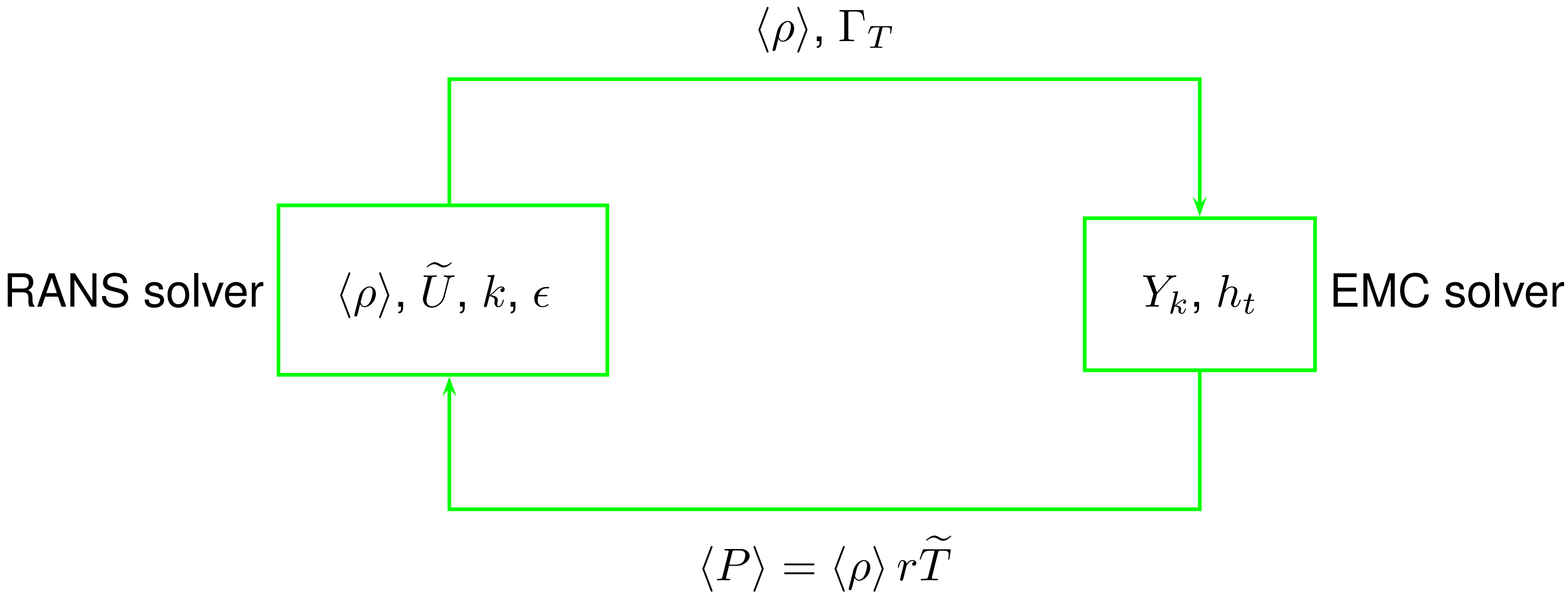
RANS & EMC solver (2/2)

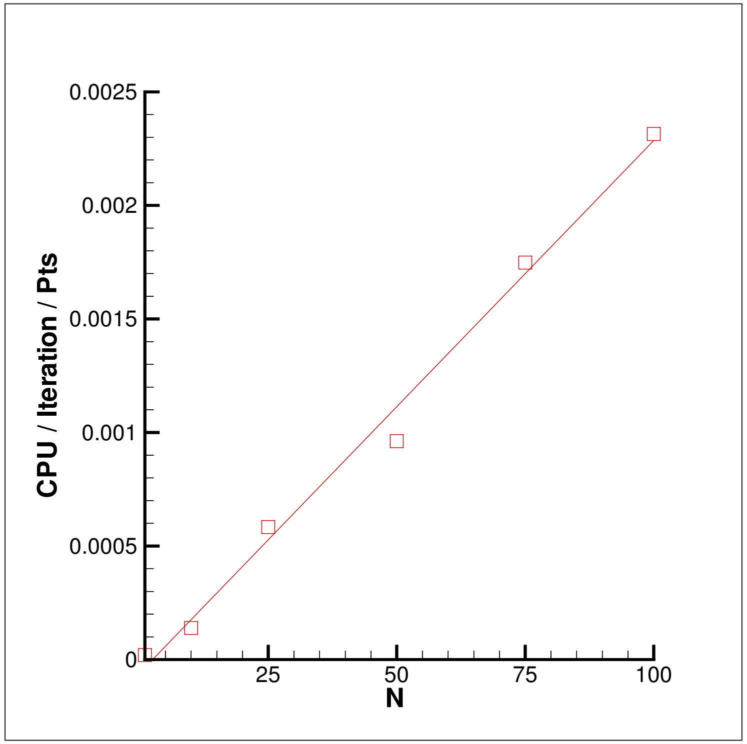
- Coupling between the solvers:



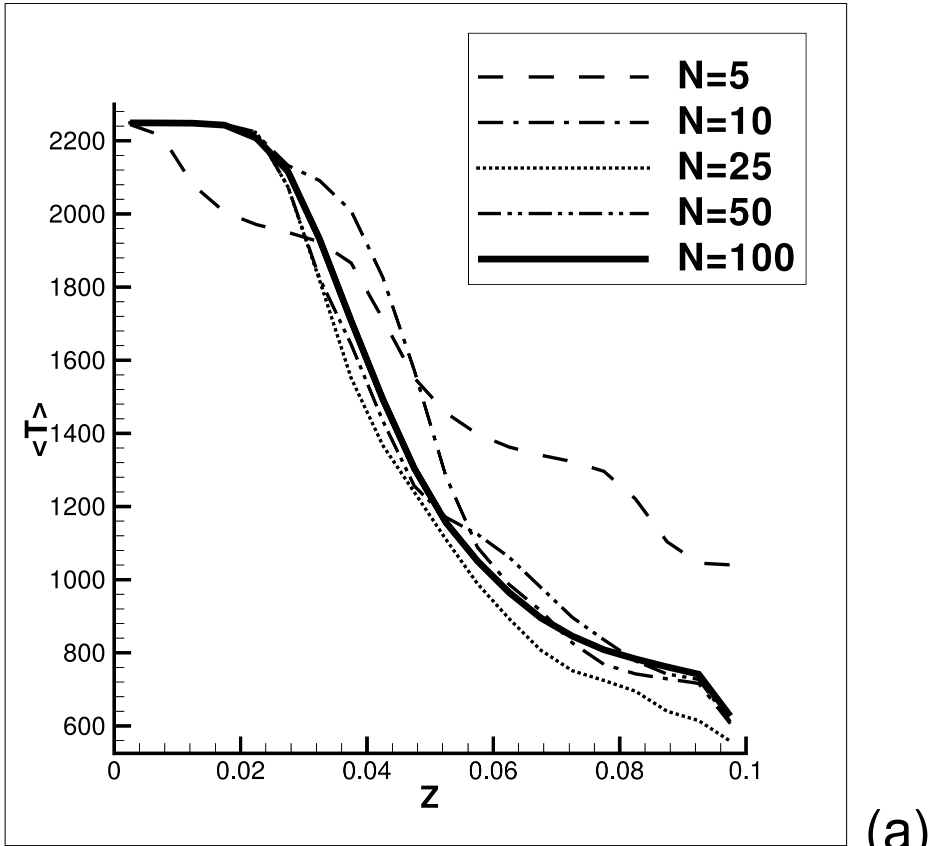
EMC solver based on Stratonovitch calculus

Parameters

- Chemistry: $CH_4 + 2O_2 + \beta N_2 \rightarrow CO_2 + 2H_2O + \beta N_2$
- Adiabatic walls
- Mesh (default value) : 100 x 40 cells
- Stochastic fields (default value): 50
- Evolution of the CPU time per iteration and per number of cells against the number of stochastic fields



Analysis of the stochastic error (1/2)



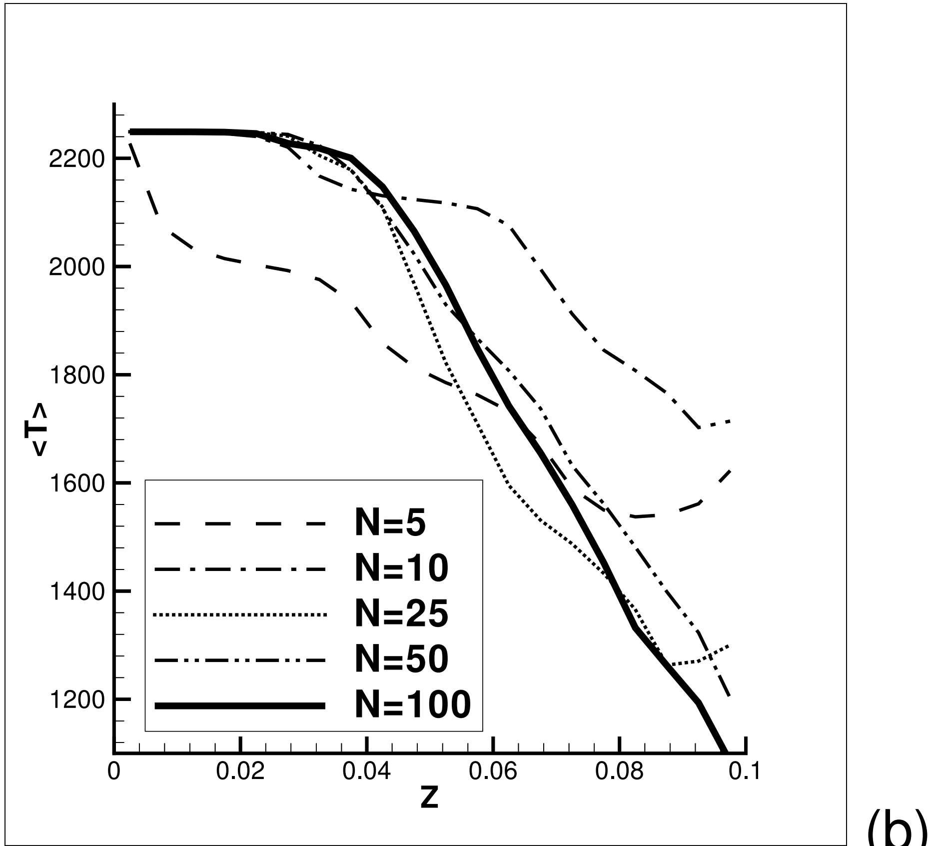


Figure 1: Influence of the number of stochastic fields N on the mean temperature vertical profiles, at $x = 0.25\ m$ (a) and $x = 0.46\ m$ (b)

Analysis of the stochastic error (2/2)

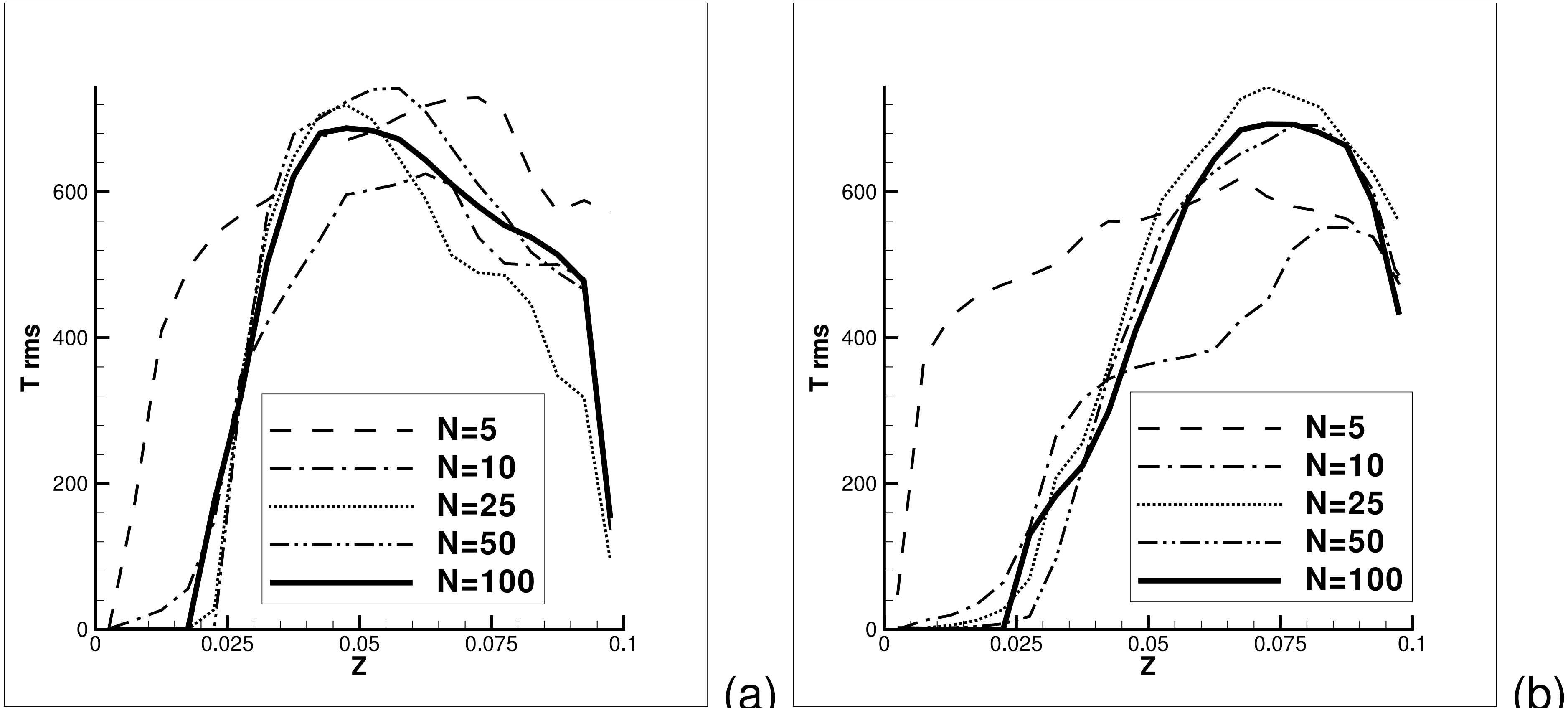


Figure 2: Influence of the number of stochastic fields N on the RMS temperature vertical profiles, at $x = 0.25\ m$ (a) and $x = 0.46\ m$ (b)

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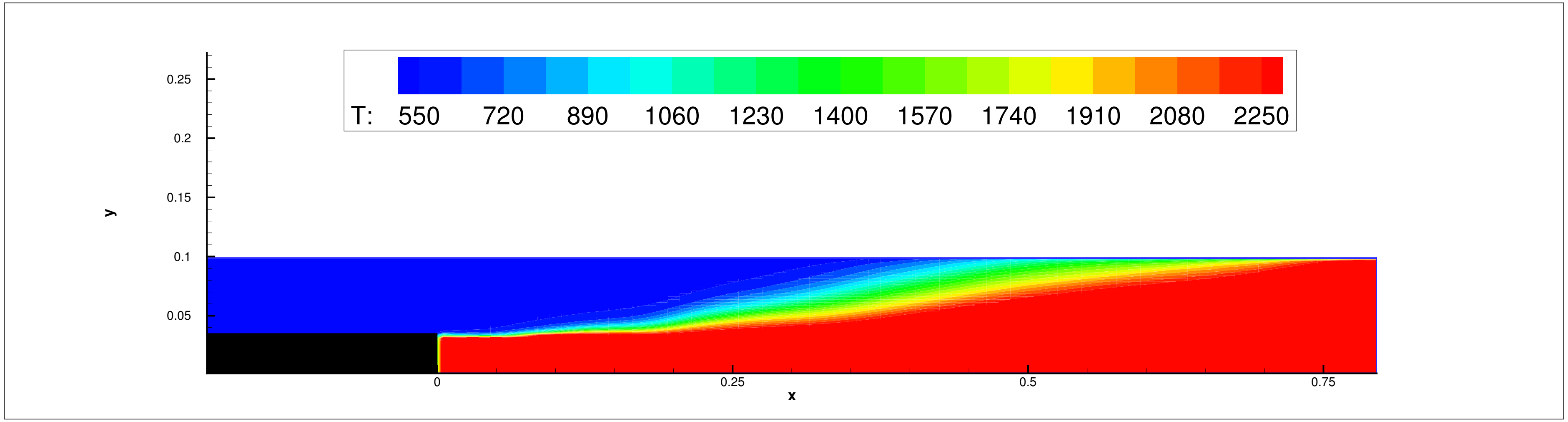
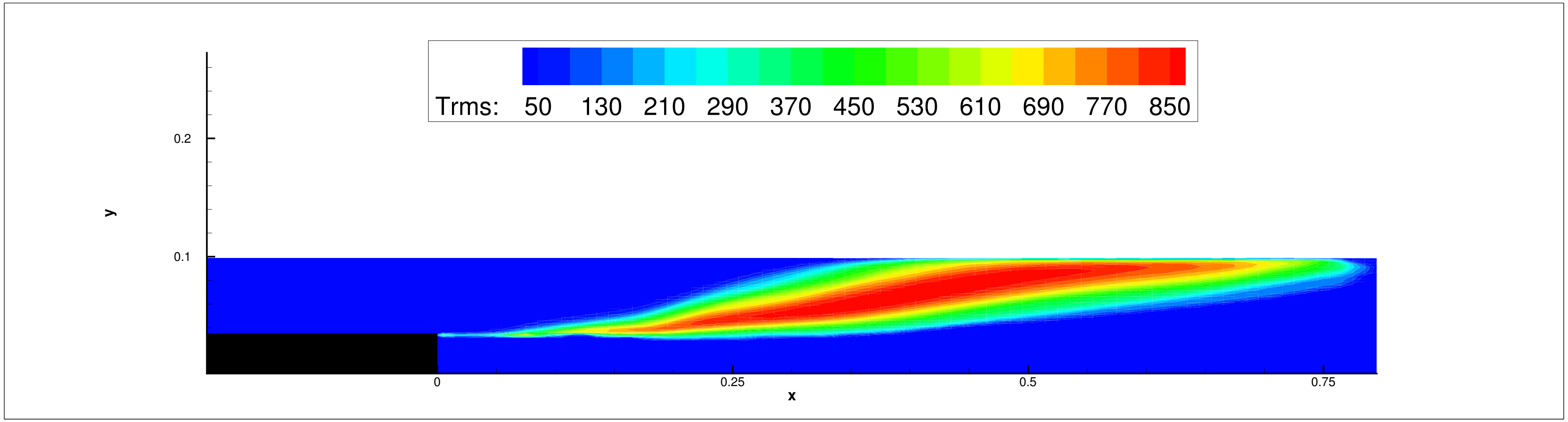
Results

- Mean and RMS temperature fields:





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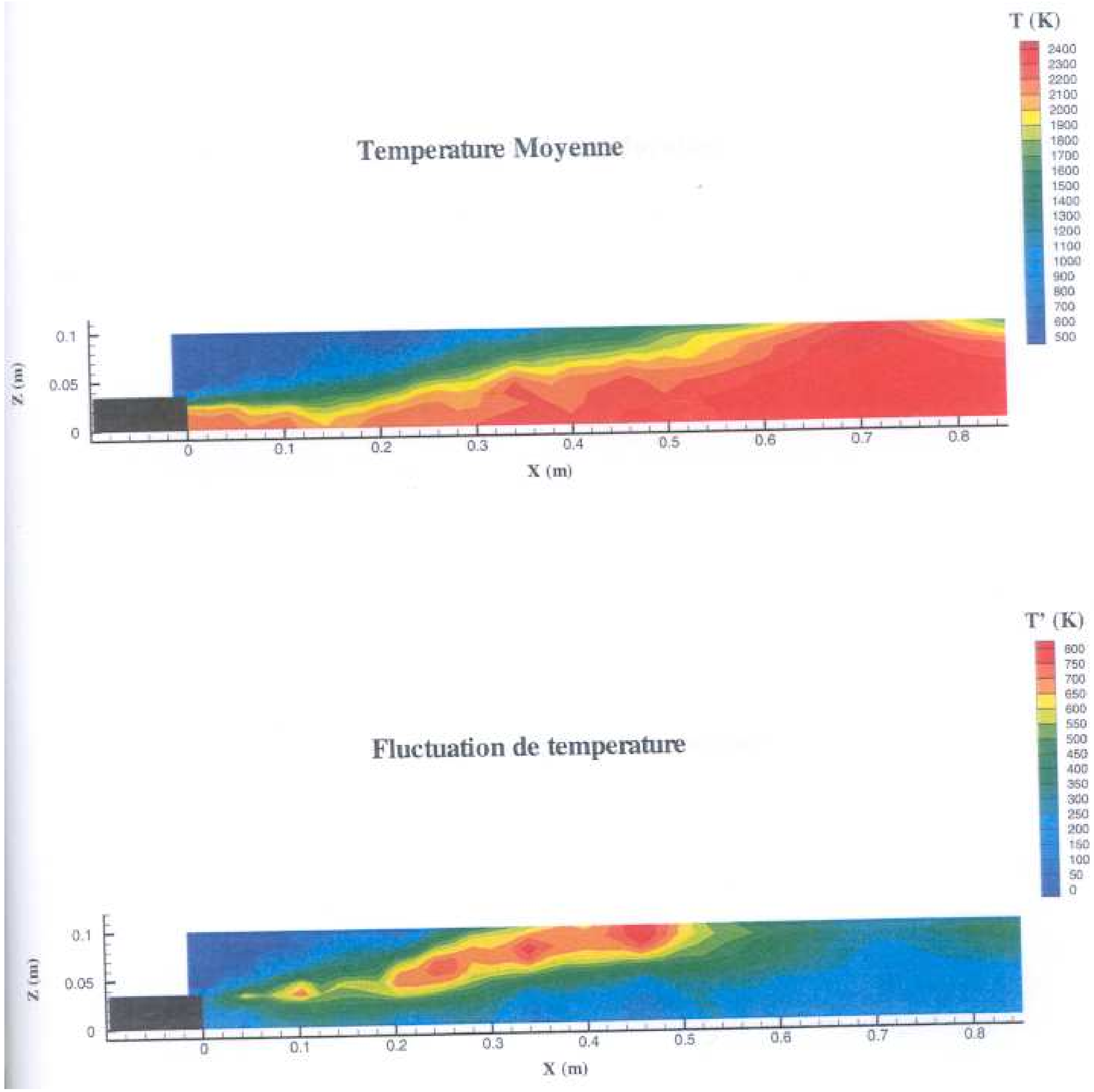
Experiments (Magre & Moreau 1988)

- Mean and RMS temperature fields:



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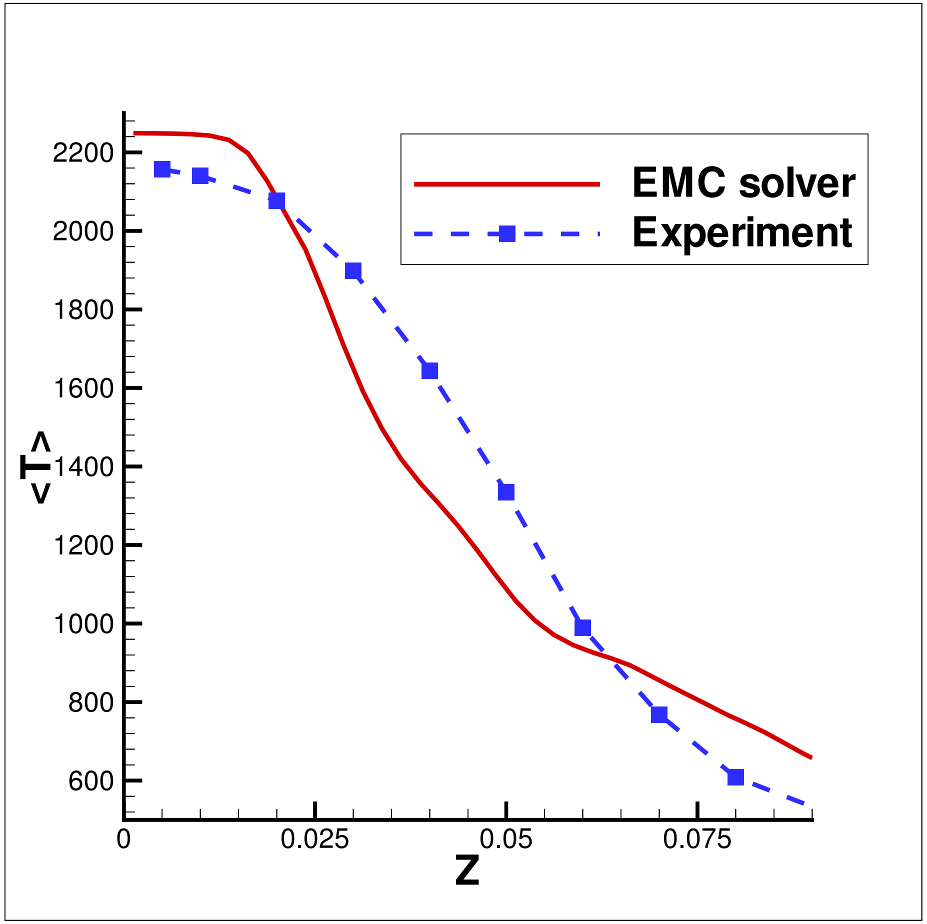
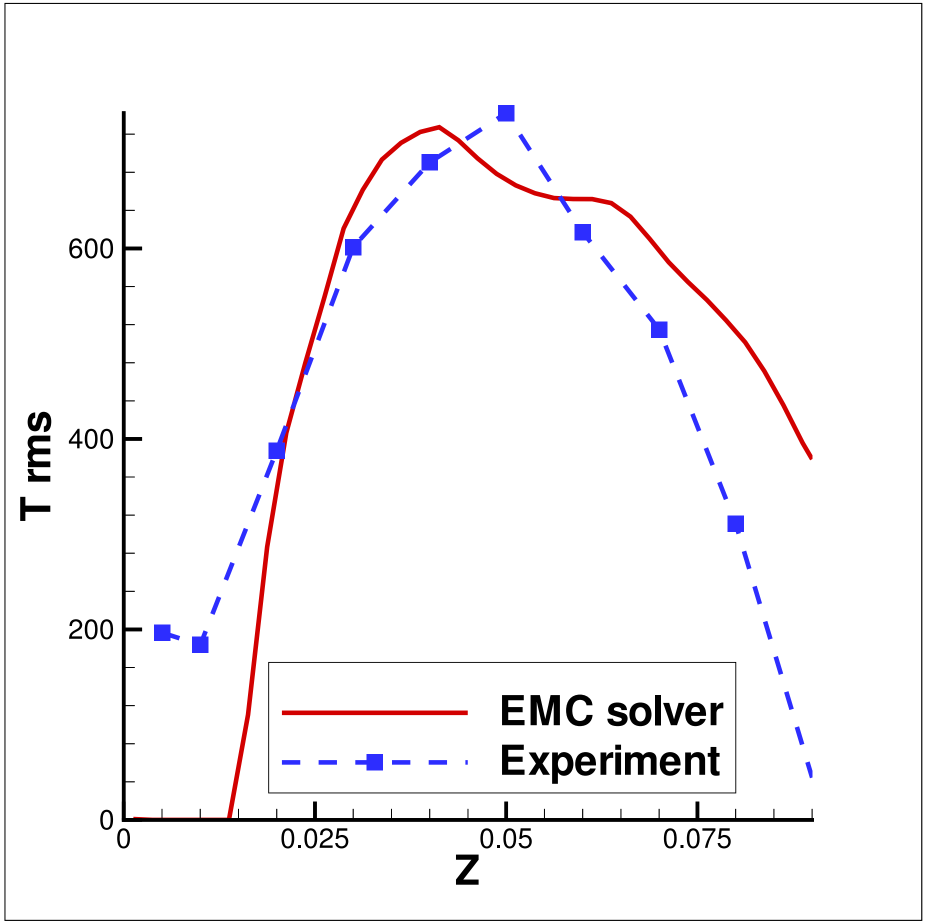
Profiles (1/3)

- Comparison of mean and RMS temperature with experiment:



Mean Temperature at x=210 mm



RMS Temperature at x=210 mm

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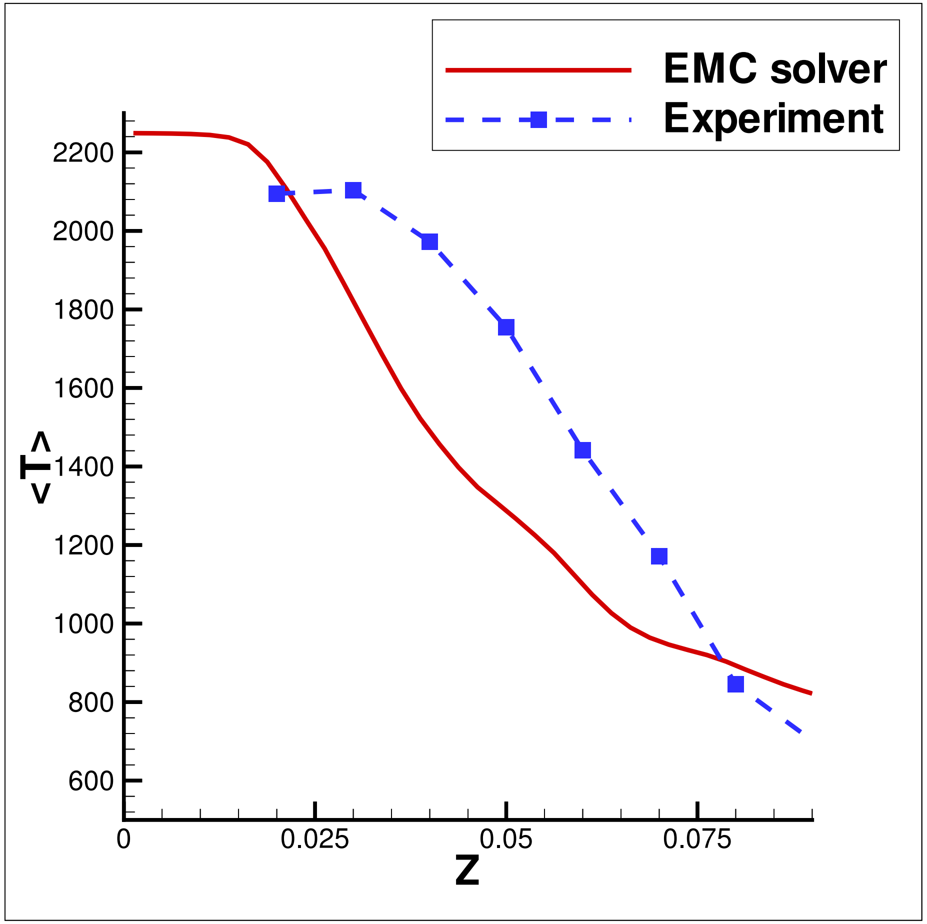
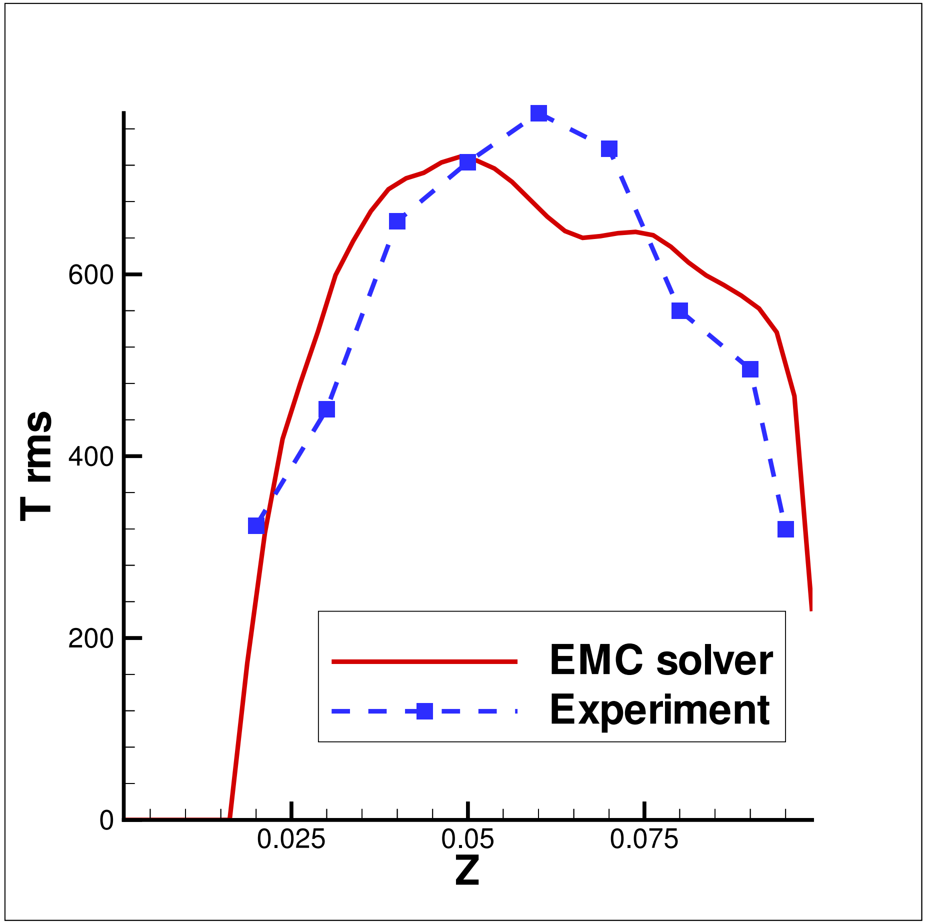
Profiles (2/3)

- Comparison of mean and RMS temperature with experiment:



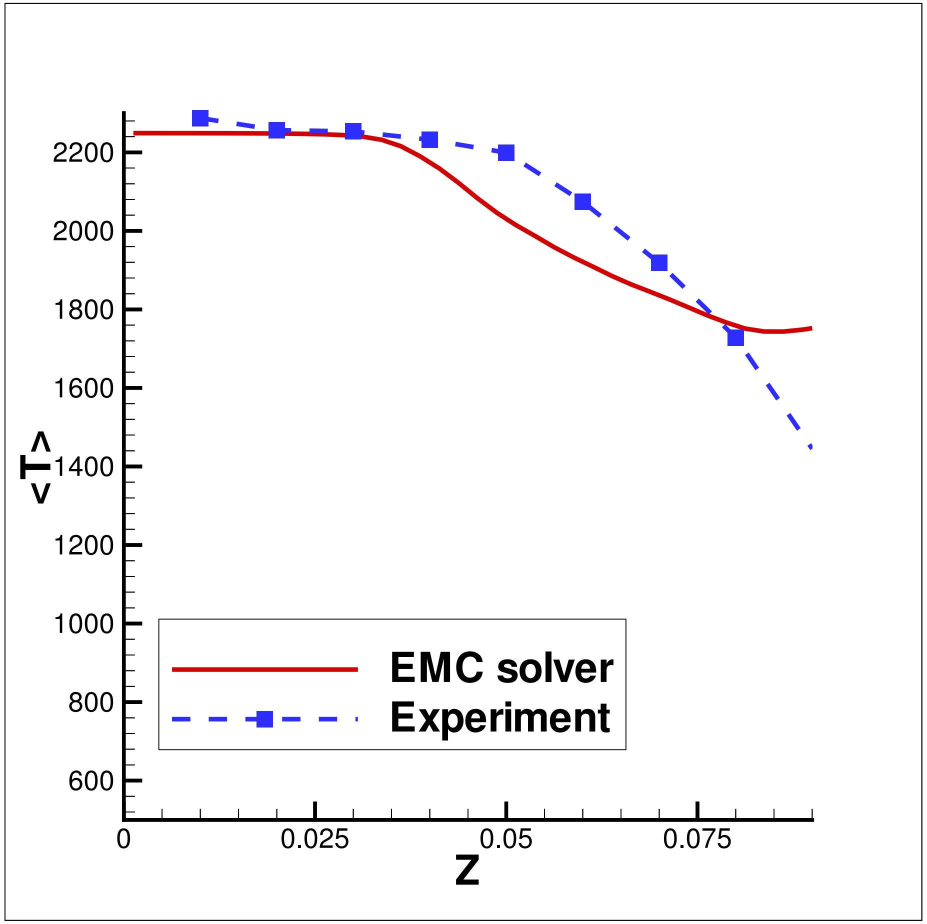
Mean Temperature at x=250 mm



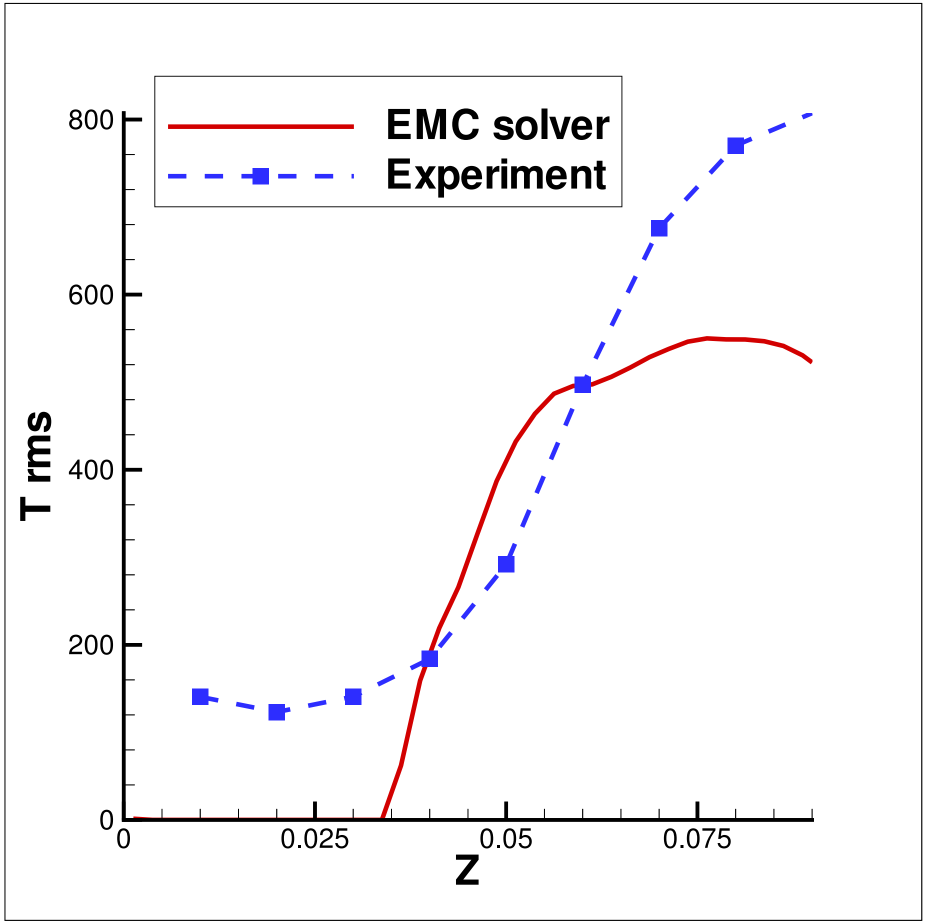
RMS Temperature at x=250 mm

Profiles (3/3)

- Comparison of mean and RMS temperature with experiment:



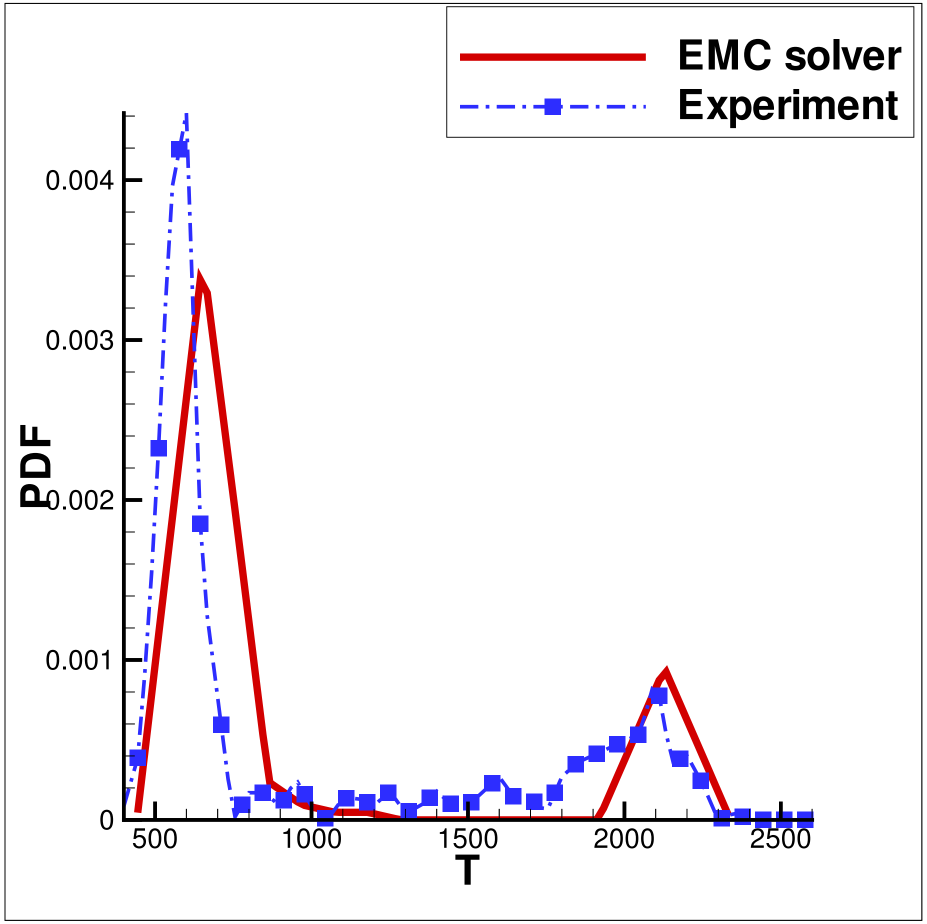
Mean Temperature at x=460 mm



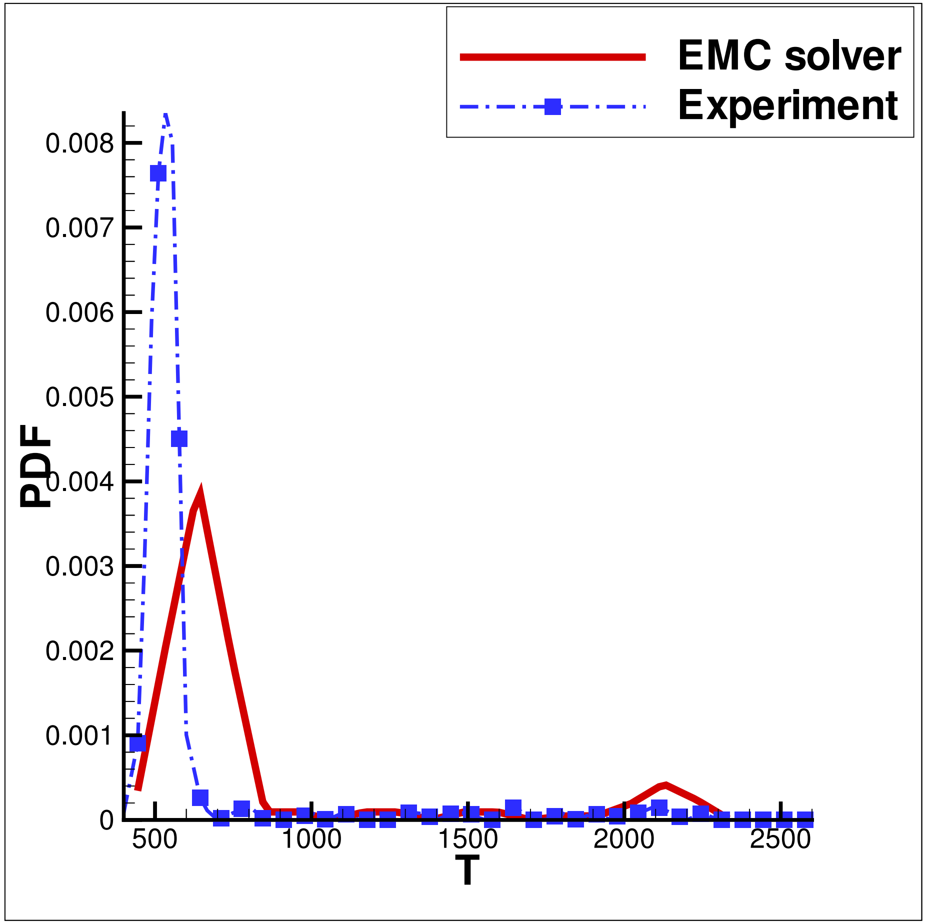
RMS Temperature at x=460 mm

PDF (1/2)

- Comparison between computed and measured PDFs at x=210 mm



$z = 6mm$



$z = 8mm$

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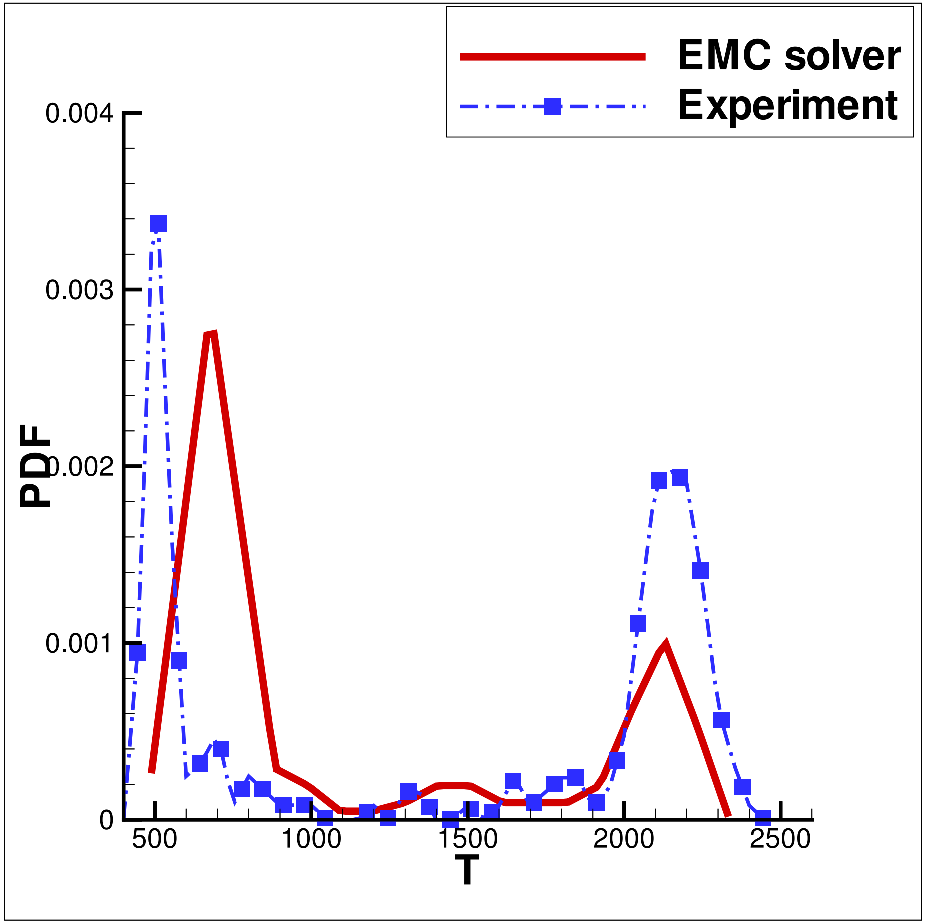
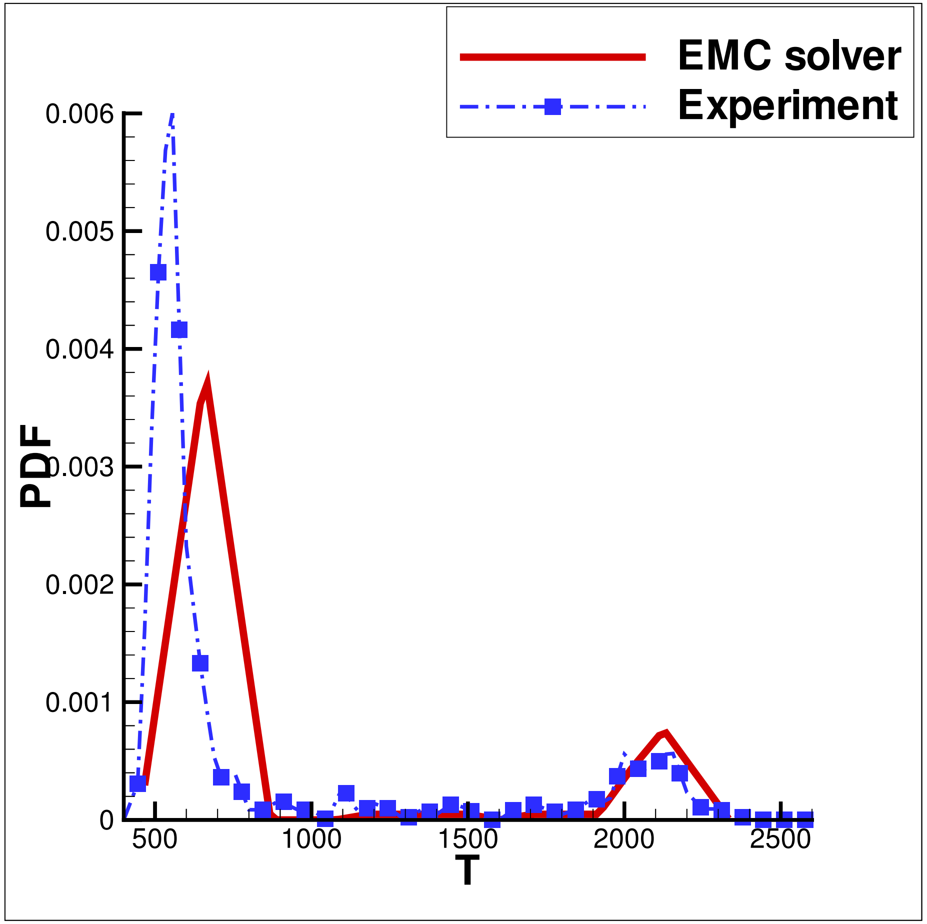
PDF (2/2)

- Comparison between computed and measured PDFs at x=250 mm



$z = 6mm$



$z = 8mm$

Conclusions for Part I

- Extension of EMC method for solving velocity-scalar PDF has been proposed
  - → Appropriate numerical scheme must be designed
  - → The derived SPDEs need to be tested on simple 1D tests
  - → The overall method needs to be compared against LMC method
- Corresponding EMC method for solving scalar PDF has also been proposed
- The EMC method for scalar PDF has been applied to the computation of a turbulent premixed methane flame over a backward facing step

Part II

Contents

① Velocity-scalar PDF
- Modeled velocity-scalar PDF
- Lagrangian and Eulerian Monte Carlo methods

② Scalar-velocity EMC method

③ Numerical scheme

④ Validation tests
- Riemann problem
- Return to Gaussianity
- Auto-ignition of a Methane-air mixture

⑤ Conclusions and perspectives

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Turbulent reacting flow

- We consider a turbulent reacting flow with density ρ, velocity $\boldsymbol{U}$, total enthalpy h_t, and mass fractions Y_α $(\alpha = 1, \cdots, N_s)$

- For variable density flows, it is usual to work with Favre statistics:

Reynolds PDF $\overline{f} = \langle \delta(Y_\alpha(x,t) - Y_\alpha)\delta(h_t(x,t) - h_t)\delta(\boldsymbol{U}(x,t) - \boldsymbol{U})\rangle$

Favre PDF $\widetilde{f} = \dfrac{\overline{(\rho|\, \boldsymbol{U}, Y_\alpha, h_t)}}{\langle \rho \rangle} \overline{f}$

Reynolds and Favre averages are noted $\overline{Q}$ and $\widetilde{Q}$: $\widetilde{Q} = \frac{\langle \rho Q \rangle}{\langle \rho \rangle}$

- Low Mach number assumption: pressure fluctuations are neglected in the thermodynamical equations

$\Rightarrow \rho$ *and the chemical source terms are functions of the reactive scalars*

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Modeled scalar-velocity PDF equation

- Modeled transport equation in 1D for the Favre PDF $\widetilde{f}$:

$$\frac{\partial}{\partial t}\left(\langle\rho\rangle\,\widetilde{f}\right)+\frac{\partial}{\partial x}\left(\langle\rho\rangle\,U\widetilde{f}\right)= \tag{24}$$

$$-\frac{\partial}{\partial U}\left(\langle\rho\rangle\left[-\frac{1}{\rho}\frac{\partial\overline{P}}{\partial x}-C_1\omega\left(U-\widetilde{U}\right)\right]\widetilde{f}\right)+\frac{1}{2}C_0\,\langle\rho\rangle\,\omega\widetilde{k}\frac{\partial^2\widetilde{f}}{\partial U^2}$$

$$-\frac{\partial}{\partial h_t}\left(\langle\rho\rangle\left[\frac{1}{\rho}\frac{\partial\overline{P}}{\partial t}-C_h\omega\left(h_t-\widetilde{h_t}\right)\right]\widetilde{f}\right)$$

$$-\frac{\partial}{\partial Y_\alpha}\left(-\langle\rho\rangle\,C_\phi\omega\left(Y_\alpha-\widetilde{Y_\alpha}\right)\widetilde{f}+\langle\rho\rangle\,S_\alpha\widetilde{f}\right)$$

→ First line: transport in physical space, treated exactly

→ Second line: pressure fluctuations and molecular diffusion modelled by the simplified Langevin model

→ Third and fourth lines: mixing modelled by the IEM model

P: pressure, S_α: source term, $\widetilde{k}$: turbulent kinetic energy, ω: turbulent frequency, $C_\#$: constants

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Solving PDF equation (24)

- PDF equation (24) has $N_d = N_s + 7$ dimensions
  where N is the number of scalars = large in practical applications

- Finite volume/element/difference methods:
  - → CPU cost increases exponentially with $N_d \Rightarrow$ Not suitable

- Monte Carlo methods:
  - → CPU cost increases linearly with $N_d \Rightarrow$ OK
  - → Two options:
    - ☞ Lagrangian Monte Carlo (LMC) methods
    - ☞ Eulerian Monte Carlo (EMC) methods

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Lagrangian Monte Carlo methods (1/2)

- PDF represented by a set of N_p stochastic particles
  - → Each particle is a sample of the physical properties of the system

$$\mathcal{F}_{N_p} = \sum_{n=1}^{N_p} w^{(n)} \delta(\boldsymbol{U} - \boldsymbol{U}^{(n)}) \delta(Y_\alpha - Y_\alpha^{(n)}) \delta(h_t - h_t^{(n)}) \delta(x - x^{(n)}) \quad ; \quad \langle \rho \rangle \widetilde{f} = \left\langle \mathcal{F}_{N_p} \right\rangle$$

$w^{(n)}$, $\boldsymbol{U}^{(n)}$, $Y_\alpha^{(n)}$, $h_t^{(n)}$, $x^{(n)}$: mass, velocity, concentration, enthalpy, position of particle (n)

- Particles evolve according to SODEs (Pope, 1985):

$$dU_j^{(n)} = -\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_j} dt - C_1 \omega \left(U - \widetilde{U} \right) dt + \sqrt{C_0 \omega \widetilde{k}} dW_j^{(n)}(t) \tag{25}$$

$$dY_\alpha^{(n)} = -C_\phi \omega \left(Y_\alpha^{(n)} - \widetilde{Y_\alpha} \right) dt + S_\alpha^{(n)} dt \tag{26}$$

$$dh_t^{(n)} = \frac{1}{\rho} \frac{\partial \overline{P}}{\partial t} dt - C_h \omega \left(h_t^{(n)} - \widetilde{h_t} \right) dt \tag{27}$$

$$dx_j^{(n)} = U_j^{(n)} dt \tag{28}$$

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Lagrangian Monte Carlo methods (2/2)

- $W_j^{(n)}$ are independent Brownian noises :
  $\left\langle dW_j^{(n)} dW_k^{(m)} \right\rangle = \delta_{nm}\delta_{ij}dt$
- The absence of symbol in the stochastic product in eq. (26) denotes the Ito interpretation
- Numerous publications document the convergence and accuracy of LMC methods
  - → LMC used in many complex calculations (including LES)
  - → LMC implemented in commercial CFD codes

Eulerian Monte Carlo methods

- Principle → PDF represented by stochastic Eulerian fields
  - → Each field is a sample of the physical properties of the system
  - → Each field evolves according to an SPDE
- Development of EMC methods is useful and stimulating
  - → LMC/EMC competition could push both approaches forward
- EMC methods already designed for joint scalar PDFs
  - → Theoretical works : Valiño (98), Sabel'nikov & Soulard (05)
  - → Calculations : Naud et al (04), Sabel'nikov & Soulard (06)

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Eulerian Monte Carlo methods

- EMC methods also designed for joint scalar-velocity PDFs
  - ➞ Theoretical derivation of SPDEs : Soulard & Sabel'nikov (05)
  - ☞ But no validation nor application

$\Rightarrow$ Purpose of this work

- ➞ to propose a numerical scheme for solving the SPDEs
- ➞ to assess its performances

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Scalar-velocity SPDEs

- SPDEs stochastically equivalent to PDF equation (24) can be derived from SODEs (25)-(28) by the notion of stochastic characteristic:

$$\frac{\partial \mathtt{r}}{\partial t} + \frac{\partial}{\partial x}(\mathtt{r}\,\mathcal{U}) = 0 \tag{29}$$

$$\frac{\partial}{\partial t}(\mathtt{r}\,\mathcal{U}) + \frac{\partial}{\partial x}(\mathtt{r}\,\mathcal{U}^2 + \overline{P}) = \left(1 - \frac{\mathtt{r}}{\rho}\right)\frac{\partial \overline{P}}{\partial x} - \mathtt{r}\,C_1\omega\left(\mathcal{U} - \widetilde{U}\right) + \mathtt{r}\sqrt{C_0\omega\widetilde{k}}\dot{W} \tag{30}$$

$$\frac{\partial}{\partial t}(\mathtt{r}\,\mathcal{H}) + \frac{\partial}{\partial x}(\mathtt{r}\,\mathcal{U}\mathcal{H}) = -\mathtt{r}\,\omega\left(\mathcal{H} - \widetilde{h}_t\right) + \frac{\mathtt{r}}{\rho}\frac{\partial \overline{P}}{\partial t} \tag{31}$$

$$\frac{\partial}{\partial t}(\mathtt{r}\,\mathcal{Y}_\alpha) + \frac{\partial}{\partial x}(\mathtt{r}\,\mathcal{U}\mathcal{Y}_\alpha) = -\mathtt{r}\,\omega\left(\mathcal{Y}_\alpha - \widetilde{Y}_\alpha\right) + \mathtt{r}\,S_\alpha \tag{32}$$

- $\mathcal{U}$ is the stochastic velocity field, $\mathcal{H}$ is the stochastic total enthalpy and $\mathcal{Y}_\alpha$ is the stochastic mass fraction. W is a standard Brownian noise and $\dot{W}$ is its time derivative
- $\mathtt{r}$ is the stochastic density. $\mathtt{r}$ is different from the physical density ρ

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Scalar-velocity SPDEs

- We note $\langle Q\rangle_s$ the average over the stochastic fields, and $\langle Q\rangle_r$ the average weighted by the density $\mathtt{r}$: $\langle Q\rangle_r = \frac{\langle \mathtt{r}Q\rangle_s}{\langle \mathtt{r}\rangle_s}$
- The corresponding PDFs are respectively denoted by f_s and $f_{\mathtt{r}}$.
  The following equivalences exist:

$$\widetilde{f} = f_{\mathtt{r}} = \frac{\langle \mathtt{r}|\mathcal{U},\mathcal{Y}_\alpha,\mathcal{H}\rangle_s}{\langle\rho\rangle} f_s \quad \text{and} \quad \overline{f} = \frac{\langle\rho\rangle}{\rho} f_{\mathtt{r}} = \frac{\langle \mathtt{r}|\mathcal{U},\mathcal{Y}_\alpha,\mathcal{H}\rangle_s}{\rho} f_s$$

- with consistency conditions: $\langle \mathtt{r}\rangle_s = \langle\rho\rangle$ and $\left\langle \frac{\mathtt{r}}{\rho}\right\rangle_s = 1$
- Favre and Reynolds averages are given by:

$$\widetilde{Q} = \langle Q\rangle_{\mathtt{r}} = \frac{\langle \mathtt{r}Q\rangle_s}{\langle\rho\rangle} \quad \text{and} \quad \overline{Q} = \left\langle \frac{\mathtt{r}}{\rho} Q\right\rangle_s$$

- Mean pressure is given by:

$$\overline{P} = \overline{\rho r_g T} = \langle \mathtt{r} r_g T\rangle_s$$

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Numerical scheme: spatial discretization

- We use a finite volume method
  - → we must define a monotone numerical flux
- Characteristic waves of SPDEs (29)-(32) are complex
  - → due to the presence of both mean and instantaneous quantities
  - ⇒ upwinding monotone fluxes (like Godunov method) are difficult to use
- We decide to use instead a centered monotone flux
  - → Only requires limited information on the characteristic wave system
  - → Many different centered scheme exist
  - → We retain the 'GFORCE' flux (Toro and Titarev, 2006)
- To achieve 2nd order, we use the 'GFORCE' flux in conjunction with a 2nd/3rd order WENO interpolation

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Numerical scheme: temporal discretization

- 3 requirements for the time discretization
  - → it should be strong stability preserving (SSP): in order to maintain monotonicity
  - → it should allow for the implicit treatment of stiff source terms
  - → it should be of weak order 2
- In the deterministic case, implicit-explicit (IMEX) Runge-Kutta (RK) schemes with the SSP property exist (Pareschi and Russo, 2005)
  - → IMEX schemes are an interesting alternative to splitting methods
  - → the stiff and non-stiff parts of the system are discretized together
  - → The stiff part is treated implicitly, and the non-stiff part explicitly
- We extend these deterministic IMEX-RK schemes to the stochastic case
  - → We procede as in Tocino et al (2002)
  - ⇒ We obtain a new class of Stochastic IMEX schemes (S-IMEX)

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First test: Riemann problem (1/4)

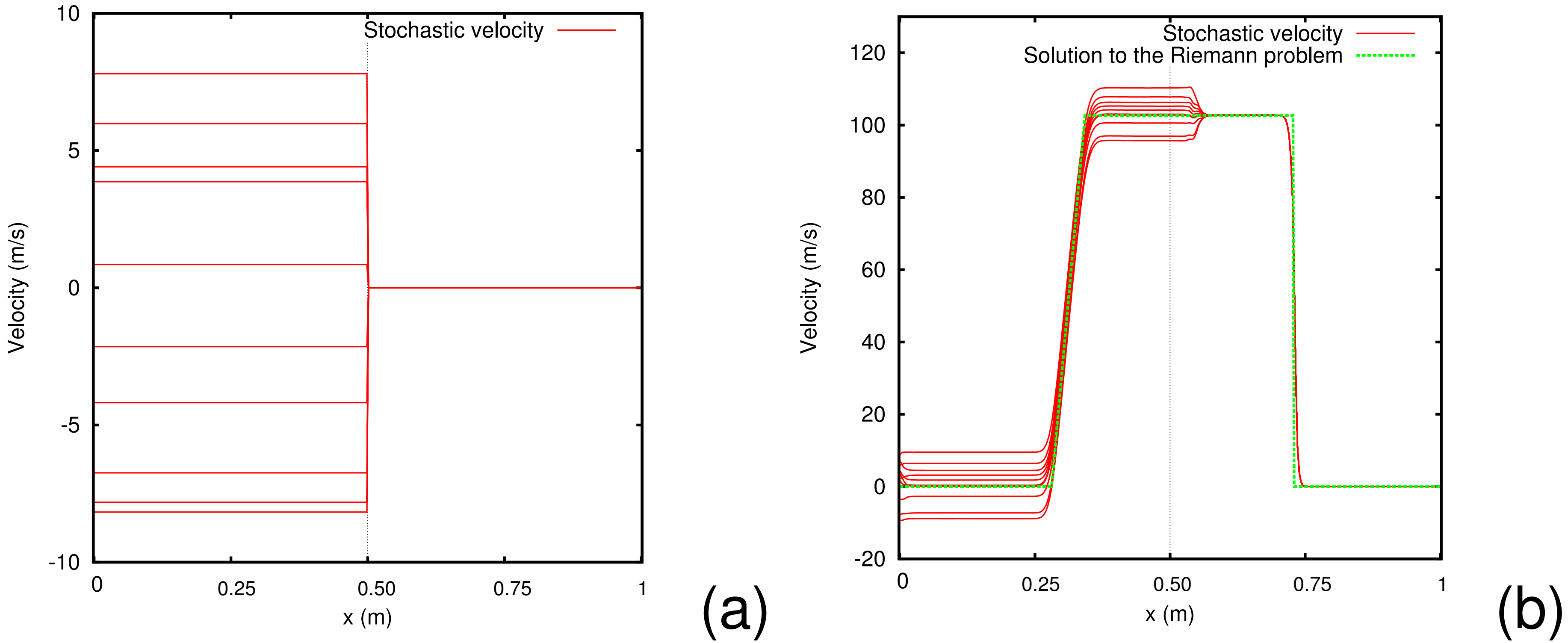
- Calculations are performed on a $L = 1\ m$ domain
  At initial time, the domain is divided into a left and a right state:

$$\text{for } x < 0.5m \quad \begin{cases} \widetilde{U}_L & = 0\ m/s \\ \widetilde{u''^2}_L & = 50\ m^2/s^2 \\ \langle\rho\rangle_L & = 0.729\ kg/m^3 \\ \overline{P}_L & = 10^5\ Pa \end{cases}$$

$$\text{for } x > 0.5m \quad \begin{cases} \widetilde{U}_R & = 0\ m/s \\ \widetilde{u''^2}_R & = 0\ m^2/s^2 \\ \langle\rho\rangle_R & = 0.456\ kg/m^3 \\ \overline{P}_R & = 5 \cdot 10^4\ Pa \end{cases}$$

- The turbulent frequency is taken equal to $\omega = 200\ s^{-1}$
- $N = 400$ stochastic fields and $N_x = 320$ cells are used

First test: Riemann problem (2/4)



First test: examples of stochastic velocity fields (a) at t=0 s and (b) at $t = 5 \cdot 10^{-4}\ s$

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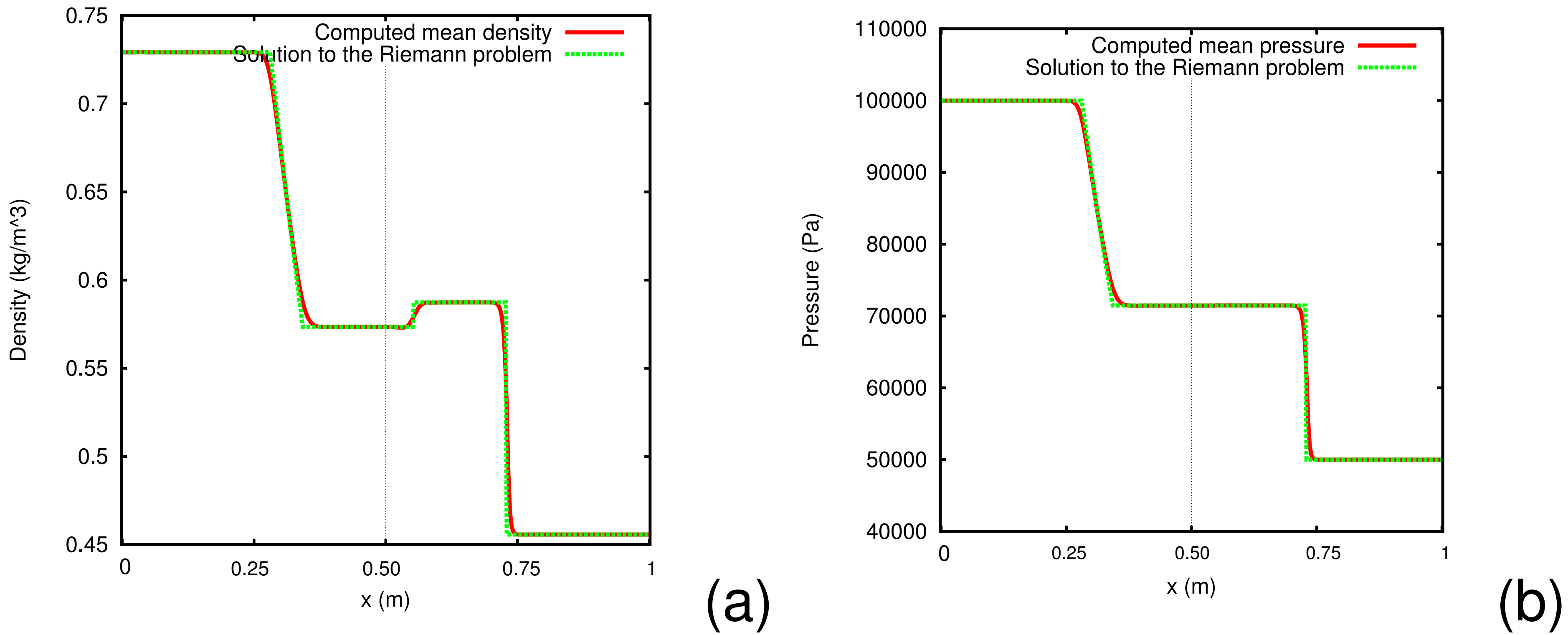
First test: Riemann problem (3/4)



First test: profiles of mean density (a), mean pressure(b) at

$$t = 5 \cdot 10^{-4}\ s$$

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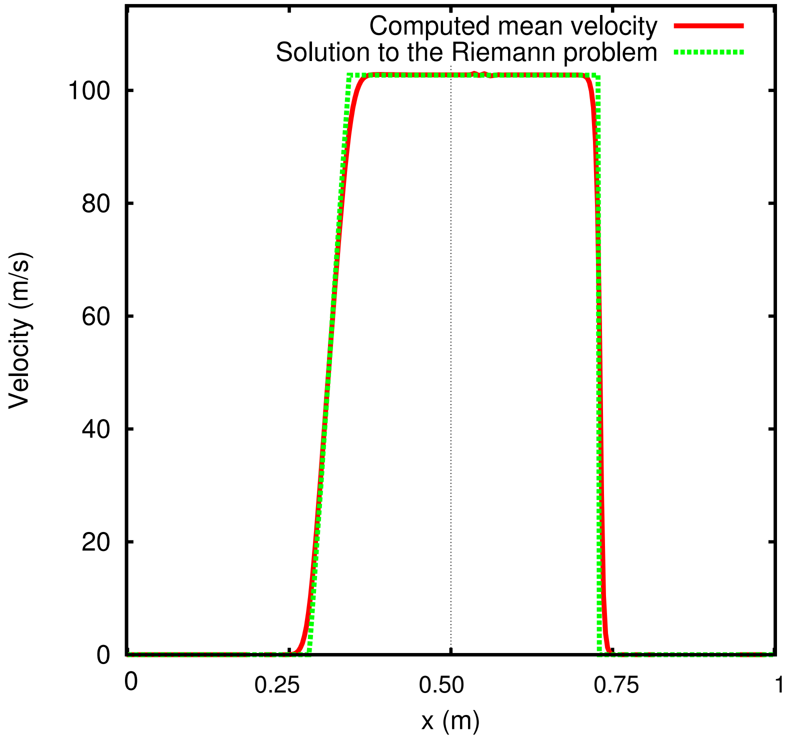
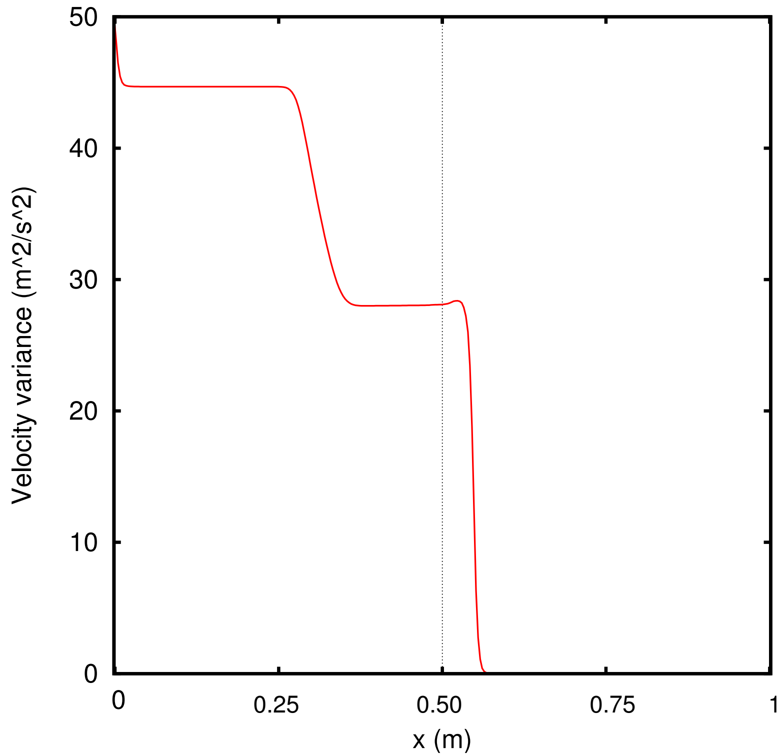
First test: Riemann problem (4/4)



(c)



(d)

First test: profiles of mean velocity (c) and velocity variance (d) at $t = 5 \cdot 10^{-4}\ s$. Mean profiles are compared against the exact solution to the Riemann problem

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Second test: Return to Gaussiannity (1/3)

- For this test only, we replace the Brownian coefficient by $\sqrt{2\omega\sigma^2}$ instead of $\sqrt{C_0\omega\widetilde{k}}$
  - → σ^2 is a constant and is taken equal to 1
  - → the velocity field PDF should tend to a Gaussian with variance σ^2
- At the left boundary: Dirac distributions are imposed, with means:

$$\widetilde{U} = 10.4m/s \ , \ \langle\rho\rangle = 0.146kg/m^3 \ , \ \overline{P} = 10^5 Pa$$

- At initial time, the stochastic fields are initialized with the left boundary conditions
- The domain has a length $L = 0.04m$ and is discretized with $N_x = 40$ cells
- The turbulent frequency is taken equal to $\omega = 2500s^{-1}$

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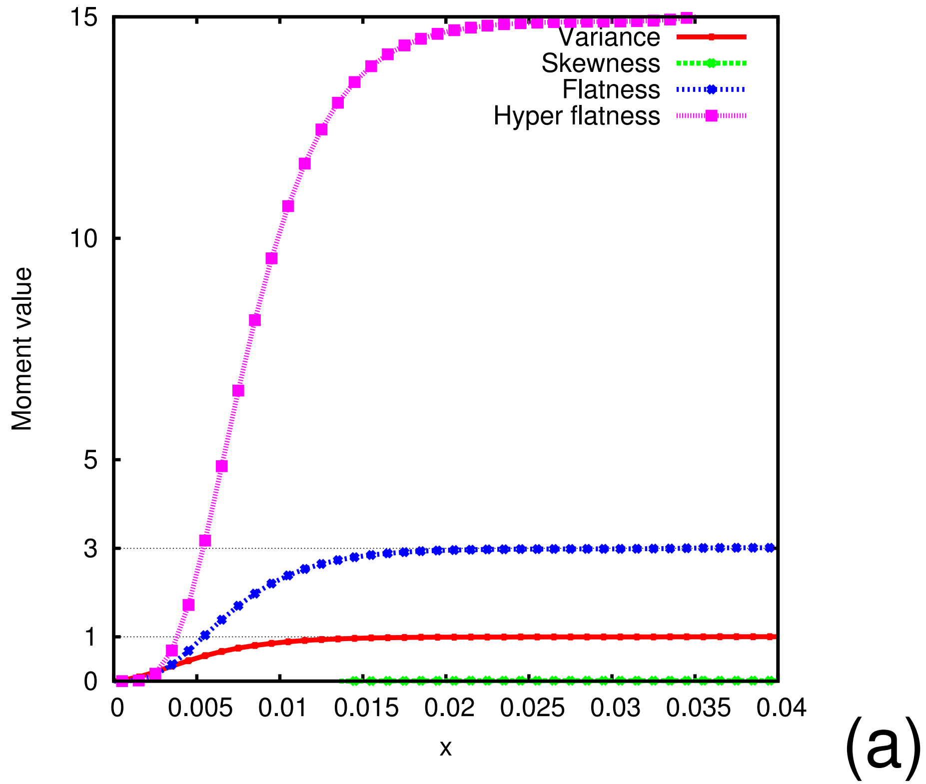
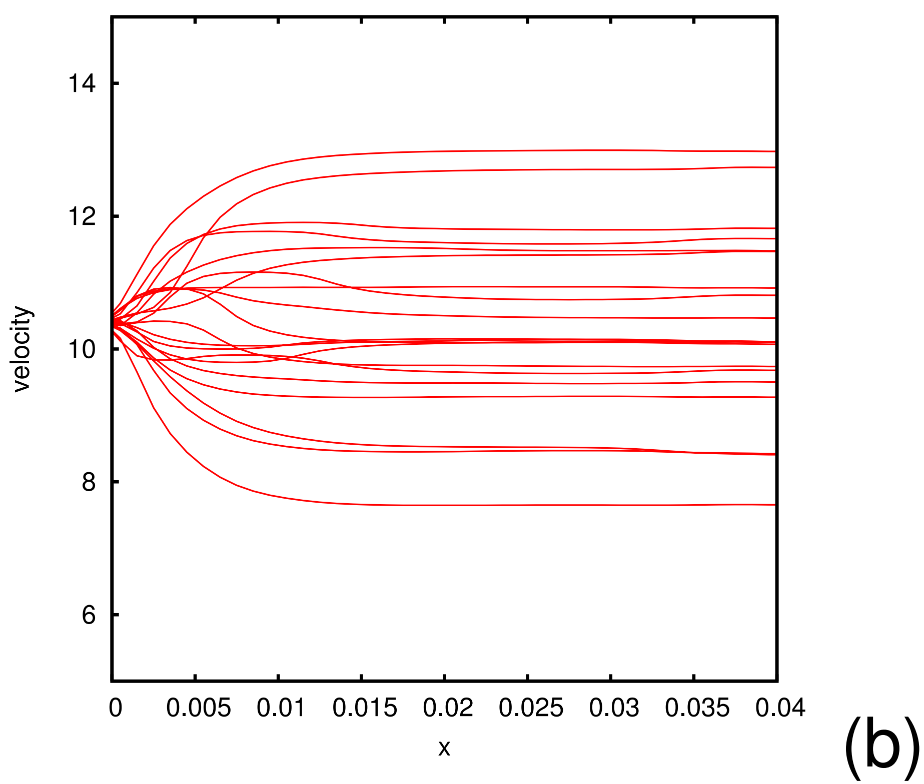
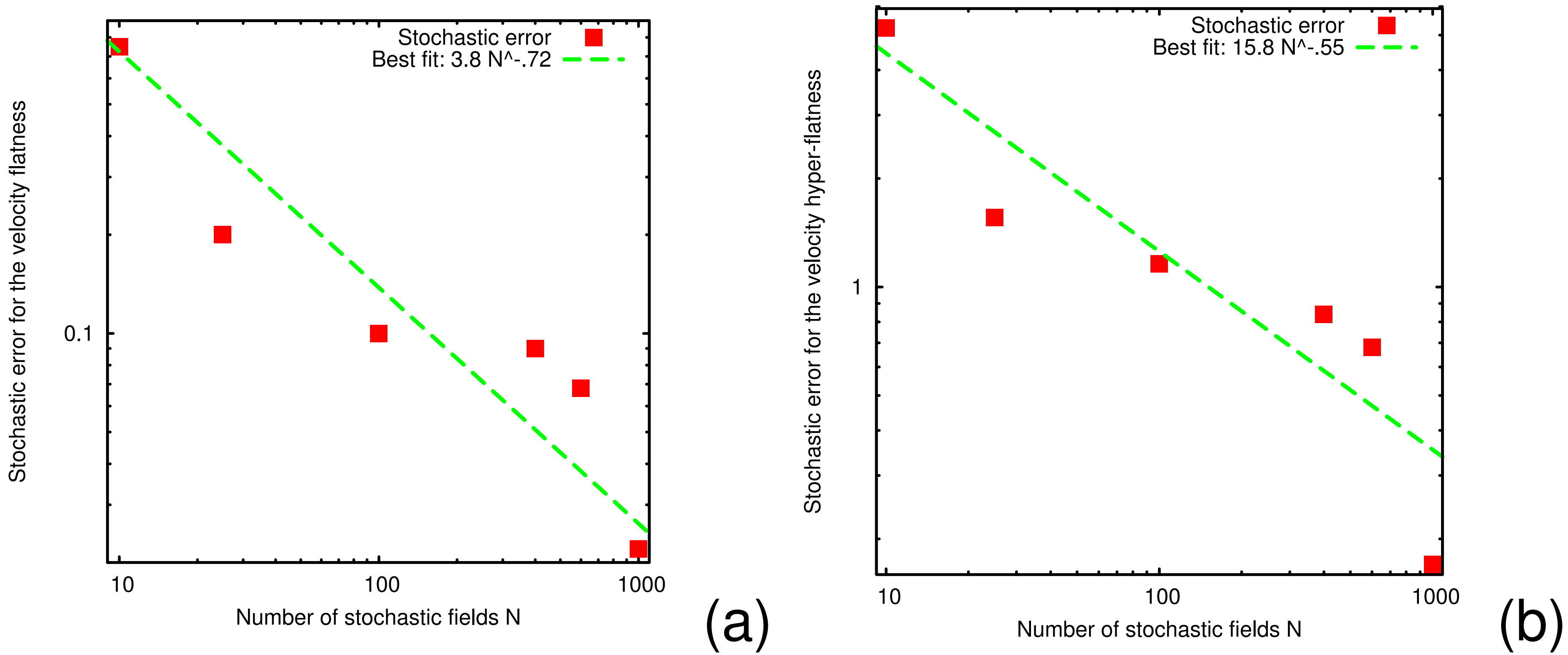
Second test: Return to Gaussiannity (2/3)





Second test: (a): evolution of the velocity variance,skewness,flatness and hyper-flatness ; (b) : stochastic velocity fields from which the moments are computed

Second test: Return to Gaussiannity (3/3)

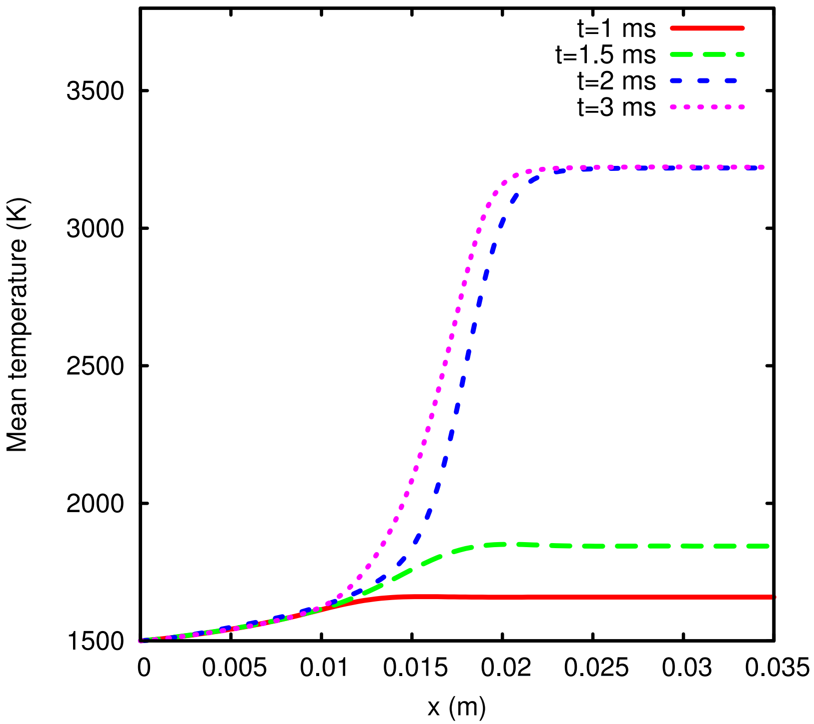


Second test : convergence rate for the velocity flatness (a) and hyper-flatness (b)

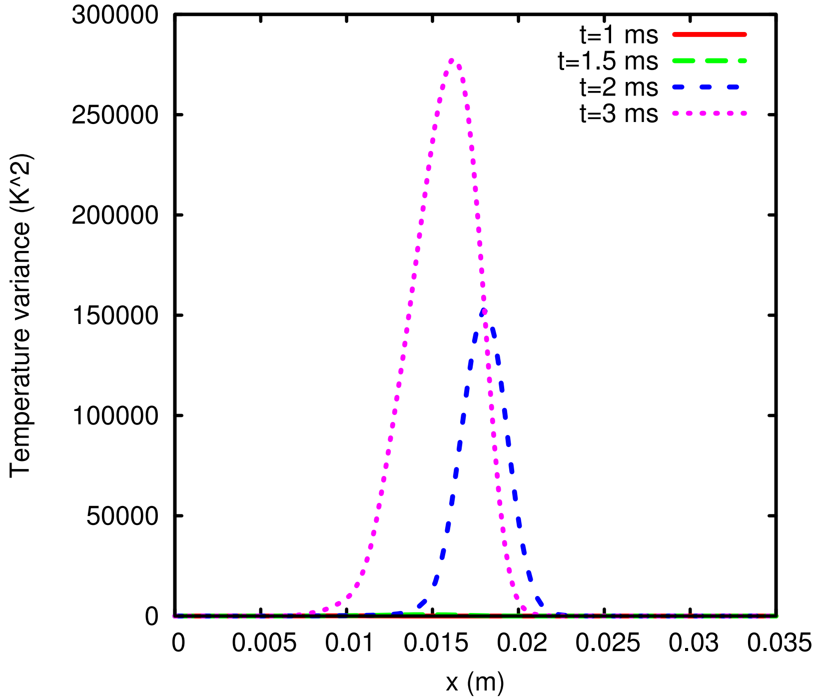
Third test: Auto-ignition (1/4)

- At inlet, a stoichiometric methane-air mixture is injected:
  - ➞ temperature $T_{in} = 1500K$
  - ➞ pressure $P_{in} = 100000Pa$
  - ➞ Gaussian random velocity with $\widetilde{U}_{in} = 10.4ms^{-1}$ and variance $\widetilde{u"^2}_{in} = 1\ m^2 s^{-2}$
- At outlet, zero gradients, except for the pressure which value is fixed at P_{in}
- The length of the 1D domain is $L = 0.035\ m$
- The methane-air chemistry is dealt with a simple one step global reaction (Westbrook, 1984)

Third test: Auto-ignition (2/4)



(a)



(b)

Third test: Time evolution of the profiles of the mean (a) and variance (b) of the temperature

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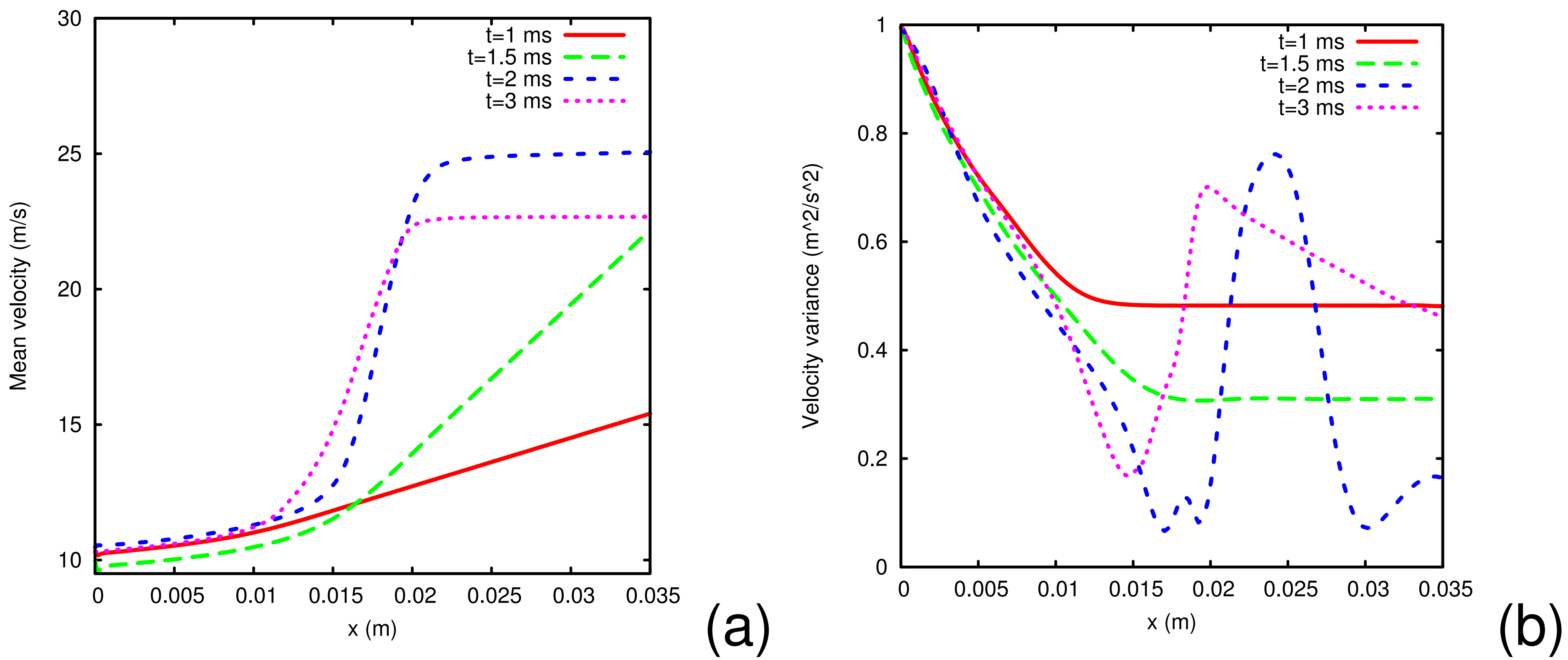
Third test: Auto-ignition (3/4)



Third test: Time evolution of the profiles of the mean (a) and variance (b) of the velocity

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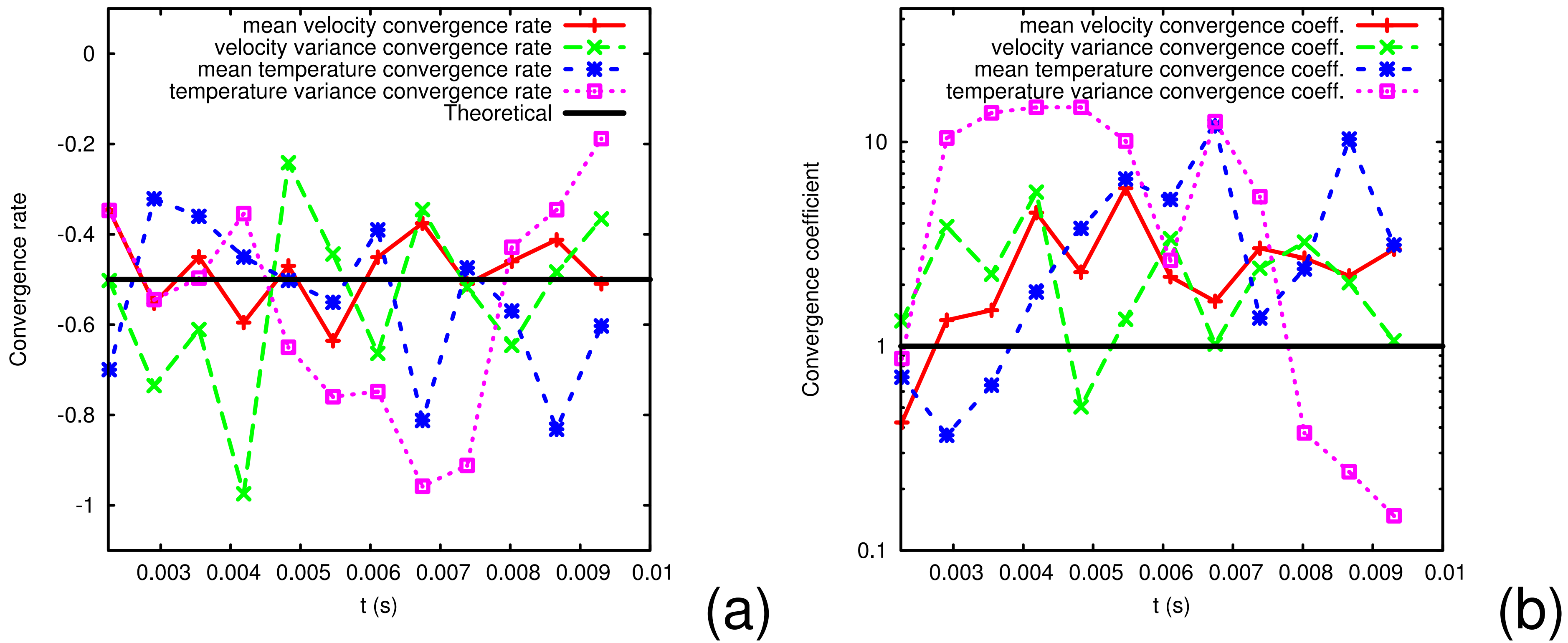
Third test: Auto-ignition (4/4)



Third test: Time evolution of the convergence rates (a) and coefficients (b) for the means and variances of velocity and temperature

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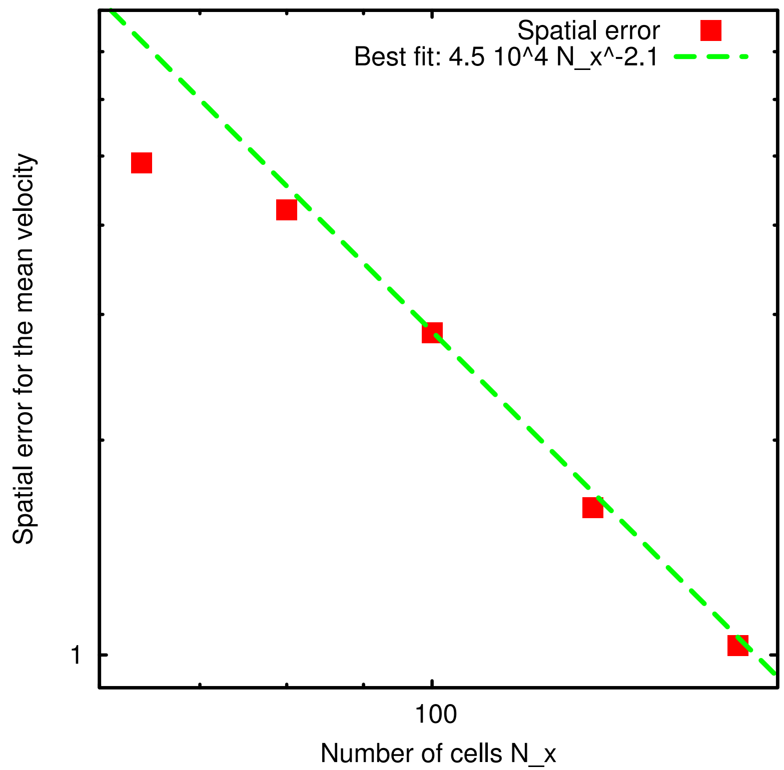
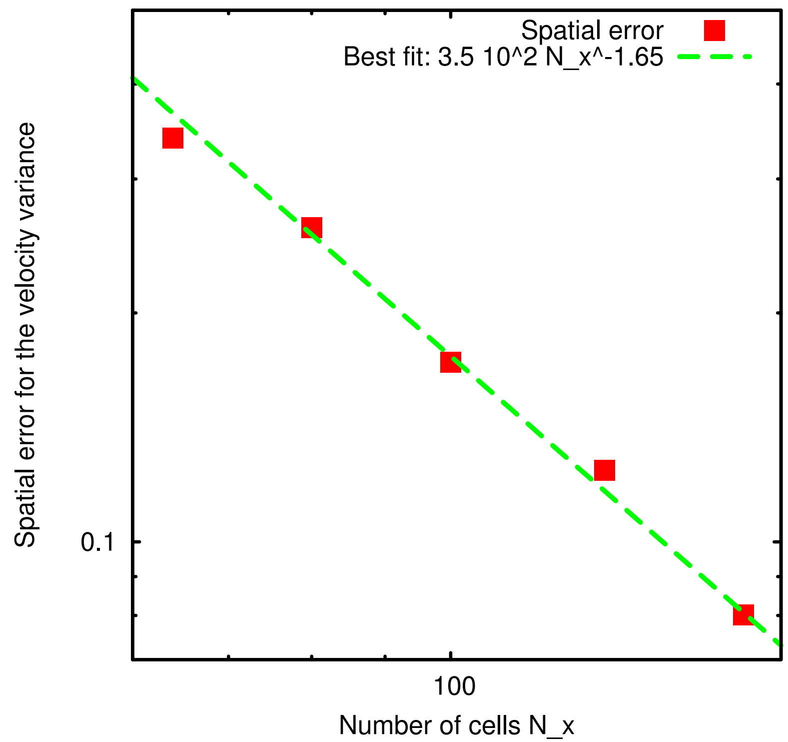
Third test: Auto-ignition



(a)



(b)

Third test: Spatial convergence of the mean (a) and variance (b) of the velocity at $t = 2.5ms$

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Conclusions for Part II

- A numerical scheme for solving the SPDEs obtained in Soulard and Sabel'nikov has been proposed
  - → finite volume scheme based on a monotone centered second order numerical flux
  - → new weak second order Runge-Kutta scheme, whith the SSP property, and an implicit treatment of chemical source terms (S-IMEX)
- 1D validation tests have been performed
  - → Monotonicity was verified on a Riemann problem
  - → Return to Gaussiannity was also checked
  - → An auto-ignition problem was studied
- Further developments of this work :
  - → extension of the numerical method to 2D problems
  - → calculation of a practical cases

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