

Groupe de travail « Schémas de Boltzmann sur réseau » — 24 février 2021.

LBM – reactive flows

P. Boivin (et al. surtout)

Outline

- ❖ Part I : M2P2 & me...
- ❖ Part II : LBM : price & prejudices
- ❖ Part III : LBM & reactive flows (theory)
- ❖ Part IV : Validations (academic & benchmarks)
- ❖ Part V: Towards complex configurations
- ❖ Part VI : Discussion, perspectives



M2P2

- ❖ ~40 EC+C (permanent staff)
- ❖ 3 tutelles, 2 sites: Ecole Centrale Marseille & Arbois
- ❖ Membre Fédération Fabri de Peiresc (IRPHE, IUSTI, LMA)
- ❖ Membre de l’Institut de Mécanique et d’Ingénierie (Idex Marseille)
- ❖ 6 équipes de recherches en mécanique et génie des procédés
- ❖ TONIC: Thermodynamique, Ondes, Numérique, Instabilités, Combustion.
7 permanents, 2 émérites.
- ❖ Financement industriel ~ 80%.

About me...



Since 2016 : CNRS research fellow

2014-2016: Post-doctoral studies

2012-2013: Snecma (Vernon)

2009-2011: PhD - UC3M (Madrid)

2007-2008: PSA (Vélizy)

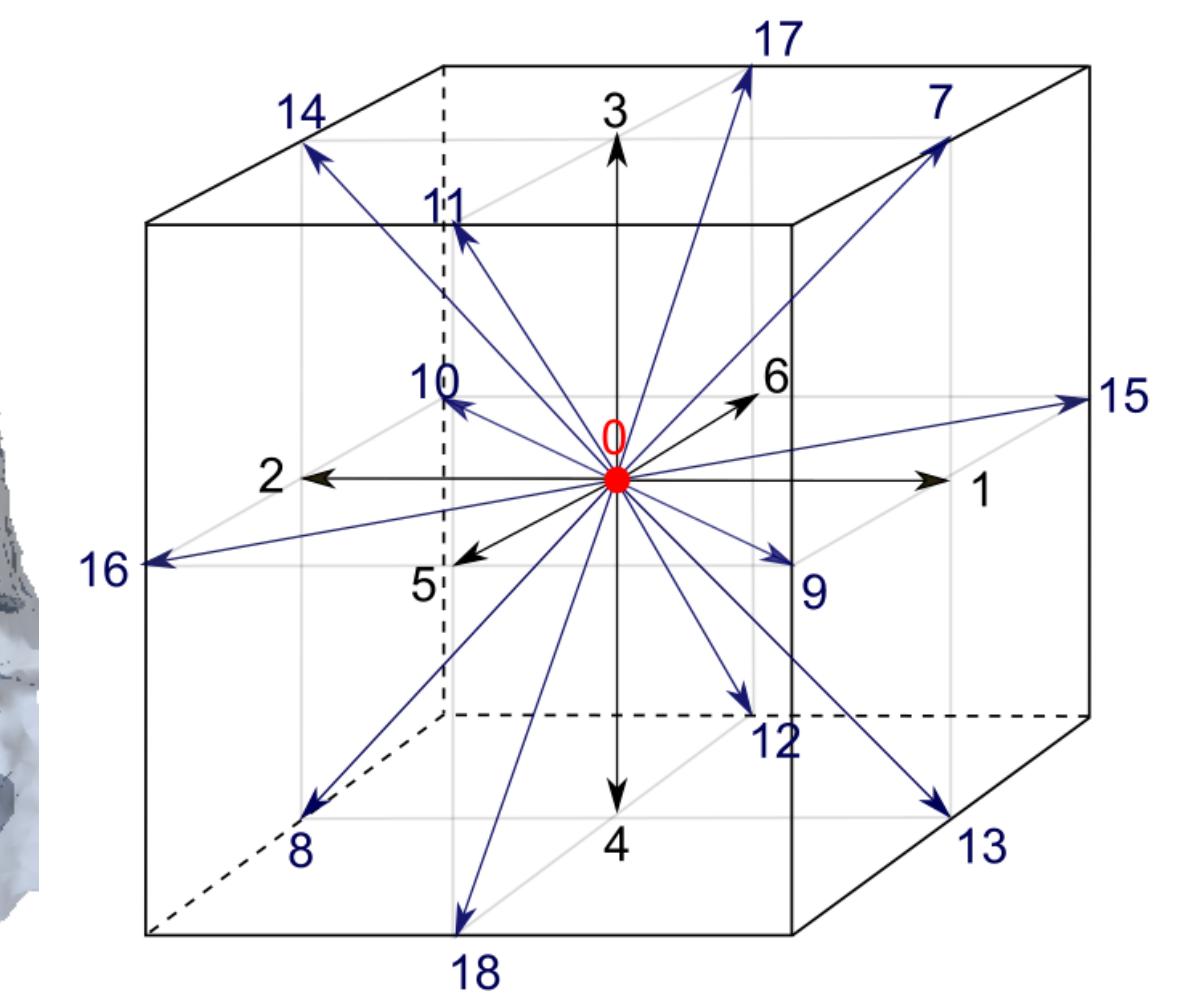
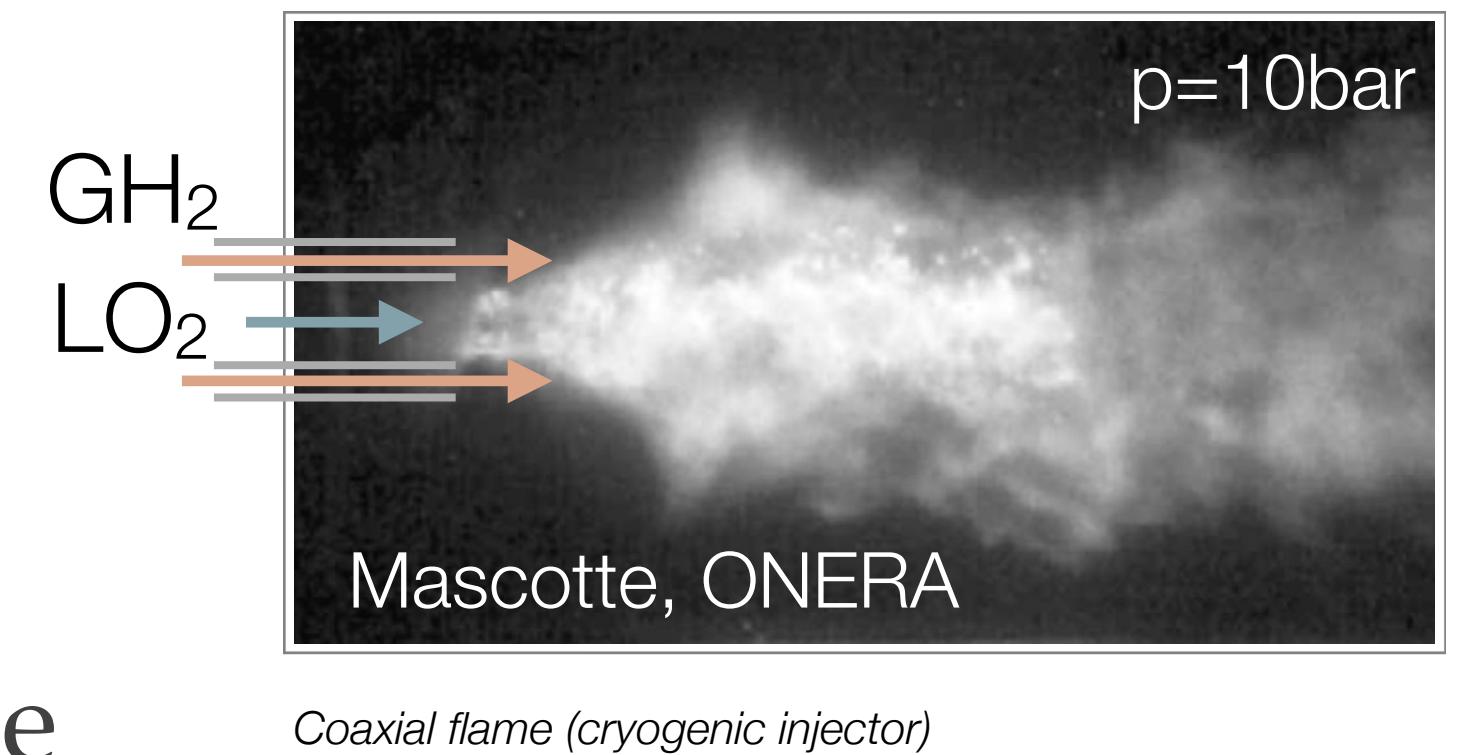
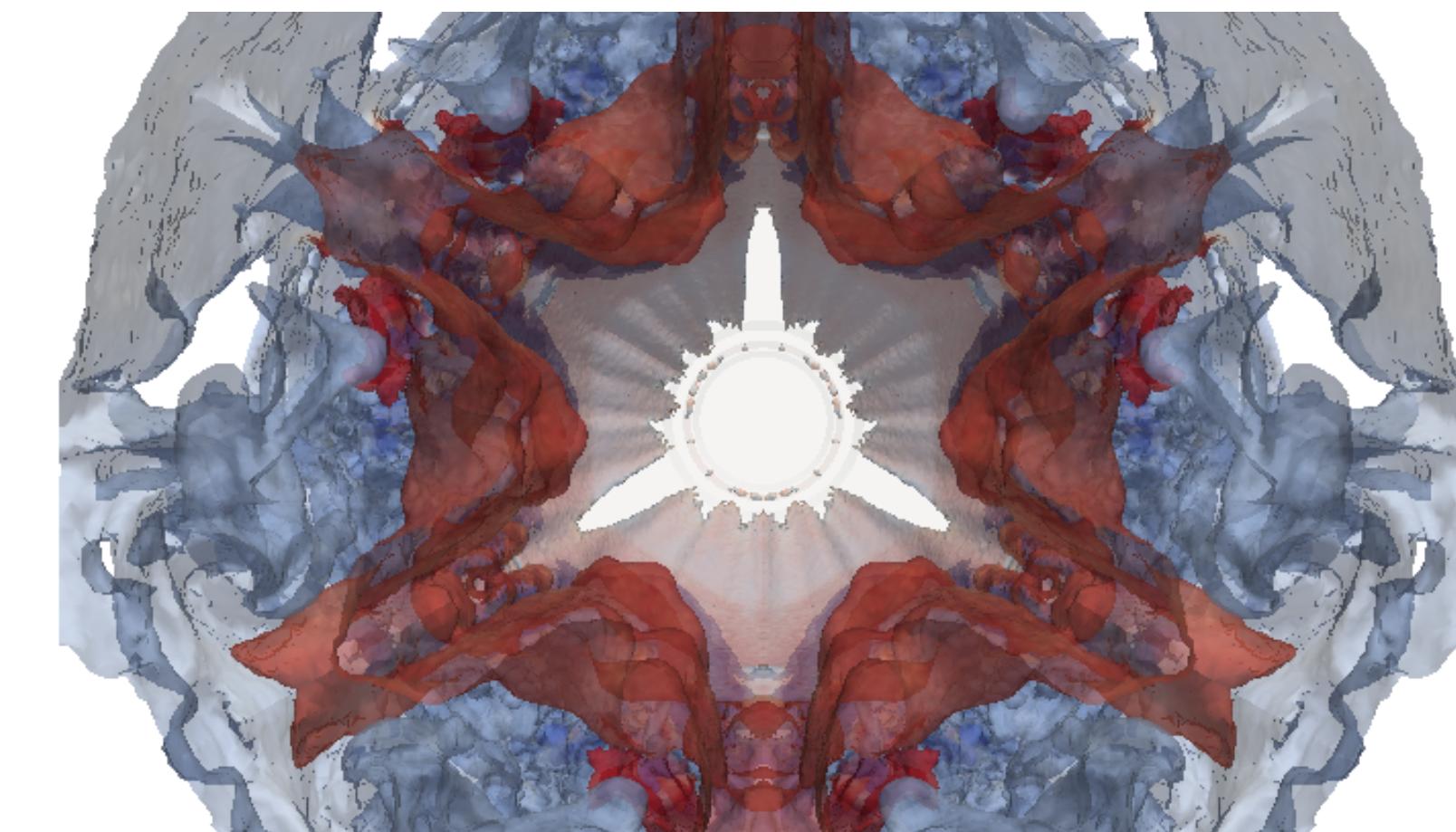
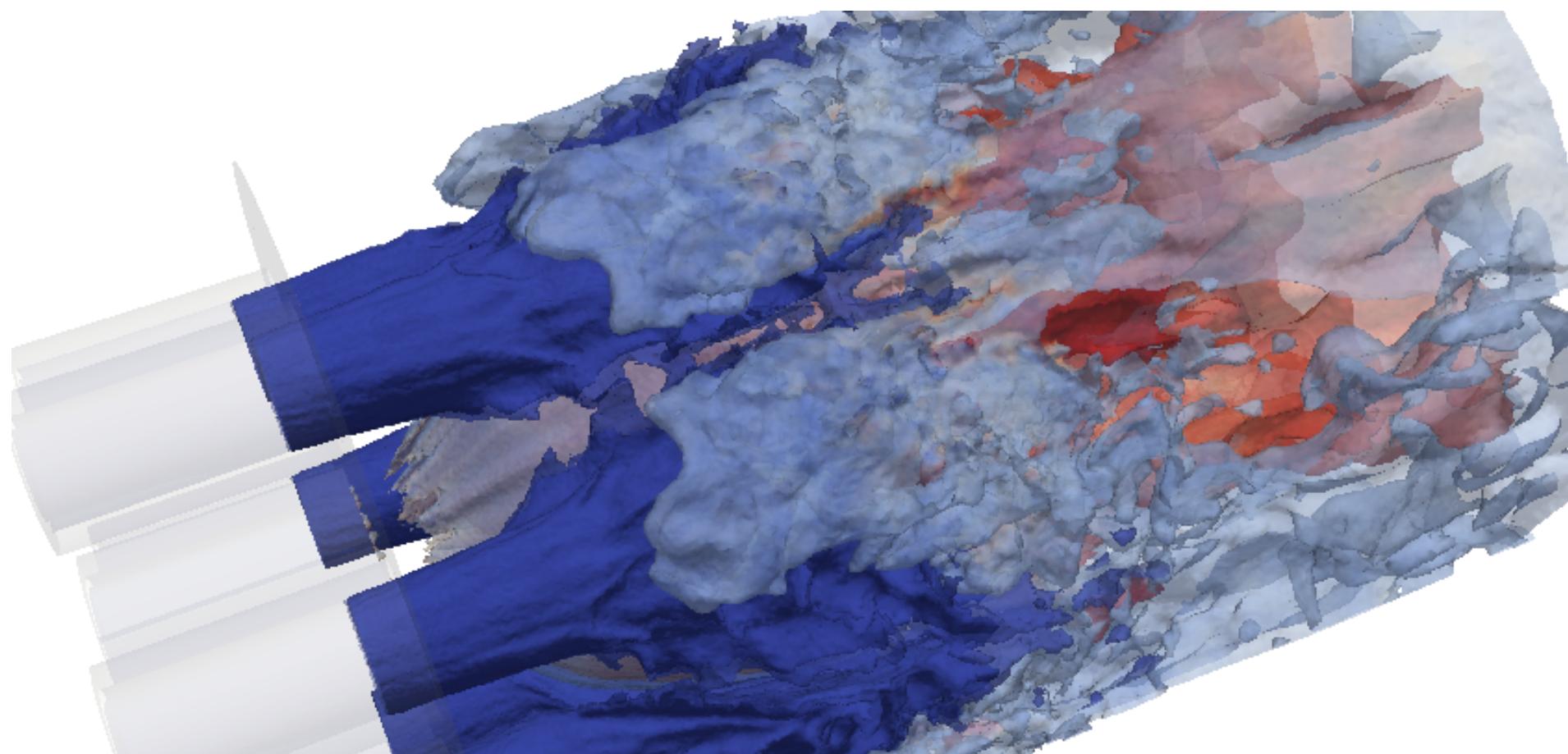
2006-2007: KTH (Stockholm)

2003-2007: Ecole Polytechnique

- ❖ TONIC team leader
- ❖ CR @ M2P2
- ❖ CNES + ANR
- ❖ UC3M
- ❖ Cryogenic engines
- ❖ Ignition specialist
- ❖ PhD *cum laude*
- ❖ MSc thesis
- ❖ Double degree
- ❖ Diplôme d'ingénieur

Main research lines

- ❖ Difficulty in developing methods able to encompass both multiphase (including a dense part) and reactive flows
 - ❖ Multiphase & reactive flows have evolved in separate disciplines
 - ❖ Development of thermodynamics & kinetics model simple enough for use in practical applications

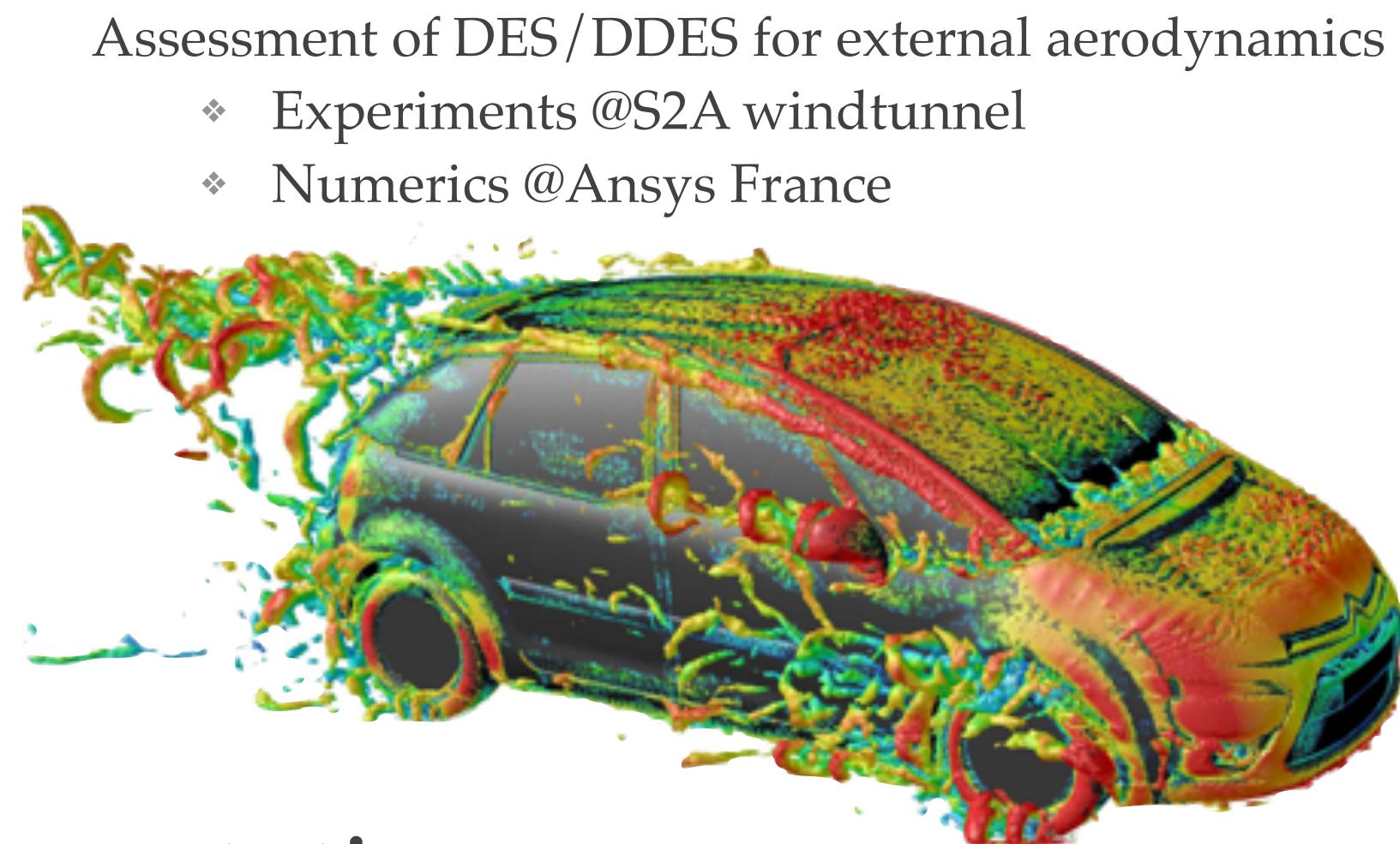


Outline

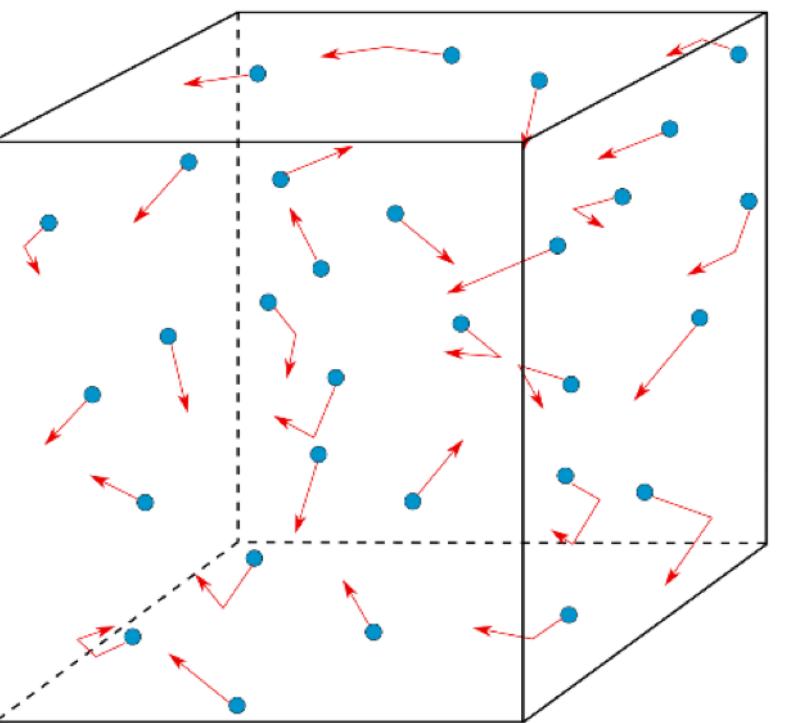
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A short & naive history of LBM

- ❖ Hard to work on real geometries:
meshing can take up to 3 weeks.
- ❖ Coding and scaling NS codes is tedious
- ❖ Powerflow came up ~2007 at PSA, doing « free » computations
- ❖ Now (2015!) claims to have 85% market share on car aerodynamics
- ❖ Expensive > ProLB, French consortium including AMU, Renault, Airbus...
.... and co-developed at M2P2



LBM - principles



Lattice Boltzmann equation

$$\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta} + F_\beta \frac{\partial f}{\partial \xi_\beta} = \Omega(f)$$

$$-\frac{1}{\tau}(f - f^0)$$

BGK

Maxwell-Boltzmann distribution function

$$f^{(0)} = \frac{\rho}{(2\pi c_T^2)^{D/2}} \exp\left(\frac{-(\vec{\xi} - \vec{u})^2}{2c_T^2}\right)$$

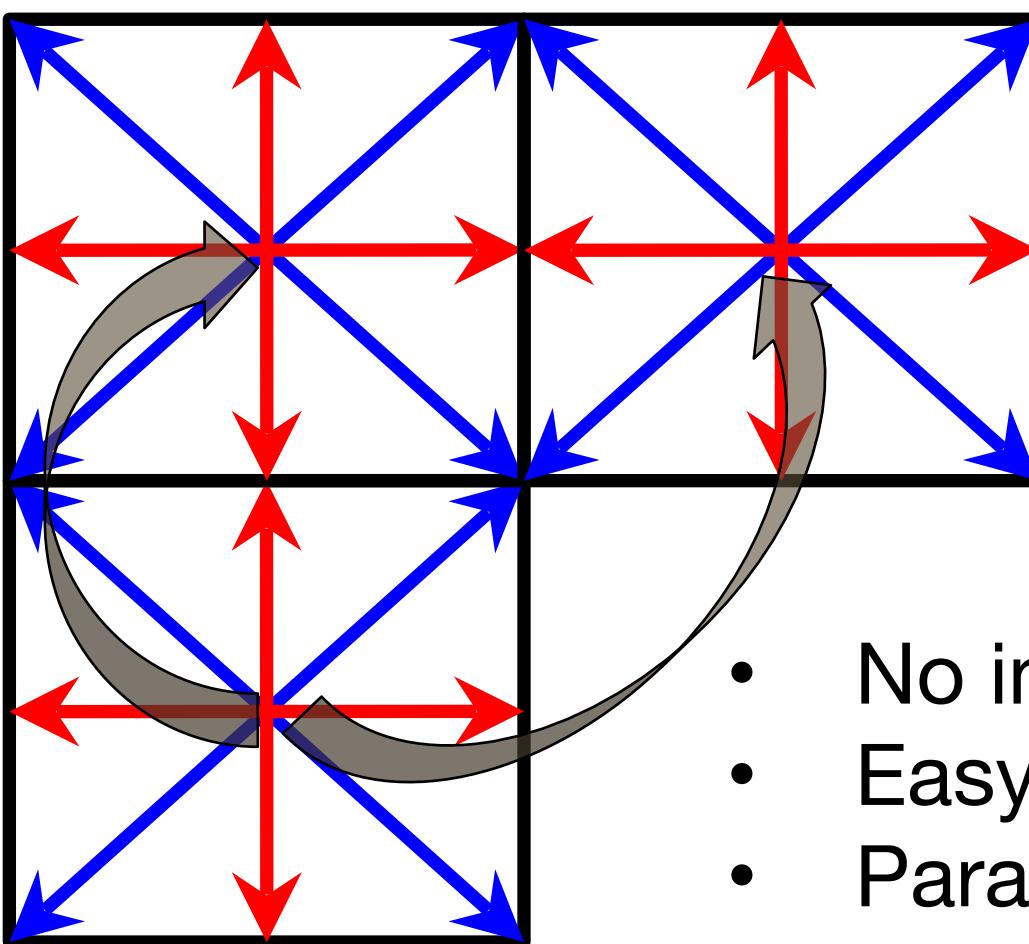
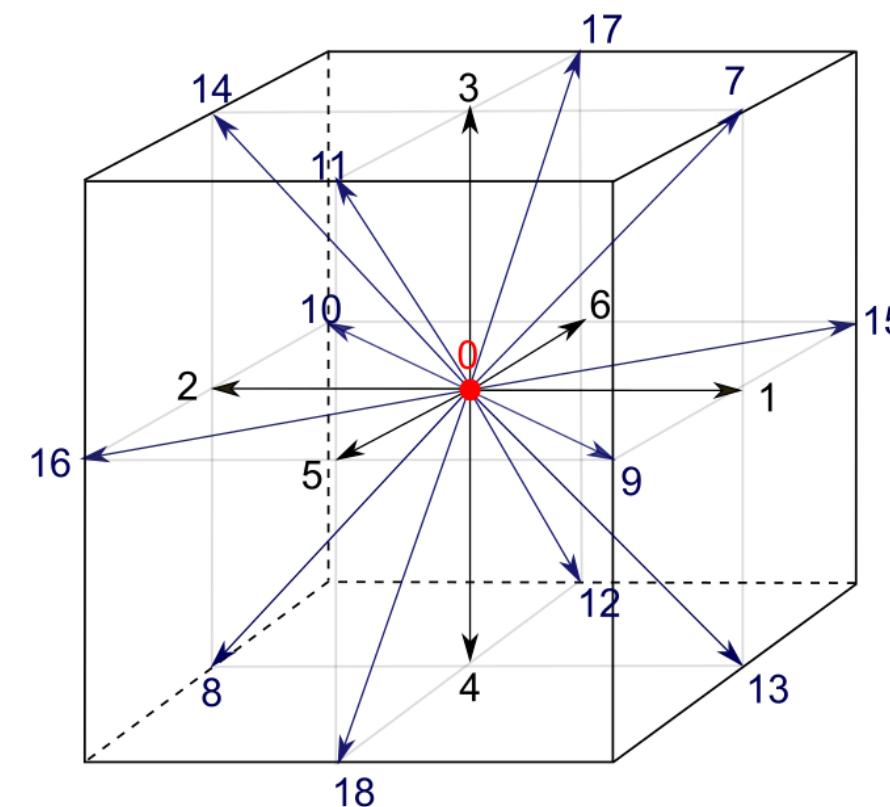
Continuum-statistical variables

$$\rho(x, t) \equiv mn(x, t) = m \int f dv$$

$$\rho u(x, t) = m \int fv dv$$

$$\rho e(x, t) = \frac{1}{2}m \int f \underbrace{|v - u|}_c dv$$

LBM - principles



- No interpolation (in transport)
- Easy to code
- Parallel Computing

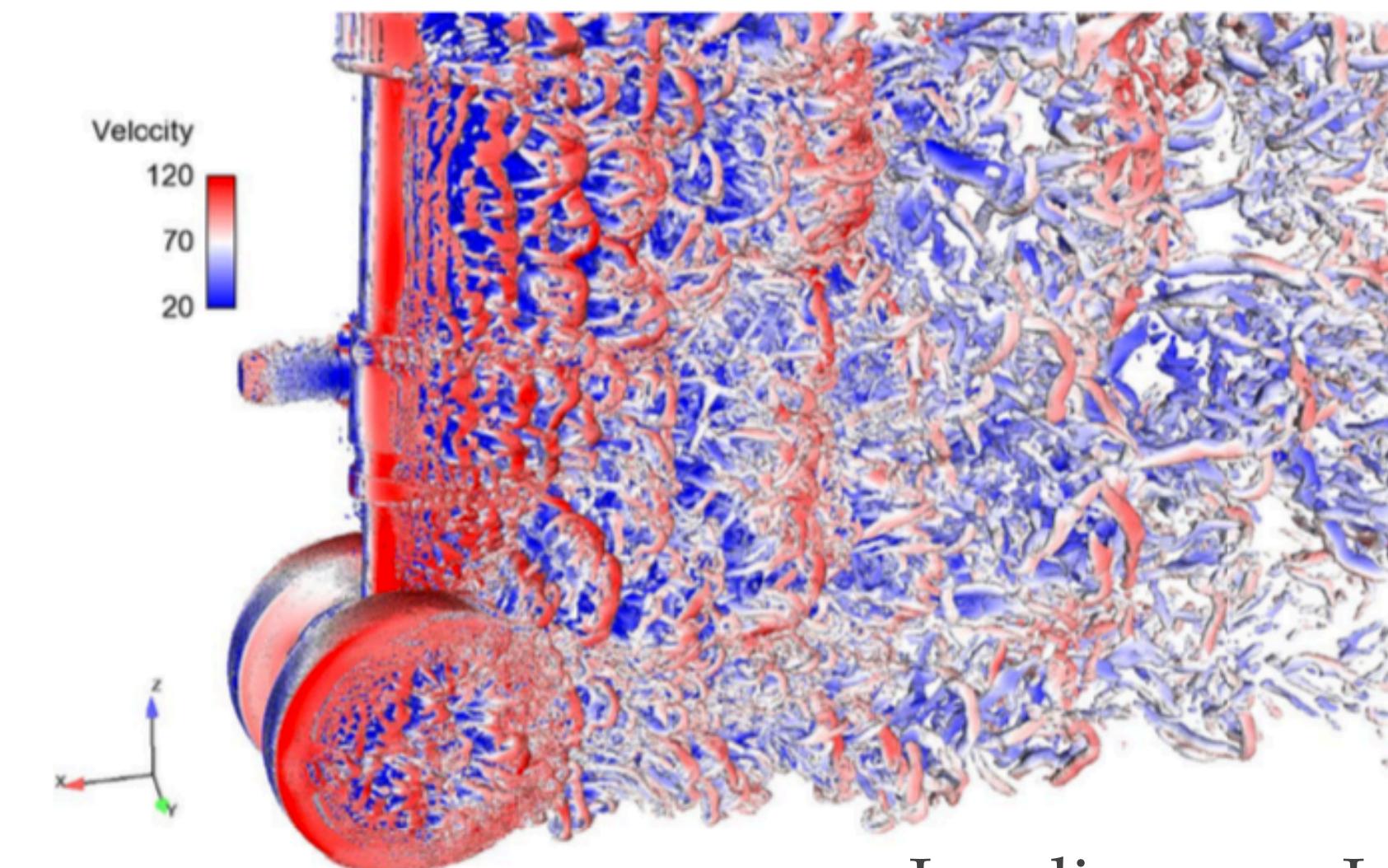
Lattice Boltzmann equation

$$f_i(\mathbf{x} + \mathbf{c}\delta t, t + \delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau} [f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)]$$

Streaming Collision

Maxwell-Boltzmann distribution function

$$f_i^{eq} = \rho w_i \left[1 + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2} \right]$$



But...

$$p = \rho \cdot c_s^2$$

Classical (athermal) LBM only solves mass & momentum equations...

Some prejudices about LBM for combustion

- ❖ LBM is for rarefied gases and the Chapman Enskog expansion is dubious, so why bother ?
- ❖ Extending LBM to multicomponent requires many distributions
 - > can become stringent in terms of memory usage
- ❖ The expensive part of a NS solver is computing combustion related quantities (diffusion / kinetics / ...).
- ❖ From the last point, one could infer that the same could be obtained with an octree cartesian NS solver.

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Combustion - macroscopic equations

Macroscopic equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\beta}{\partial x_\beta} = 0$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta + p \delta_{\alpha\beta} - \mathcal{T}_{\alpha\beta}}{\partial x_\beta} = 0$$

$$\rho \frac{\partial h}{\partial t} + \rho u_\alpha \frac{\partial h}{\partial x_\alpha} = \frac{Dp}{Dt} - \frac{\partial q_\alpha}{\partial x_\alpha} + \mathcal{T}_{\alpha\beta} \frac{\partial u_\alpha}{\partial x_\beta}$$

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_\alpha \frac{\partial Y_k}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha} (-\rho Y_k V_{k,\alpha}) + \dot{\omega}_k$$

Thermodynamic closure

$$p = \rho \bar{r} T$$

$$\bar{r} = R/\bar{W}$$

$$h = \sum_{k=1}^N h_k Y_k, \quad h_k = \int_{T_0}^T C_{p,k}(T) dT + \Delta h_{f,k}^0$$

Viscous term

$$\mathcal{T}_{\alpha\beta} = \rho \nu \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \delta_{\alpha\beta} \frac{2}{3} \frac{\partial u_\gamma}{\partial x_\gamma} \right)$$

$$\mu = \mu_0 \left(\frac{T}{T_0} \right)^\beta$$

Diffusion terms

$$V_{k,\alpha} = - D_k \frac{\partial X_k}{\partial x_\alpha} \frac{W_k}{\bar{W}} + V_\alpha^c Y_k \quad D_k = \frac{\mu}{\rho S c_k}$$

$$V_\alpha^c = \sum_{k=1}^N D_k \frac{\partial X_k}{\partial x_\alpha} \frac{W_k}{\bar{W}} \quad \lambda = \frac{\mu}{Pr} \sum_{k=1}^N Y_k C_{p,k}$$

$$q_\alpha = -\lambda \frac{\partial T}{\partial x_\alpha} + \rho \sum_{k=1}^N h_k Y_k V_{k,\alpha}$$

Fully defined provided

- EOS given (NASA polynomials)
- $S c_k$ provided for each species
- Pr provided
- $\mu(T)$ law given
- $\dot{\omega}_k$ given via kinetic scheme

LBM - Multi-physics

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot [\rho \nu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)]\end{aligned}$$

→ **LBM**

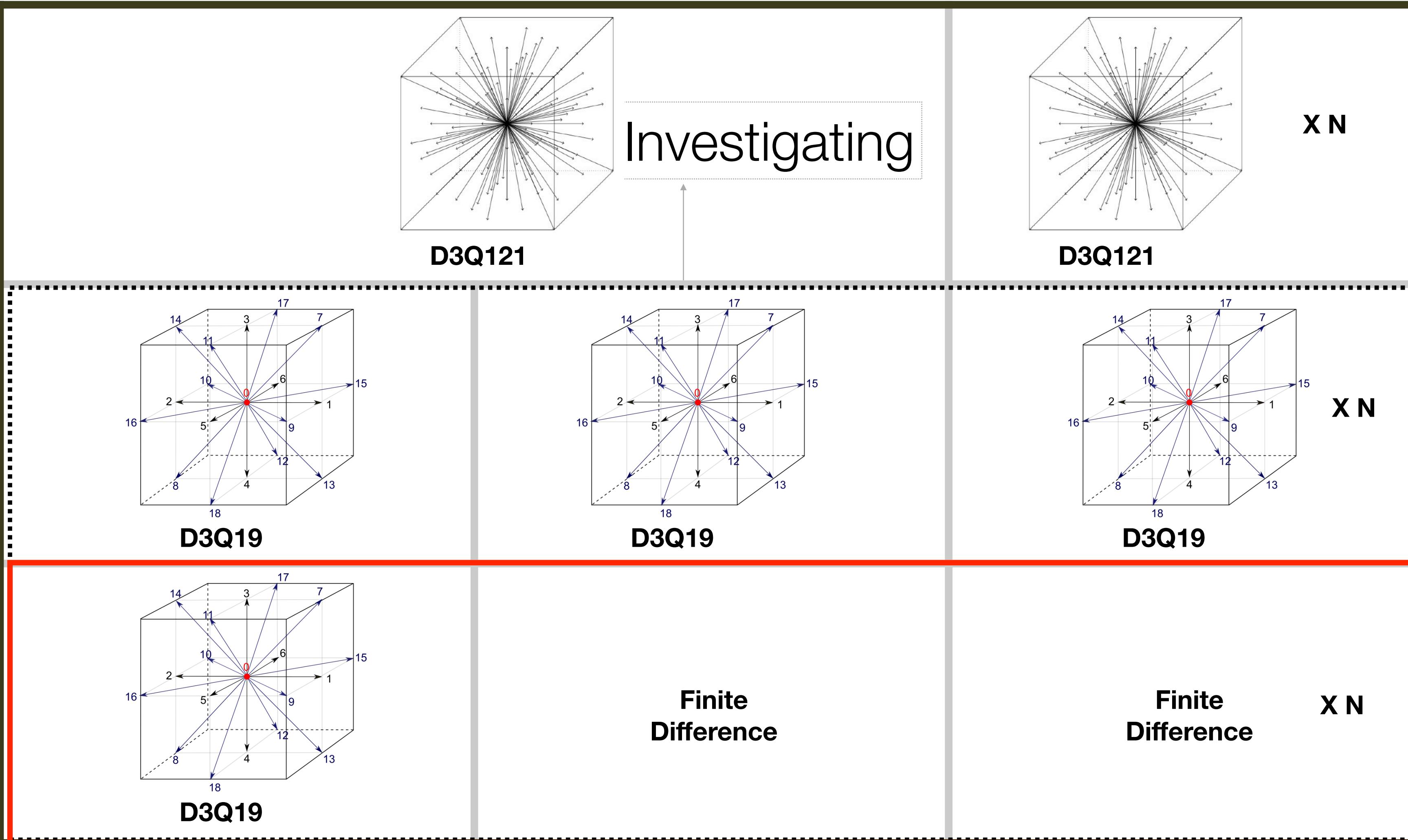
+

$$\begin{aligned}\frac{\partial T}{\partial t} + u_\alpha \frac{\partial}{\partial x_\alpha} T &= \frac{1}{\rho} \frac{\partial}{\partial x_\alpha} (\rho D_T \frac{\partial T}{\partial x_\alpha}) + \frac{\omega_h}{\rho c_p} \\ \frac{\partial Y_k}{\partial t} + u_\alpha \frac{\partial}{\partial x_\alpha} Y_k &= \frac{1}{\rho} \frac{\partial}{\partial x_\alpha} (\rho D_k \frac{\partial Y_k}{\partial x_\alpha}) + \frac{\omega_k}{\rho}\end{aligned}$$

→ **???**

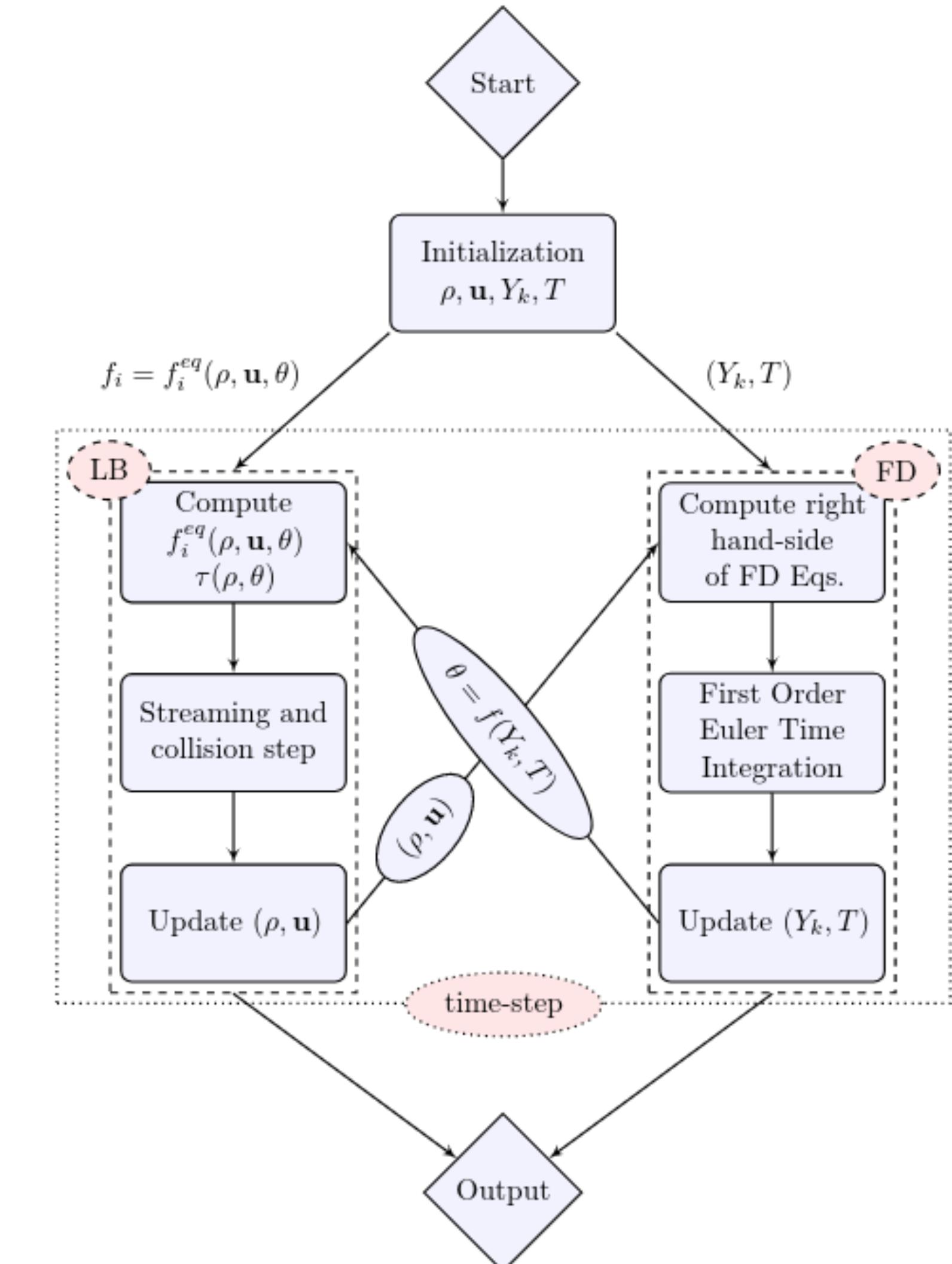
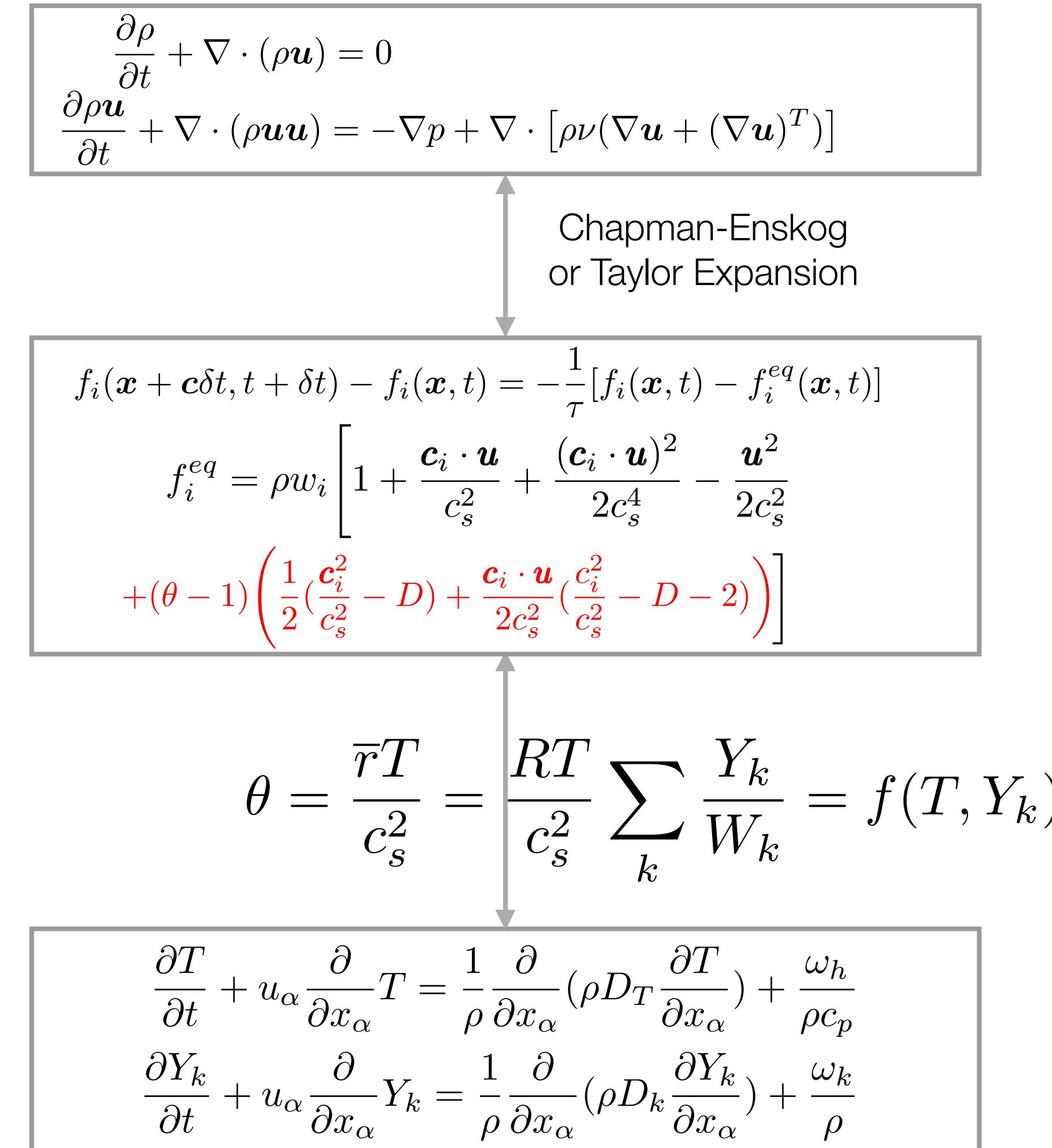
Possible Strategies

Mass/Momentum



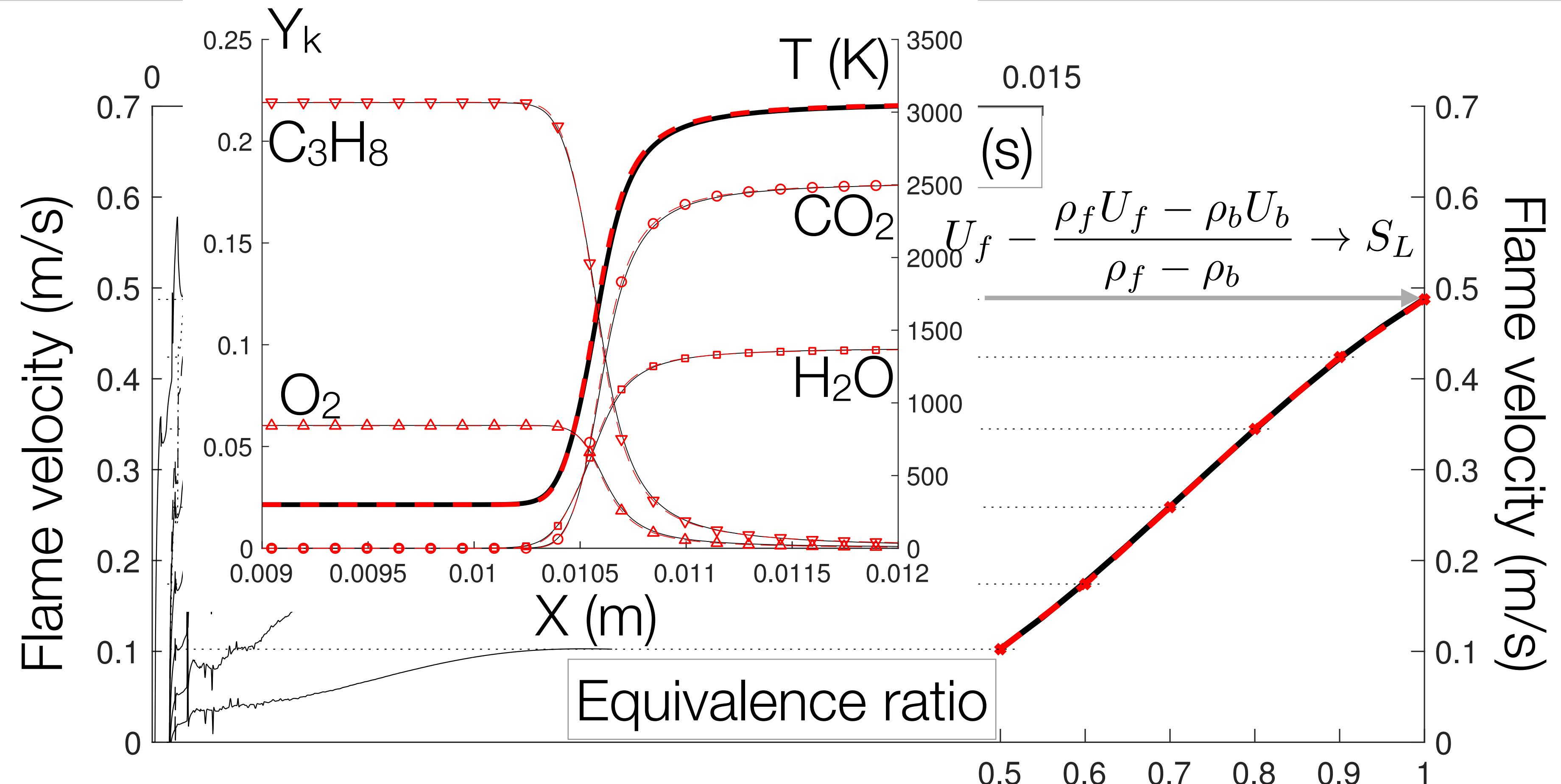
Hybrid LBM (v1: density - based)

- ❖ Mass conservation
- ❖ Momentum conservation

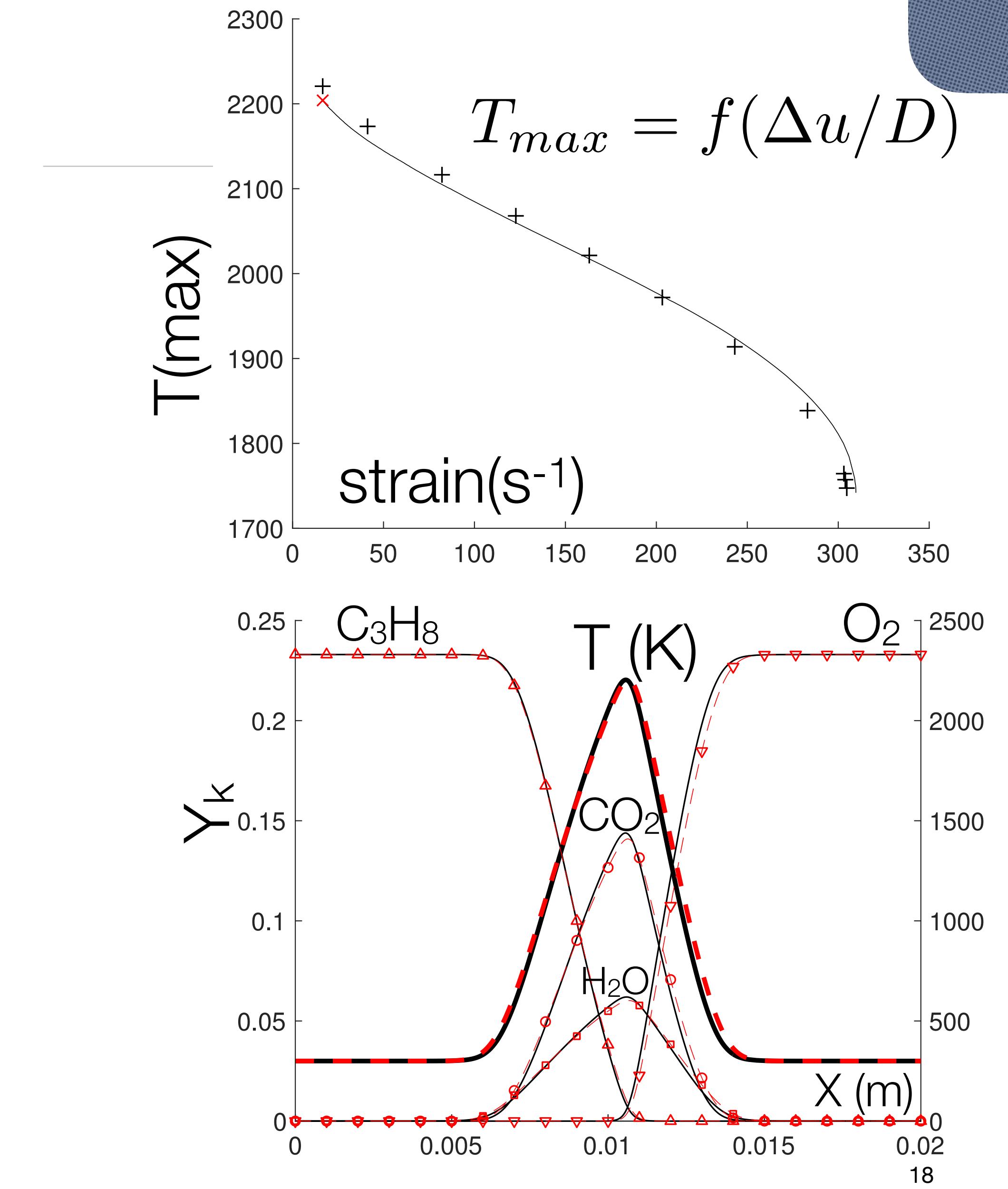
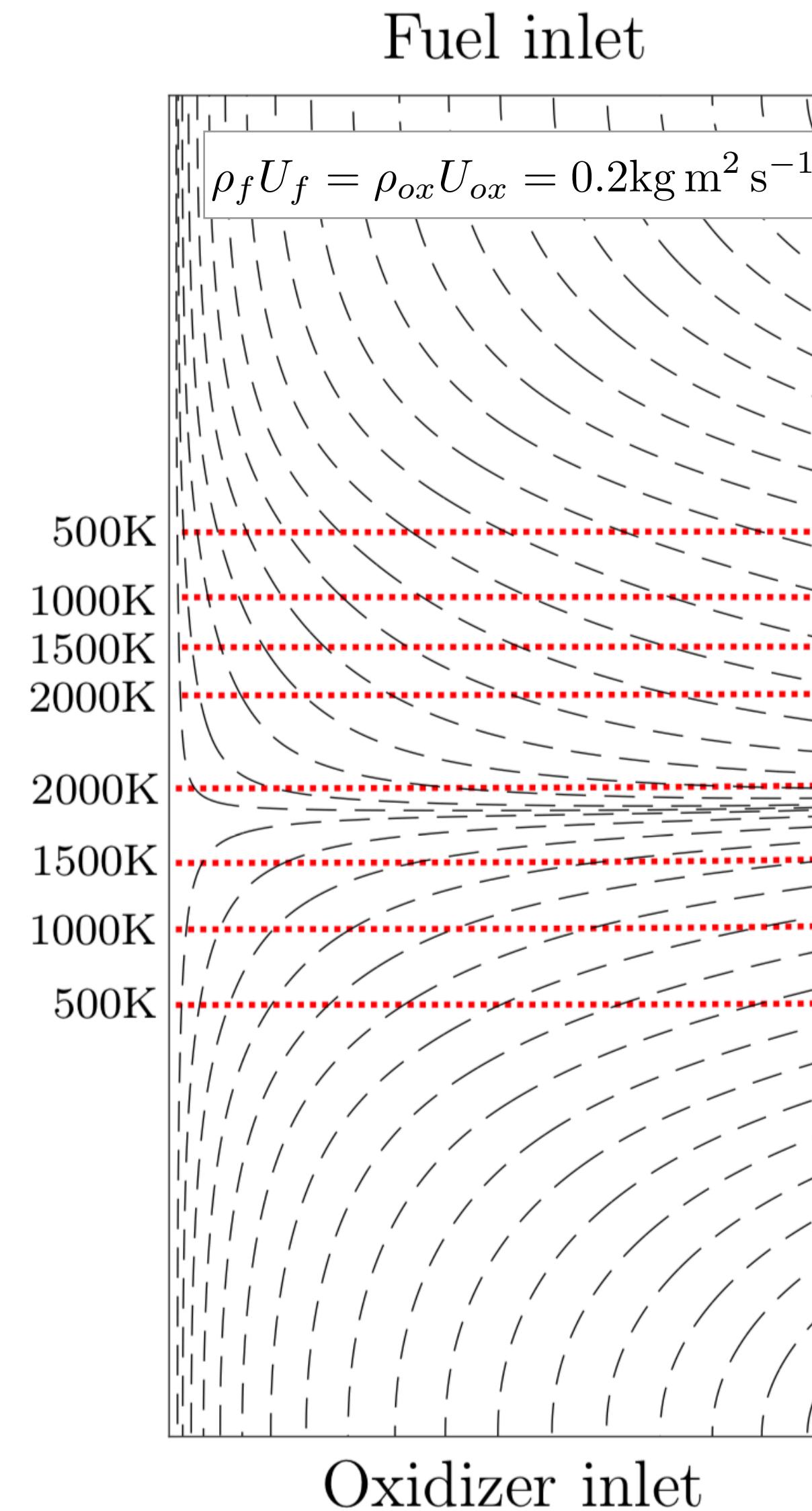


- ❖ Energy conservation
- ❖ Species conservation

Successes with v1: premixed flame.



Diffusion flame



Going more complex...

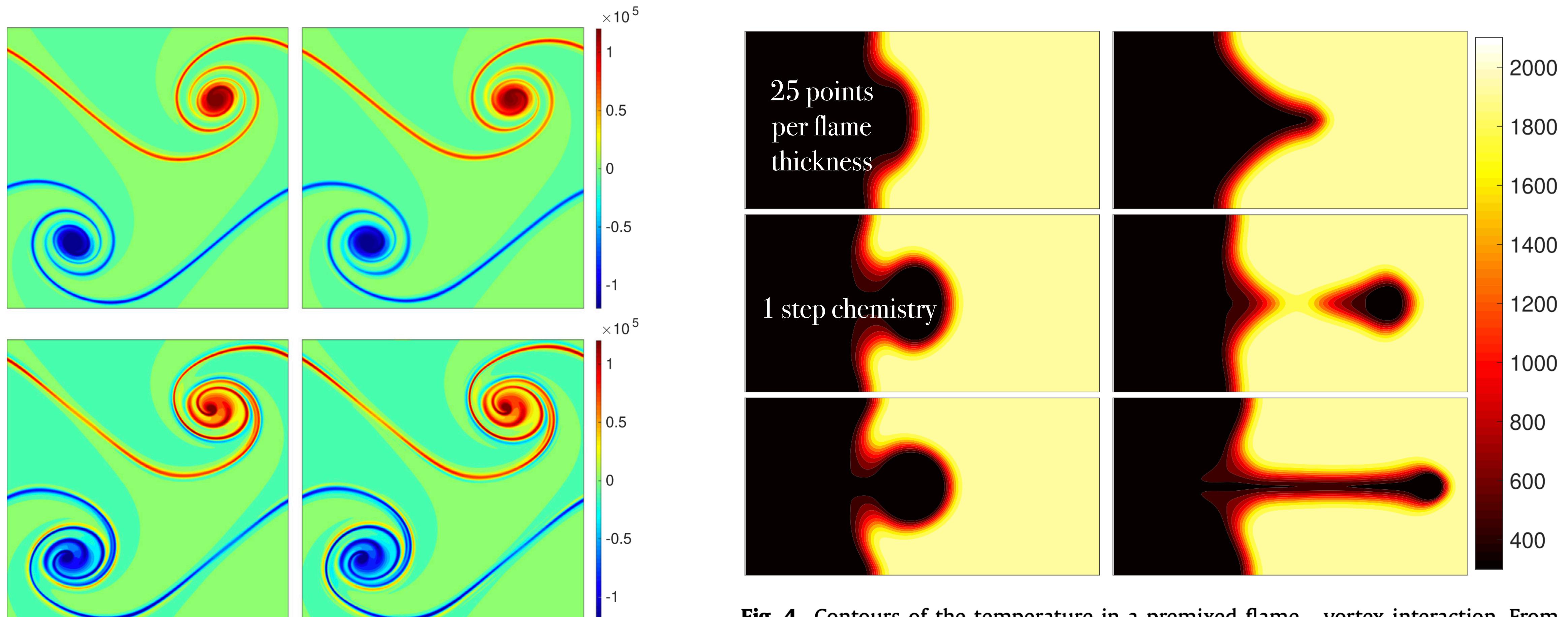
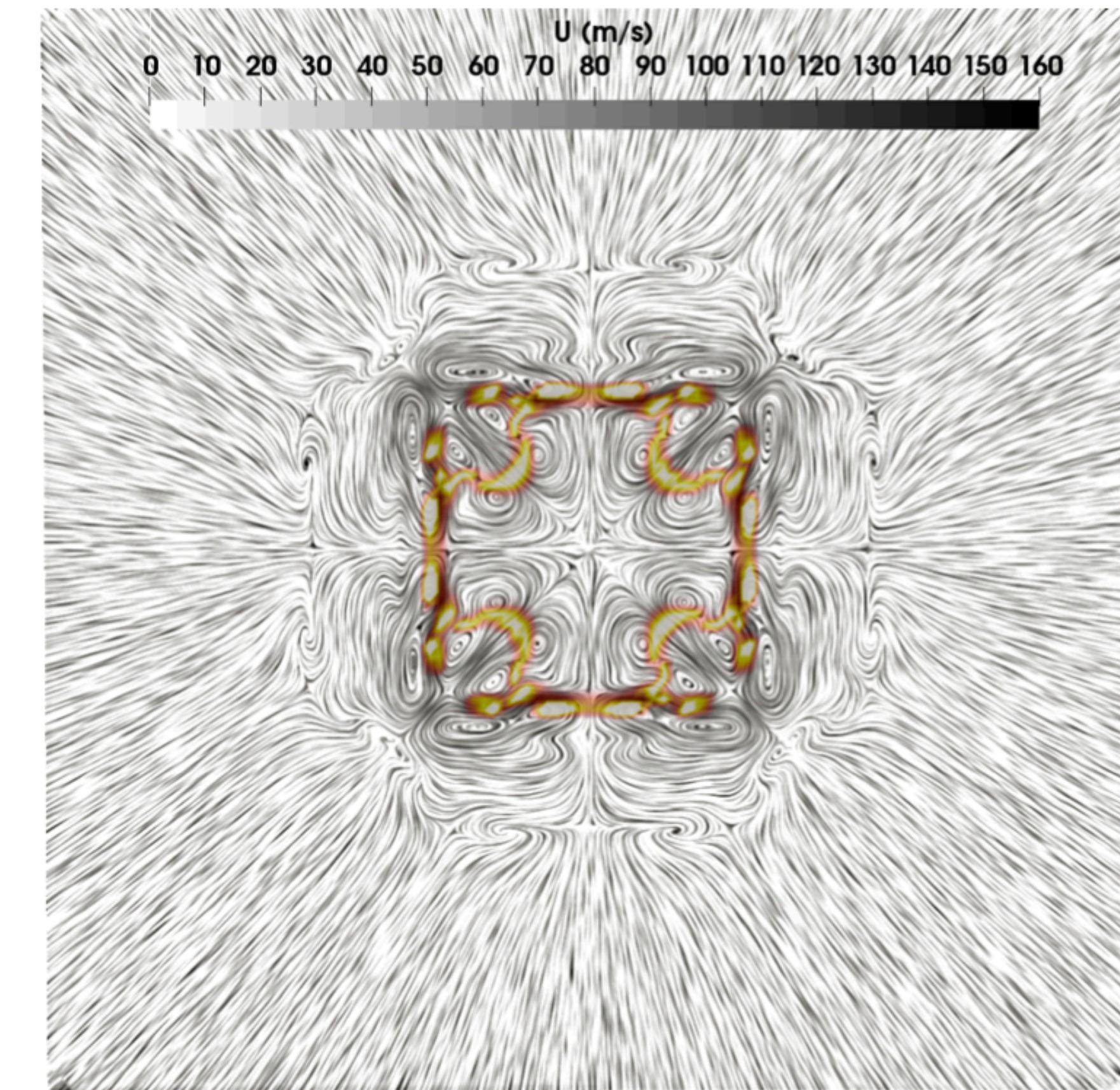
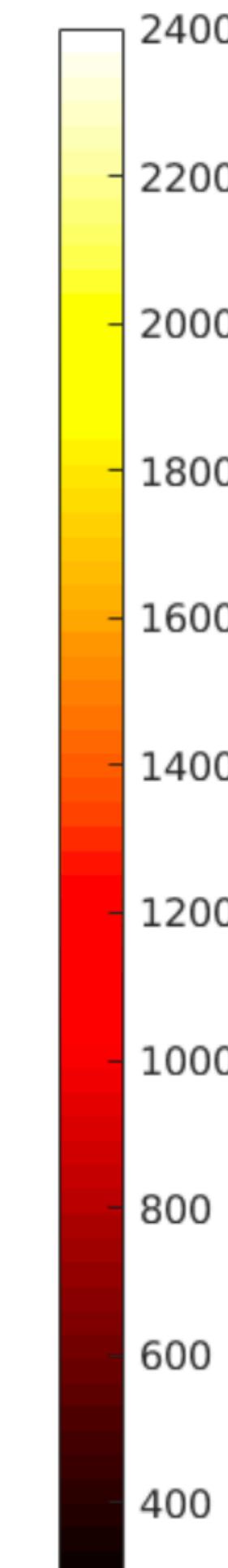
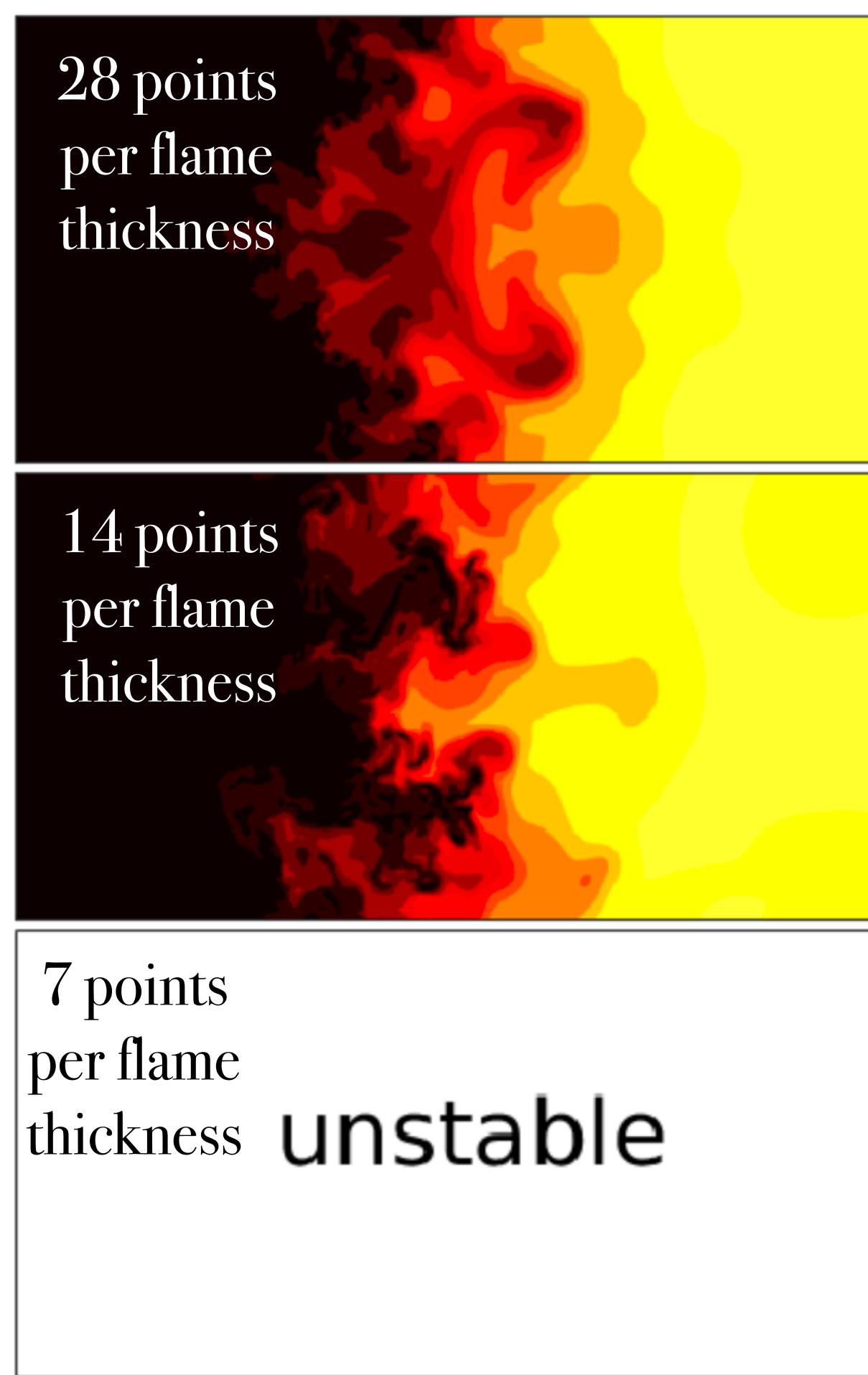


Fig. 6. Doubly periodic shear layer at $Re = 3.10^4$. Vorticity contours (magnitude of the z-component) at $t = t_c$. NTMIX contours (left) compared with the LBM contours (right), for the compressible “cold” flow (top) and the “hot” flow (bottom), e.g. including the chemical source term, on a 1024×1024 grid.

Fig. 4. Contours of the temperature in a premixed flame - vortex interaction. From top to bottom: case A at $t = 2.12$ and $t = 2.83$; case B at $t = 1.42$ and $t = 1.80$; case C at $t = 0.90$ $t = 1.09$.

... and quickly reaching limitations ...



General idea for model 2.0

- ❖ About segregated density / pressure-based methods
 - ❖ A classical CFD approach (1980s - now) for "all speed methods"
 - ❖ used in FLUENT, STARCCM+, some OpenFoam versions ...
- ❖ Generic structure
 - ❖ Predictor step (starting from (u^n, p^n, T^n, ρ^n))
 - ❖ compute intermediary variables (u^*, p^*, T^*, ρ^*) solving a (nearly) incompressible problem with a robust (usually implicit) method
 - ❖ Segregated = energy equation solved separately from mass+momentum
 - ❖ Corrector step
 - ❖ Solve an equation for pressure / density correction to recover full compressibility
 - ❖ update other variables using the new pressure / density $(u^*, p^*, T^*, \rho^*) \rightarrow (u^{n+1}, p^{n+1}, T^{n+1}, \rho^{n+1})$

Model 1.0 « density »

- ❖ Resolution for f
- ❖ $(\theta - 1)$ term in f_{eq}
- ❖ 3rd order eq. Distribution

$$\begin{cases} \sum_i f_i = \rho \\ \sum_i c_{i,\alpha} f_i = \rho u_\alpha \\ \sum_i c_{i,\alpha} c_{i,\beta} f_i = \rho u_\alpha u_\beta + \rho c_s^2 \delta_{\alpha\beta} \end{cases}$$

- ❖ Collision kernel:
hybrid regularized ($\sigma \in [0,0.5]$)
- ❖ Correction term to account for the lattice defect
(stress tensor)

[1] Y. Feng, M. Tayyab, and P. Boivin, “A lattice-boltzmann model for low-mach reactive flows,” Combustion and Flame, vol. 196, pp. 249 – 254, 2018.

[2] Y. Feng, P. Boivin, J. Jacob, and P. Sagaut, “Hybrid recursive regularized thermal lattice boltzmann model for high subsonic compressible flows,” Journal of Computational Physics, vol. 394, pp. 82 – 99, 2019.

Model 2.0 « pressure »

- ❖ Resolution for g
- ❖ Athermal formulation for g_{eq} (orders > 0)
- ❖ 2nd order is enough...

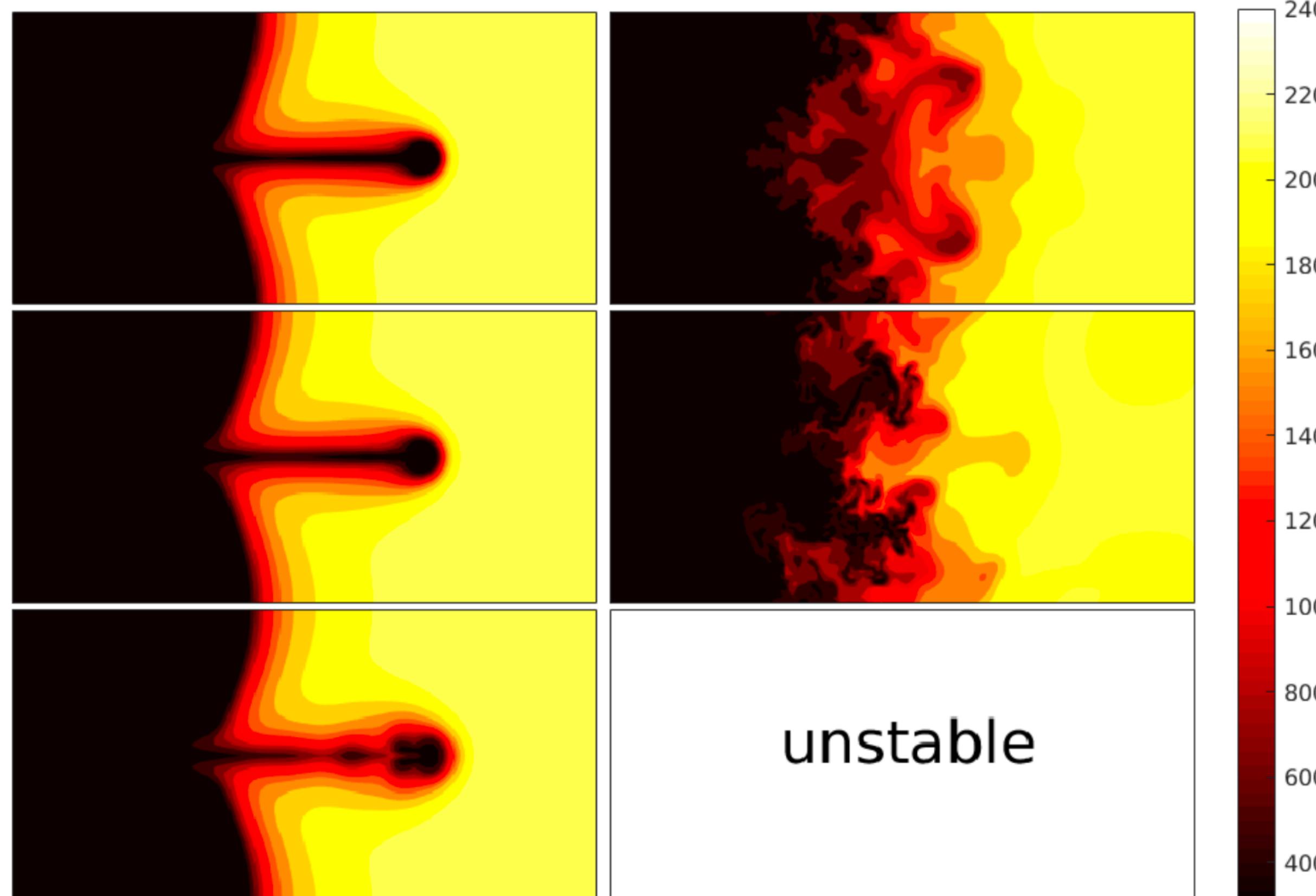
$$\begin{cases} \sum_i g_i = \rho\theta \\ \sum_i c_{i,\alpha} g_i = \rho u_\alpha \\ \sum_i c_{i,\alpha} c_{i,\beta} g_i = \rho u_\alpha u_\beta + \rho\theta c_s^2 \delta_{\alpha\beta} \end{cases}$$

- ❖ Modified macroscopic variable reconstruction
- $$\rho(t + \Delta t, x) = \sum_i [g_i^*(t + \Delta t, x)] - \rho(t, x)\theta(t, x) + \rho(t, x)$$

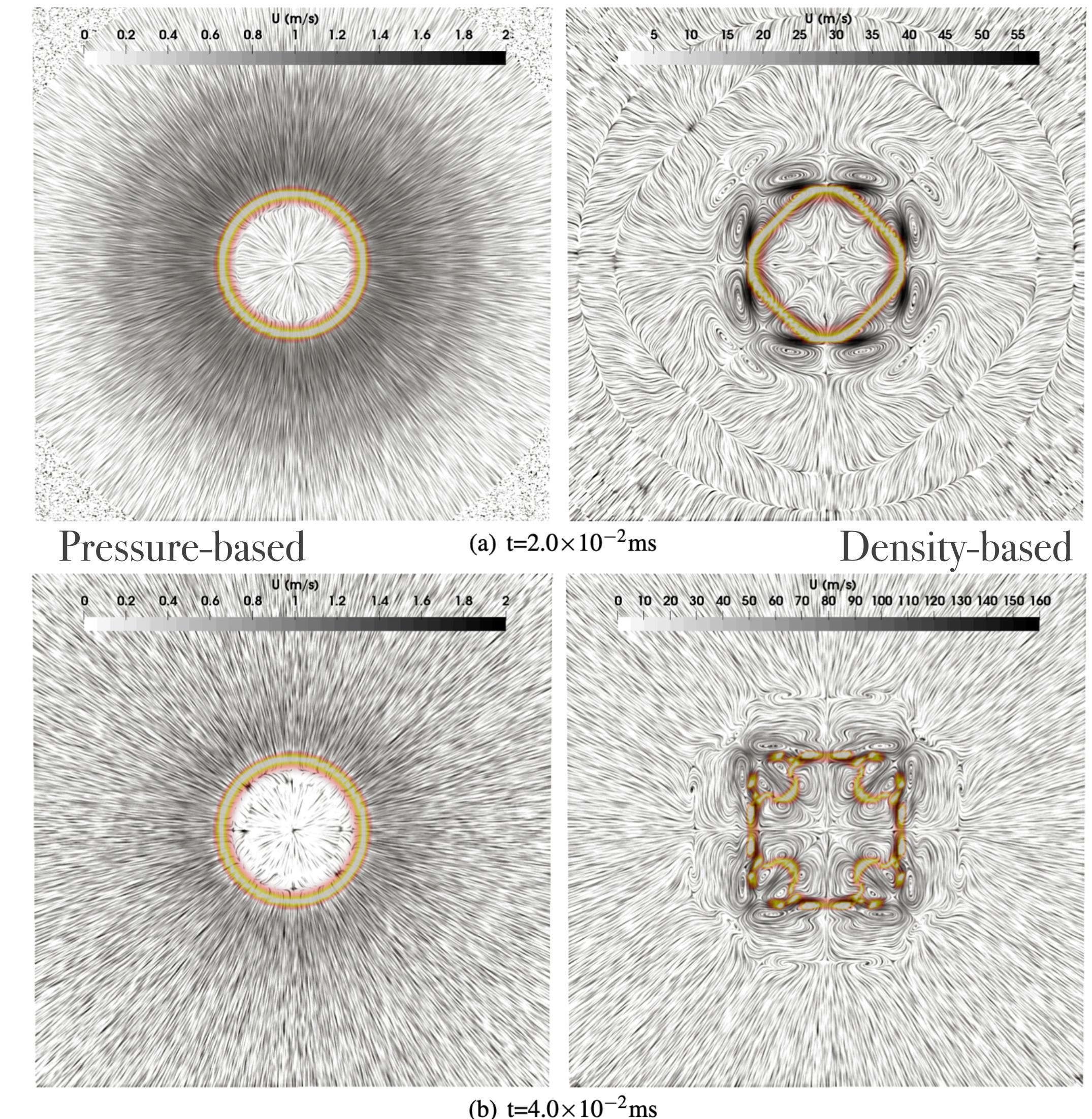
- ❖ Additional 2nd order correction needed
- $$a_{\alpha\beta}^{\text{cor}} \equiv c_s^2 \delta_{\alpha\beta} [\rho(t + \Delta t, x)(1 - \theta(t + \Delta t, x)) - \rho(t, x)(1 - \theta(t, x))]$$

[1] G. Farag, S. Zhao, T. Coratger, P. Boivin, G. Chiavassa, and P. Sagaut, “A pressure-based regularized lattice-boltzmann method for the simulation of compressible flows,” Physics of Fluids, vol. 32, no. 6, p. 066106, 2020.

Pressure-based vs Density-based



Vortex/flame interaction for 3 for H₂-air flames (28, 14, 7 pts/flame thickness)



References

- ❖ Y. Feng, M. Tayyab, and P. Boivin, “A lattice-boltzmann model for low-mach reactive flows,” *Combustion and Flame*, vol. 196, pp. 249 – 254, 2018. **(v1)**
- ❖ Y. Feng, P. Boivin, J. Jacob, and P. Sagaut, “Hybrid recursive regularized thermal lattice boltzmann model for high subsonic compressible flows,” *Journal of Computational Physics*, vol. 394, pp. 82 – 99, 2019. **(v1)**
- ❖ M. Tayyab, S. Zhao, Y. Feng, and P. Boivin, “Hybrid regularized lattice-boltzmann modelling of premixed and non-premixed combustion processes,” *Combustion and Flame*, vol. 211, pp. 173–184, 2020. **(v1)**
- ❖ G. Farag, S. Zhao, T. Coratger, P. Boivin, G. Chiavassa, and P. Sagaut, “A pressure-based regularized lattice-boltzmann method for the simulation of compressible flows,” *Physics of Fluids*, vol. 32, no. 6, p. 066106, 2020. **(v2)**
- ❖ M. Tayyab, B. Radisson, C. Almarcha, B. Denet, and P. Boivin, “Experimental and numerical lattice- boltzmann investigation of the darrieus-landau instability,” *Combustion and Flame*, vol. 221, pp. 103–109, 2020. **(v2)**
- ❖ S. Zhao, G. Farag, P. Boivin, and P. Sagaut, “Toward fully conservative hybrid lattice boltzmann methods for compressible flows,” *Physics of Fluids*, vol. 32, no. 12, p. 126118, 2020. **(v2)**
- ❖ M. Tayyab, S. Zhao, and P. Boivin, “Lattice-boltzmann modelling of a turbulent bluff-body stabilized flame,” *Physics of Fluids*, 2021. **(v2)**
- ❖ G. Farag, S. Zhao, G. Chiavassa, and P. Boivin, “Consistency study of lattice-boltzmann schemes macroscopic limit,” *Physics of Fluids*, 2021. **(Theory)**

Remarks

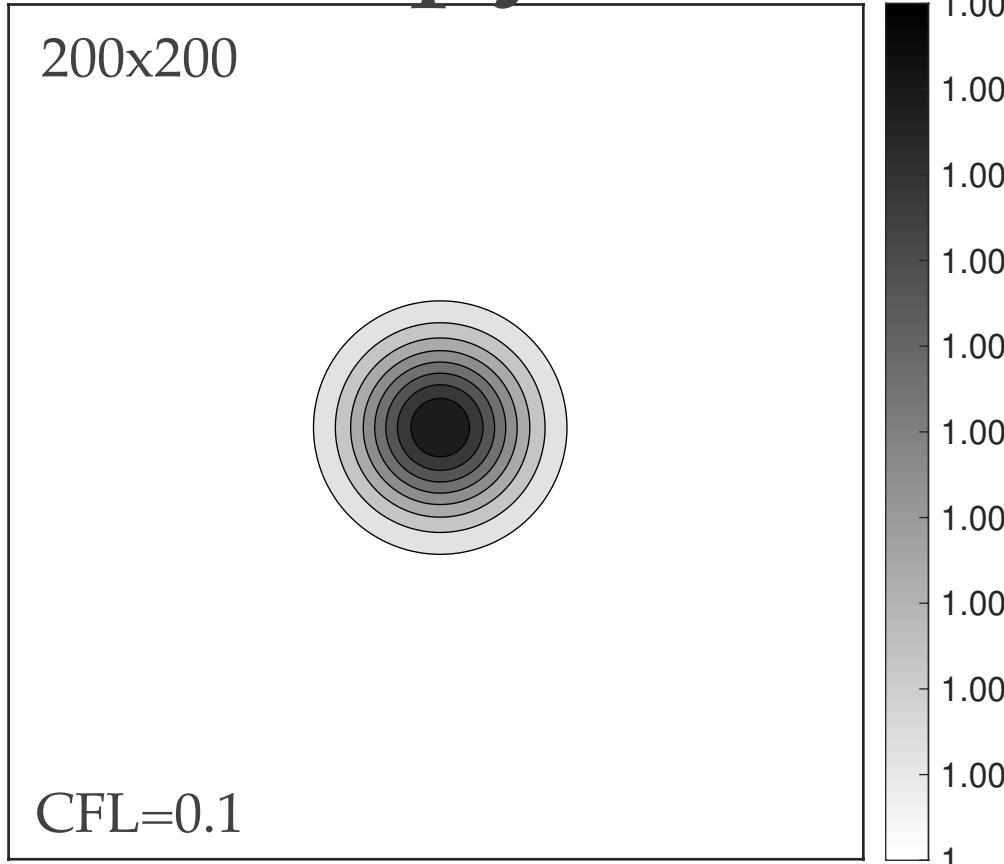
- ❖ Mass is (non-trivially) globally conserved as before for closed periodic domains
- ❖ A priori compatible with your favorite collision kernel...

And the scalar equations ?

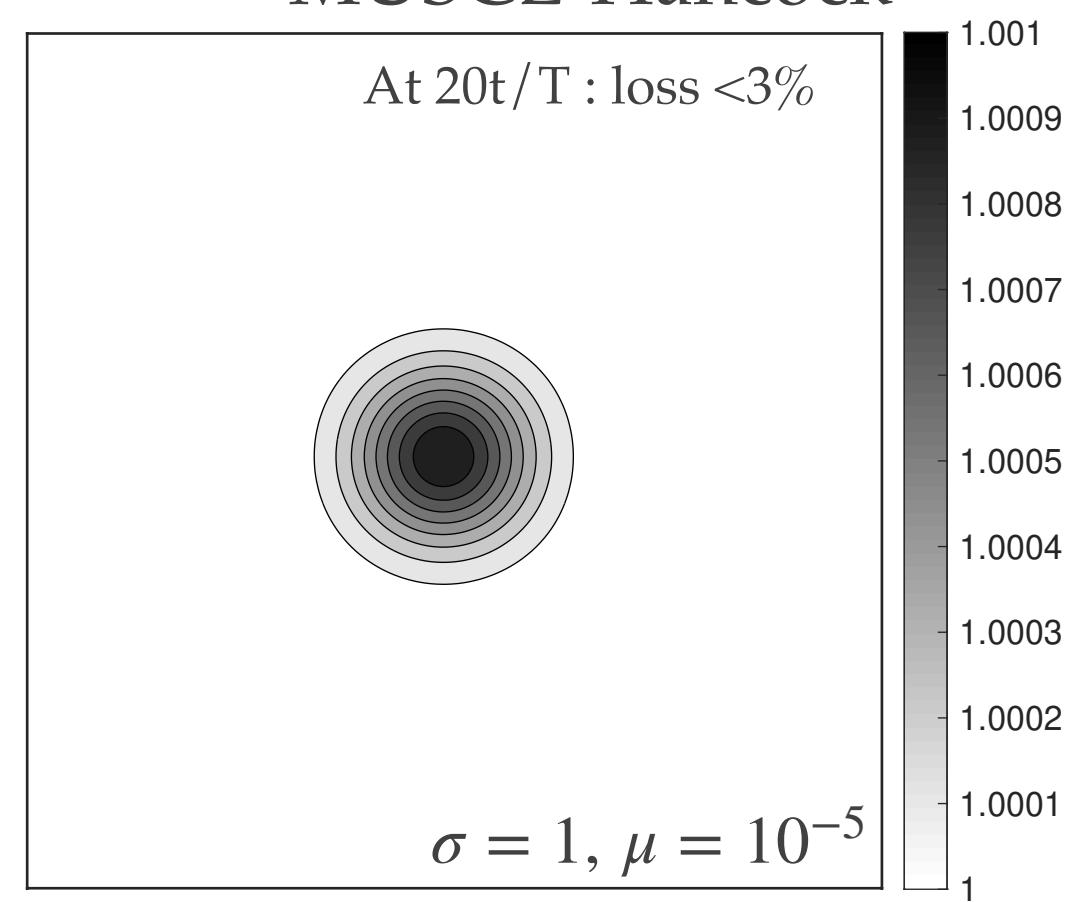
- ❖ Scalar equations are solved on the same grid.
- ❖ Explicit time-stepping is used (same time-step as LB time-step) - yet, the method is 2nd order in time
- ❖ Finite volume methods to compute all RHS terms
 - ❖ Second-order isotropic operator = non-conservative form (OK for $\text{Ma} < 0,3$)
 - ❖ Or MUSCL = non-conservative form (necessary for higher speeds)
 - ❖ Or (new) flux reconstruction from LB mass fluxes = conservative form
 - ❖ Coupling is paramount...
- ❖ Any number of explicit advection/diffusion equation can be included (energy / mass fraction / liquid / spray / ...)

Compressible core

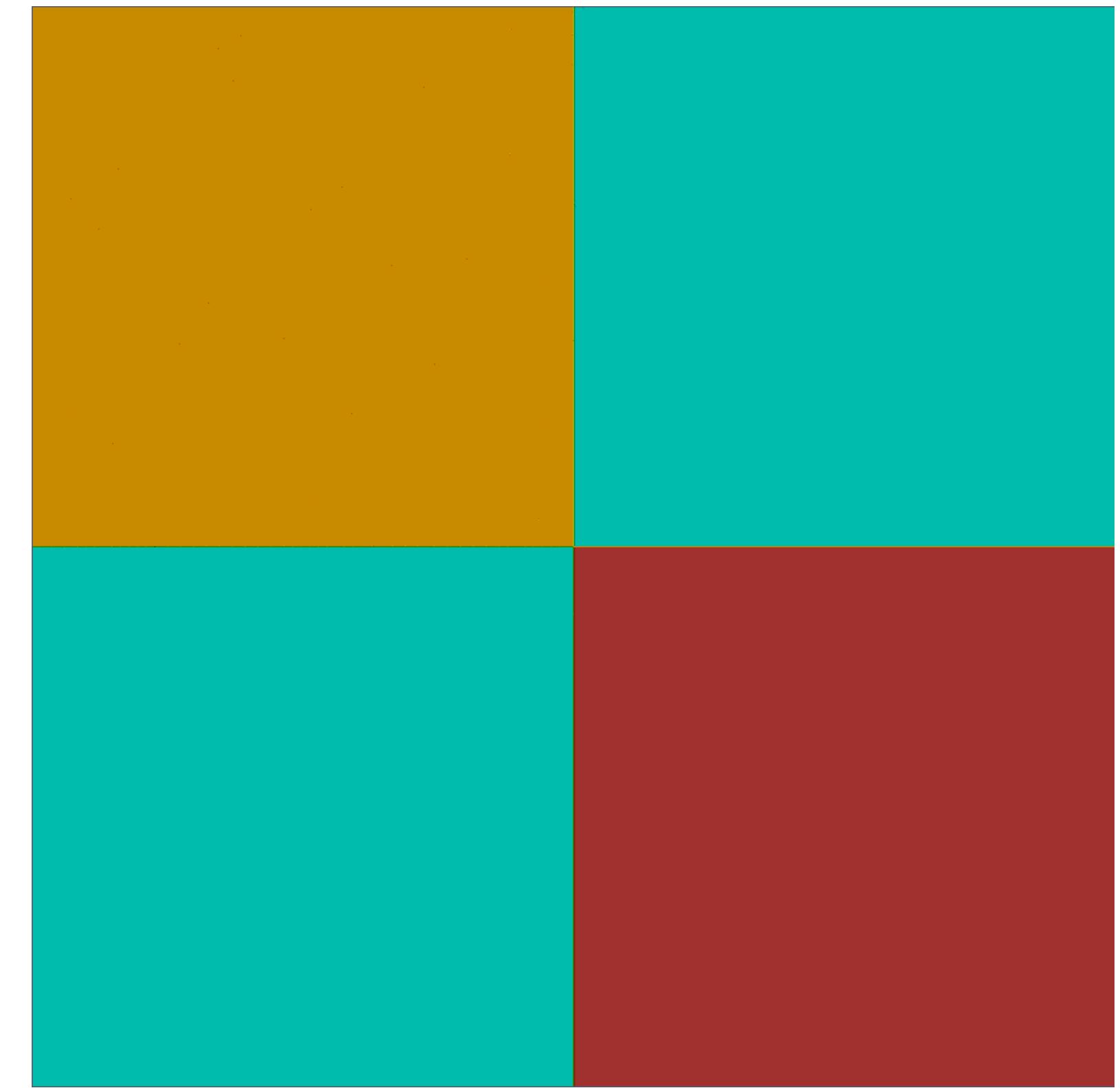
Entropy mode



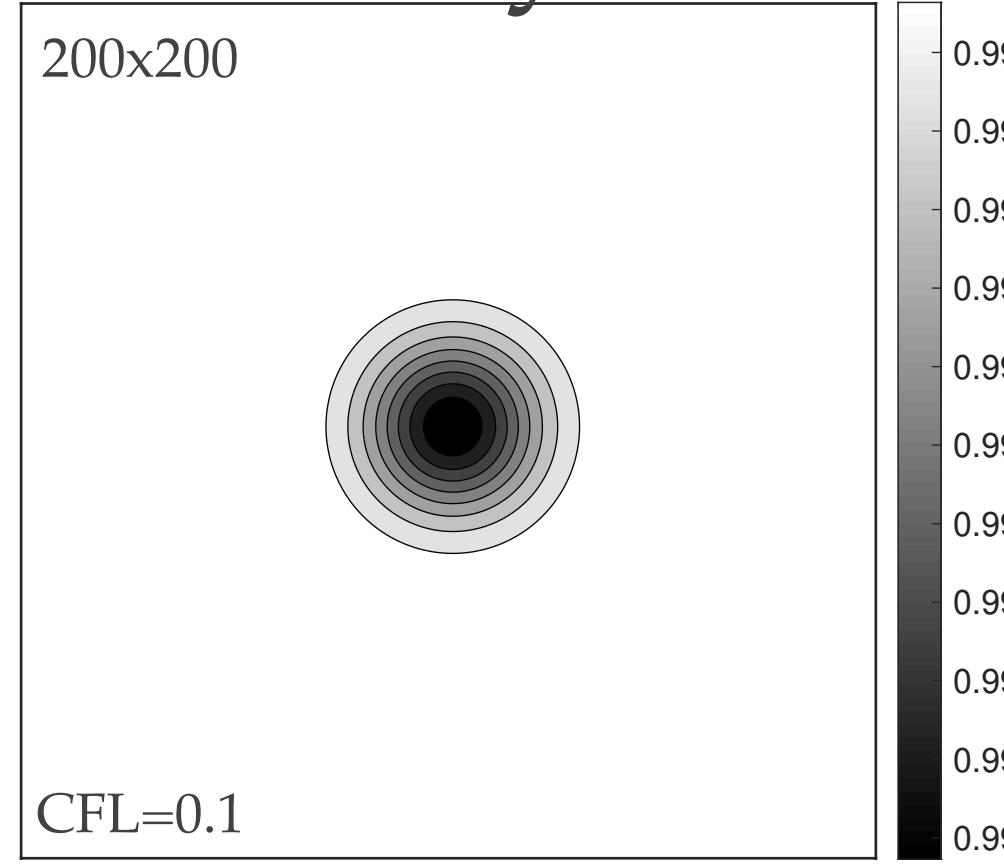
MUSCL-Hancock



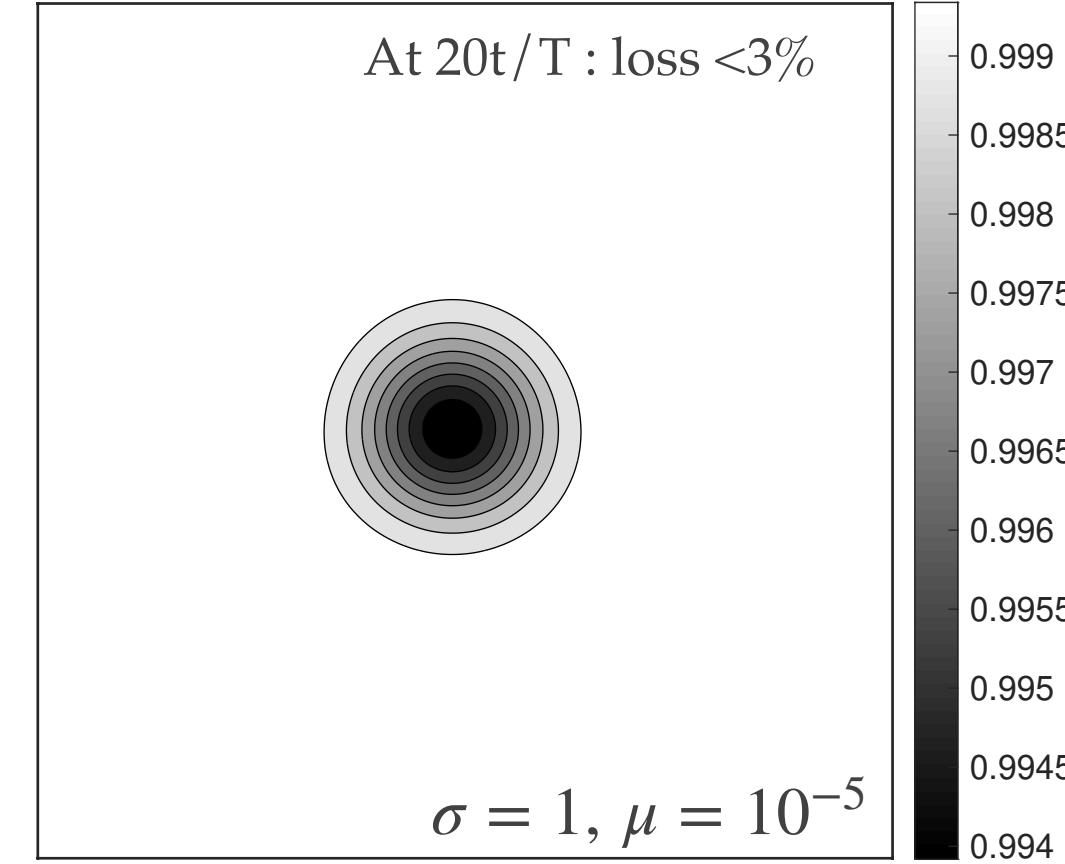
$Ma = 1.5$



Vorticity mode



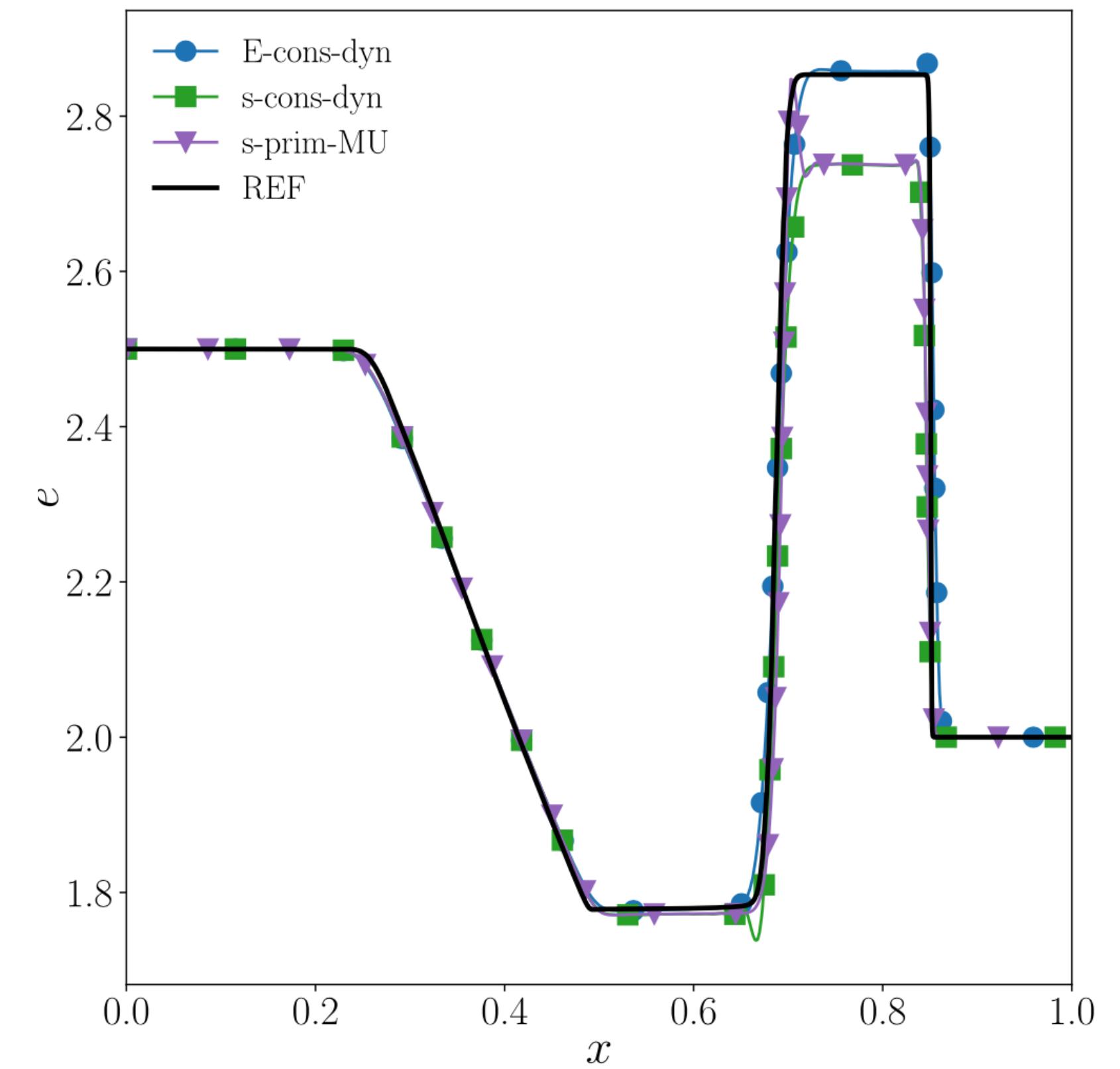
MUSCL-Hancock



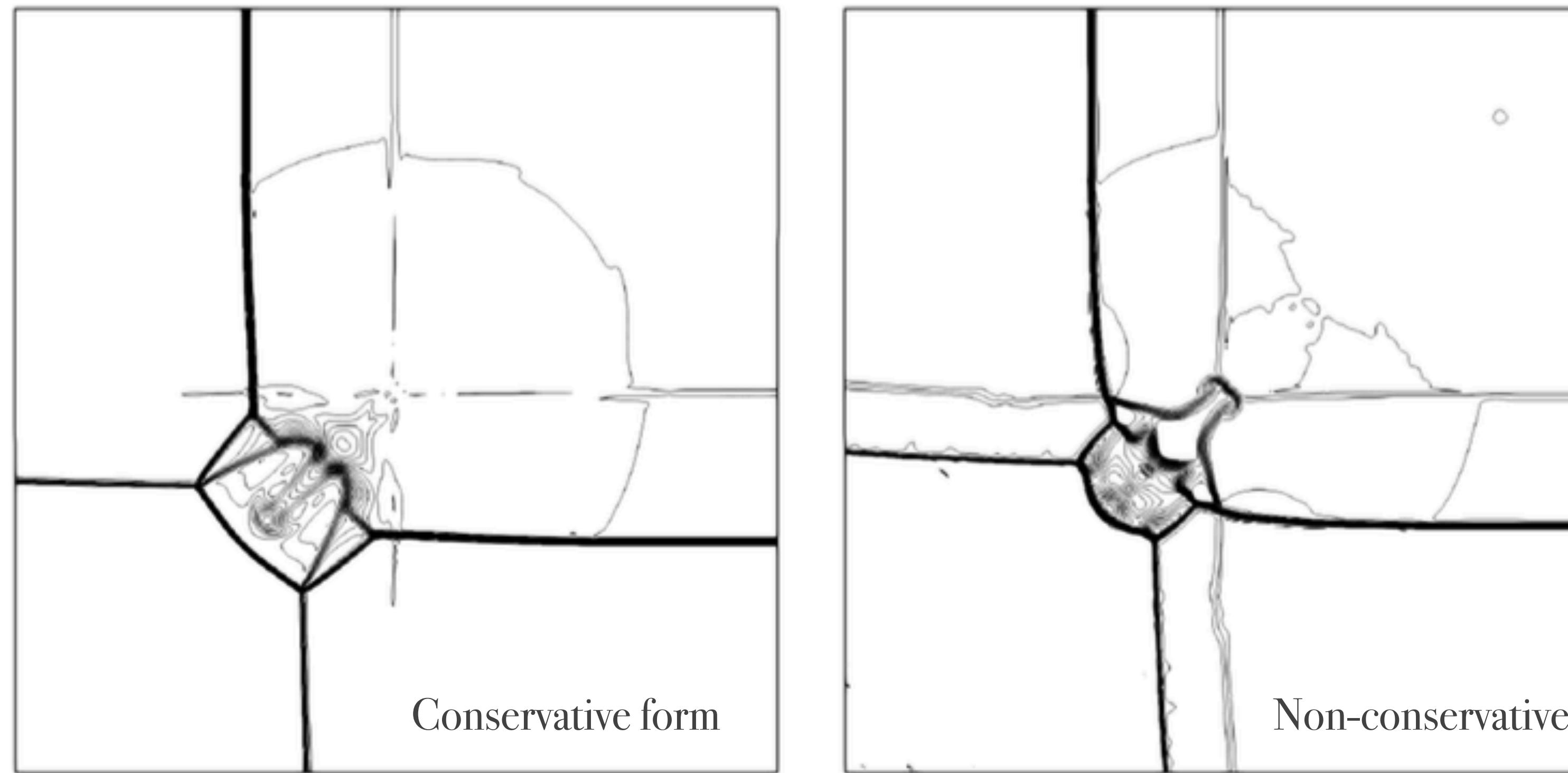
Entropy equation (MUSCL)

Conserving Scalars...

- ❖ For any advection equation $\frac{\partial \rho\phi}{\partial t} + \nabla \cdot (\rho u \phi) = 0$,
- ❖ (= mass conservation + non-conservative scalar eq)
- ❖ $\nabla^C \cdot (\rho u \phi) \equiv \frac{1}{\Delta t} \sum_i \left[f_i^{\text{col}} \frac{\phi^+ + \phi^-}{2} - f_i^{\text{col}} \frac{\phi^+ + \phi^-}{2} \right]$
- ❖ ~ Match the LBM mass flux computation to compute scalar eqs.
- ❖ => numerically conserve $\rho\phi$ and $\rho\phi^2$
- ❖ And respect the Hugoniot jump conditions !
- ❖ *S. Zhao, G. Farag, P. Boivin, and P. Sagaut, "Toward fully conservative hybrid lattice boltzmann methods for compressible flows," Physics of Fluids, vol. 32, no. 12, p. 126118, 2020.*



Conserving Scalars...

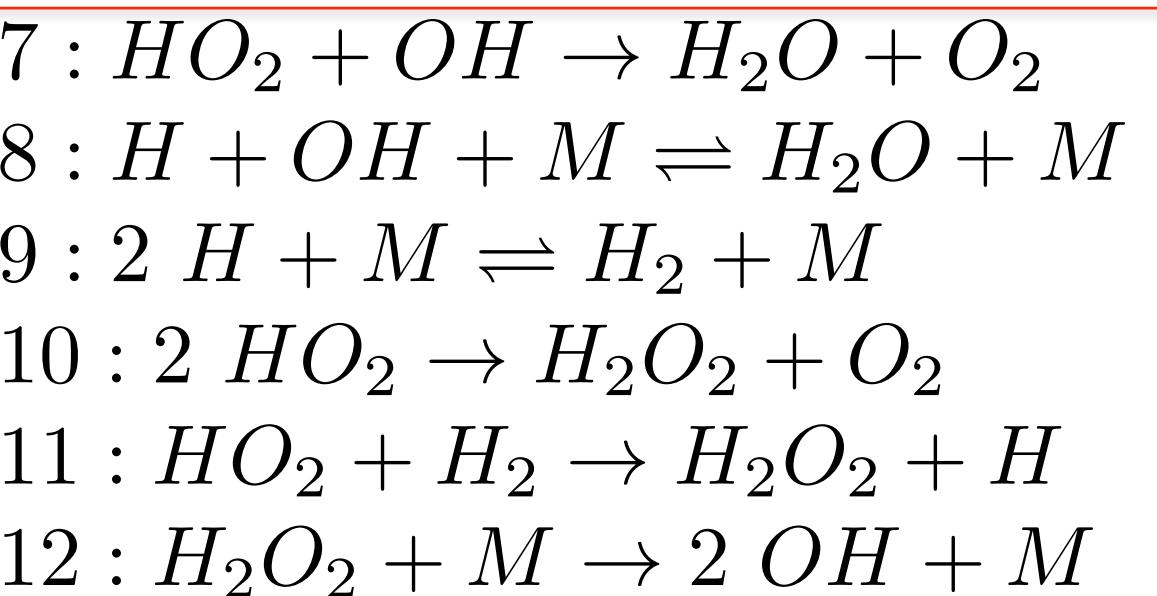
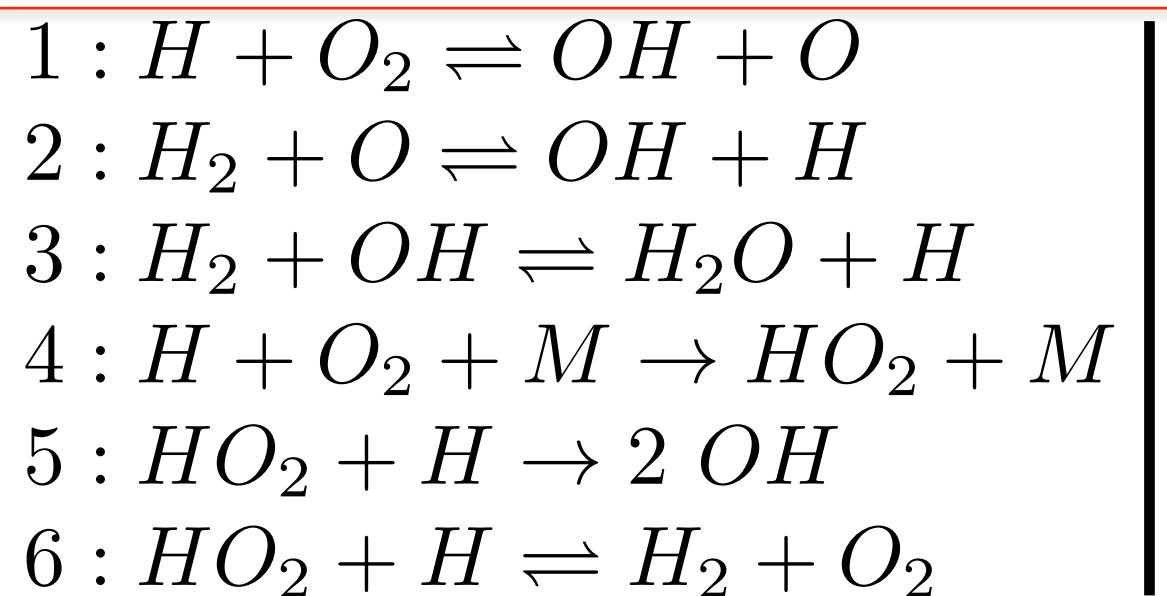


2D Riemann problem. Conservative form is mandatory to properly capture Hugoniot jumps...

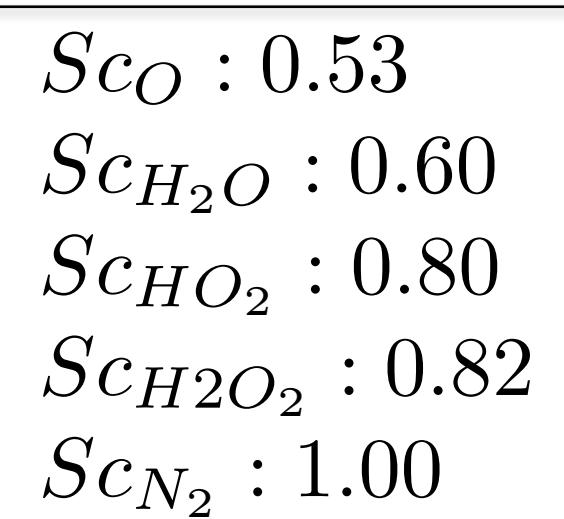
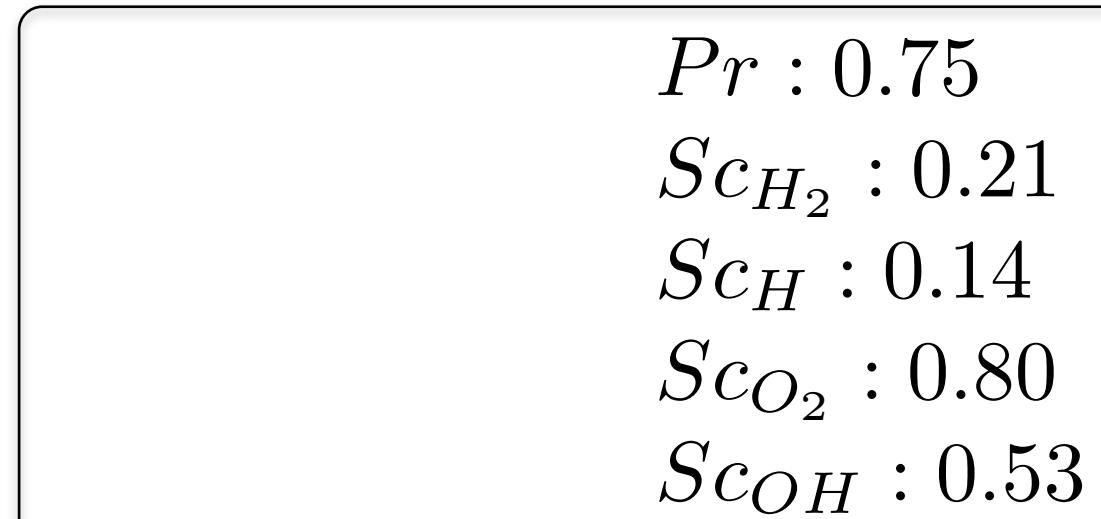
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Validation



12-Step



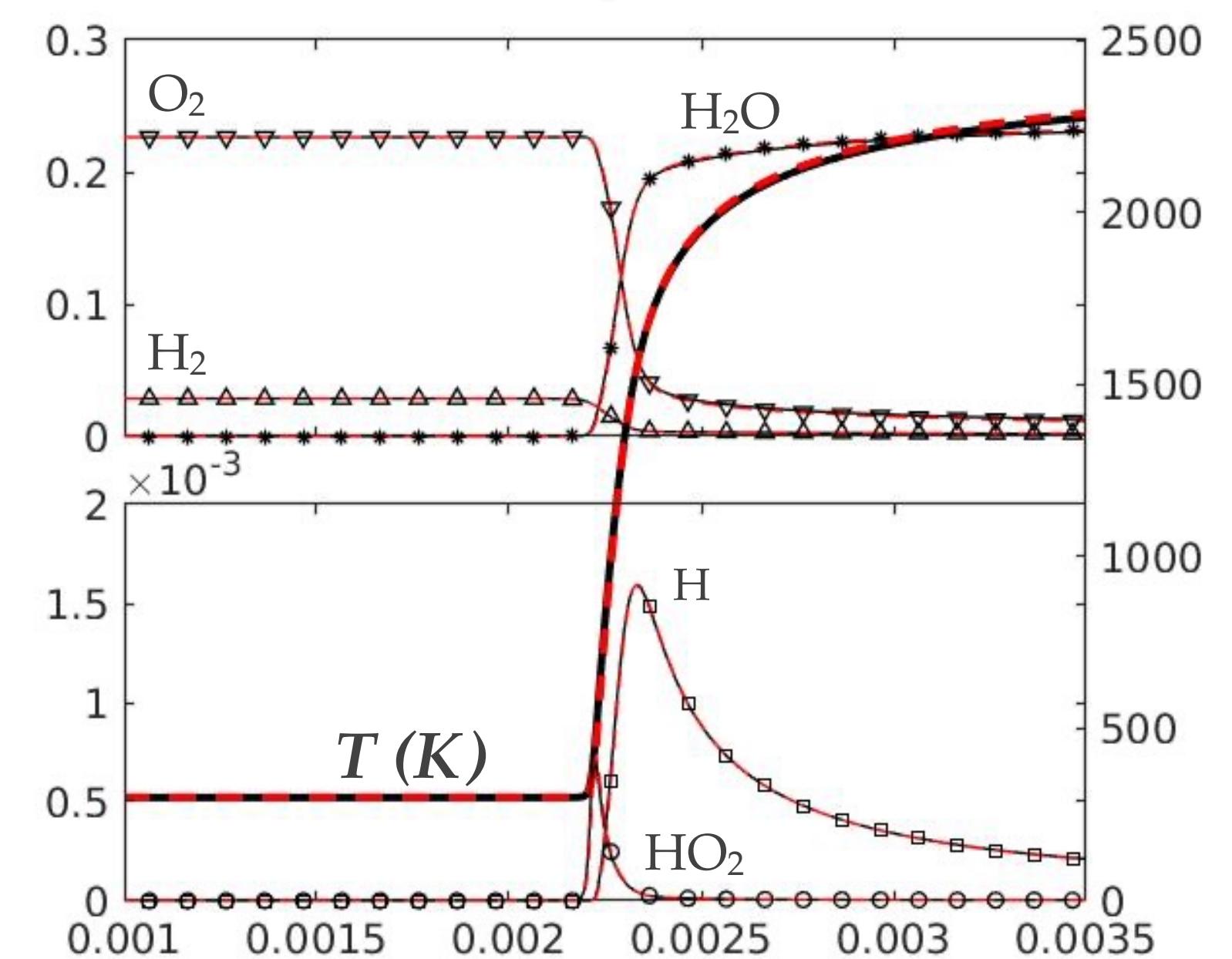
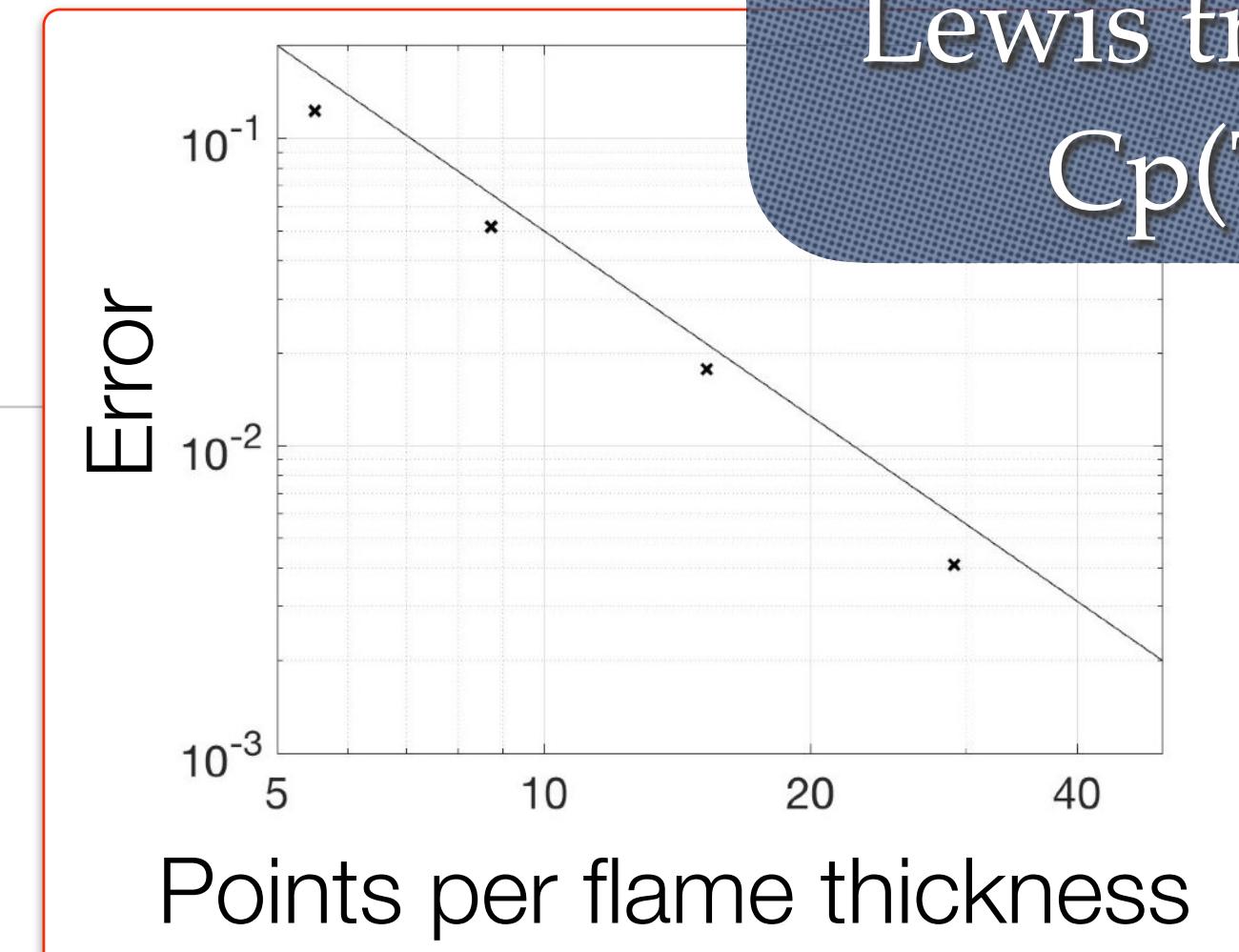
Heat and Diffusion

Variable Heat Capacity

Viscosity's Power Law

$$C_p(T) = R(a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4)$$

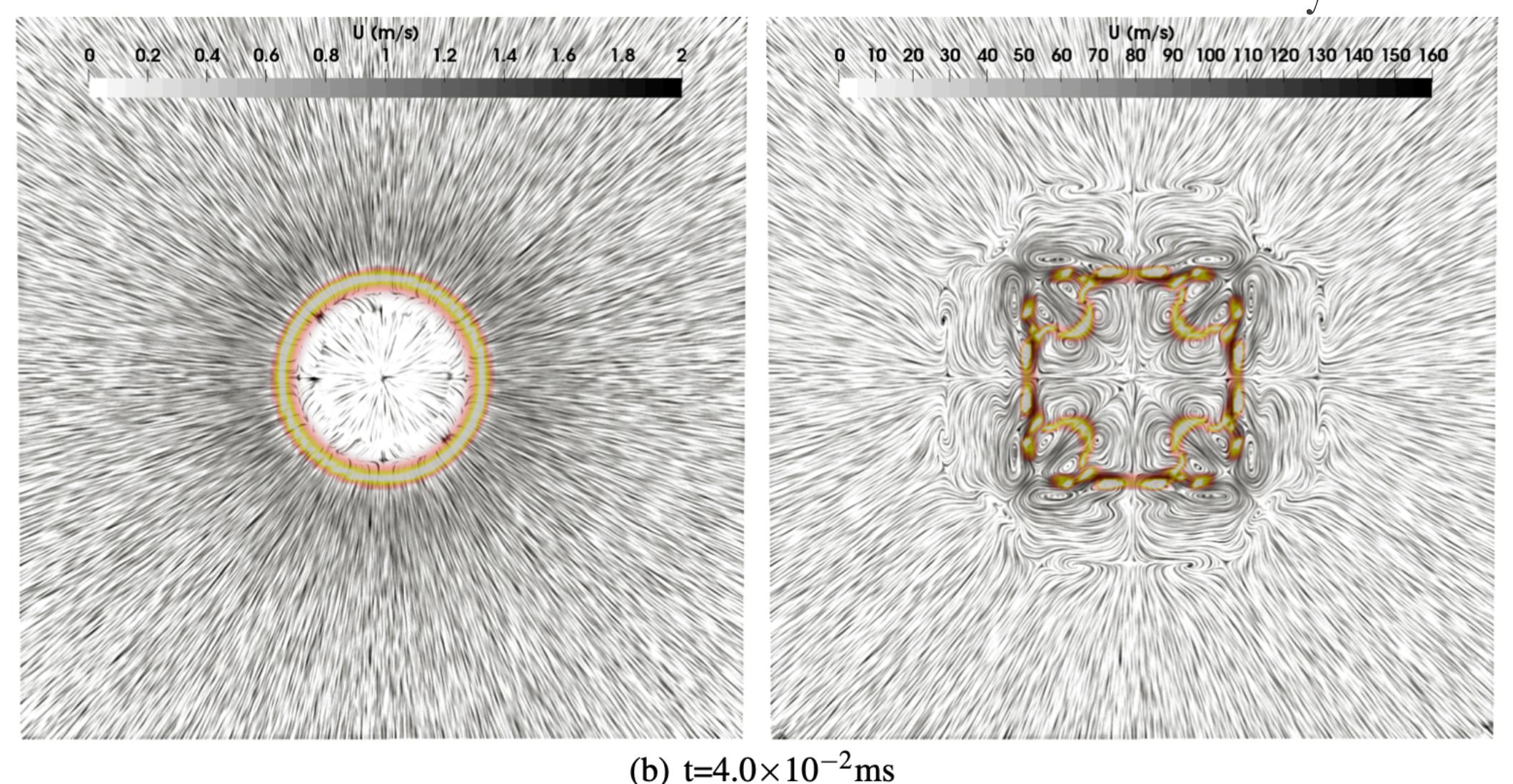
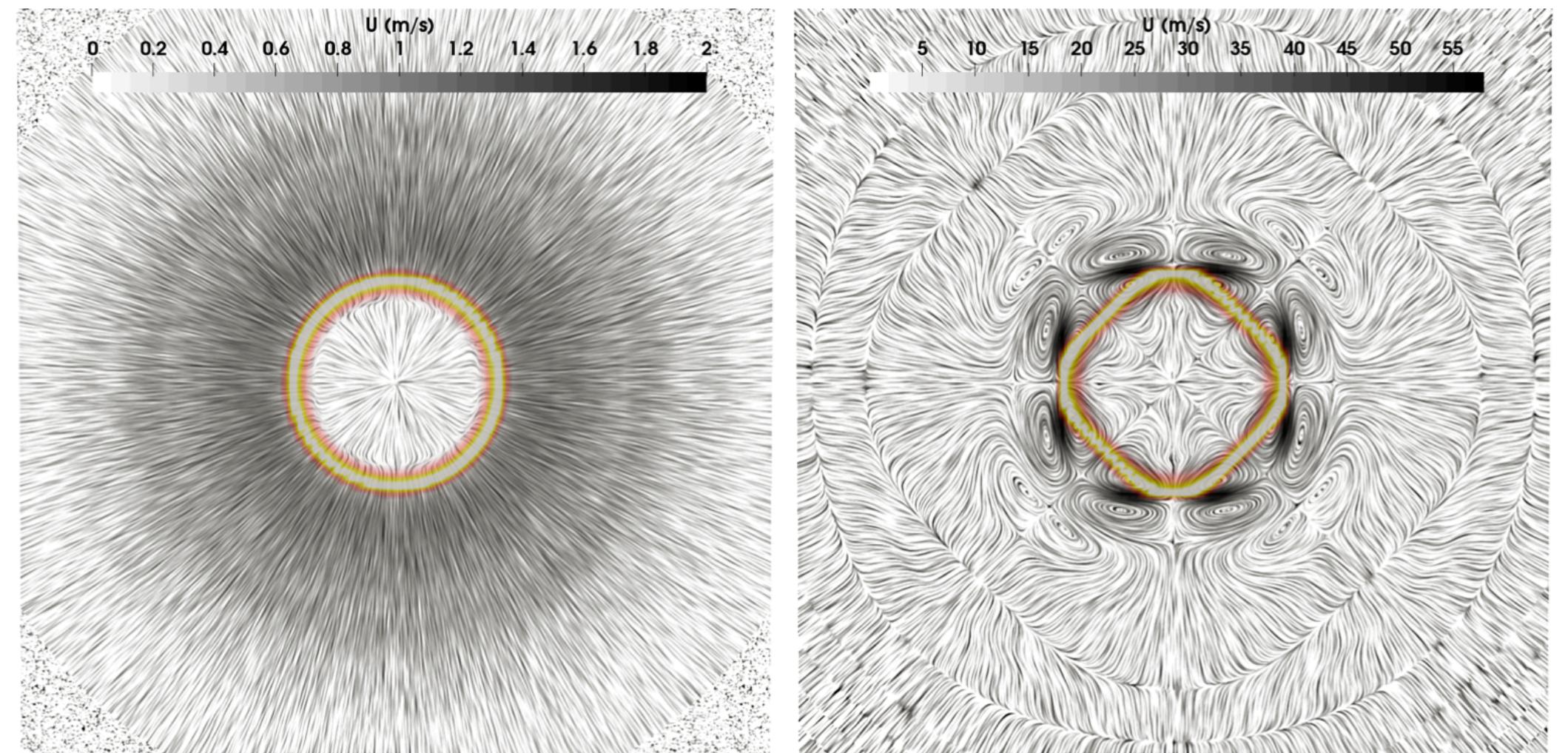
$$\mu = \mu_0 \left(\frac{T}{T_0} \right)^\beta$$



Stoichiometric H₂-air premixed flame.
 Ref: Cantera.

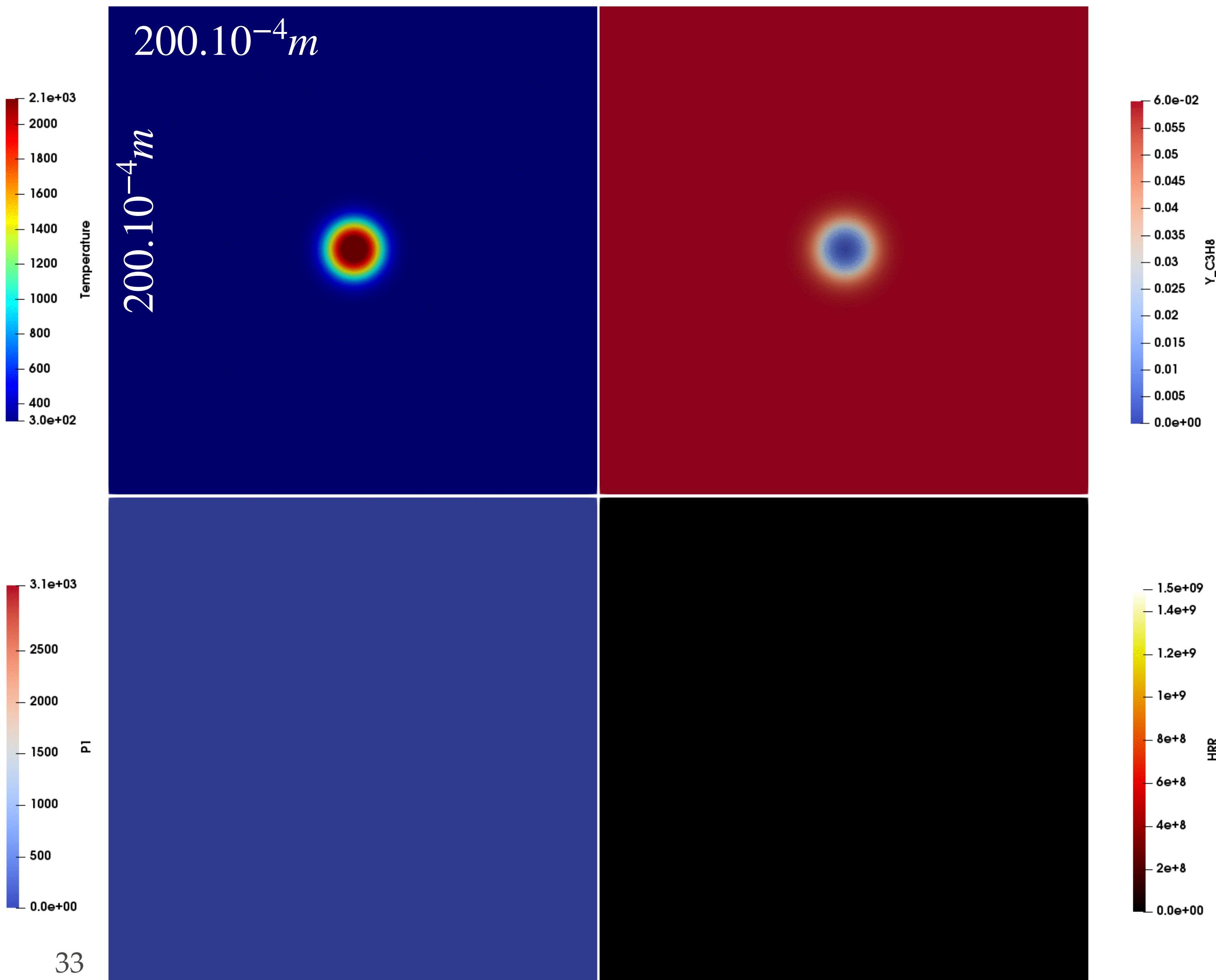
Spherical premixed flame

- ❖ Isotropy & stability test
- ❖ ~3 pts in flame thickness
- ❖ Excellent isotropy

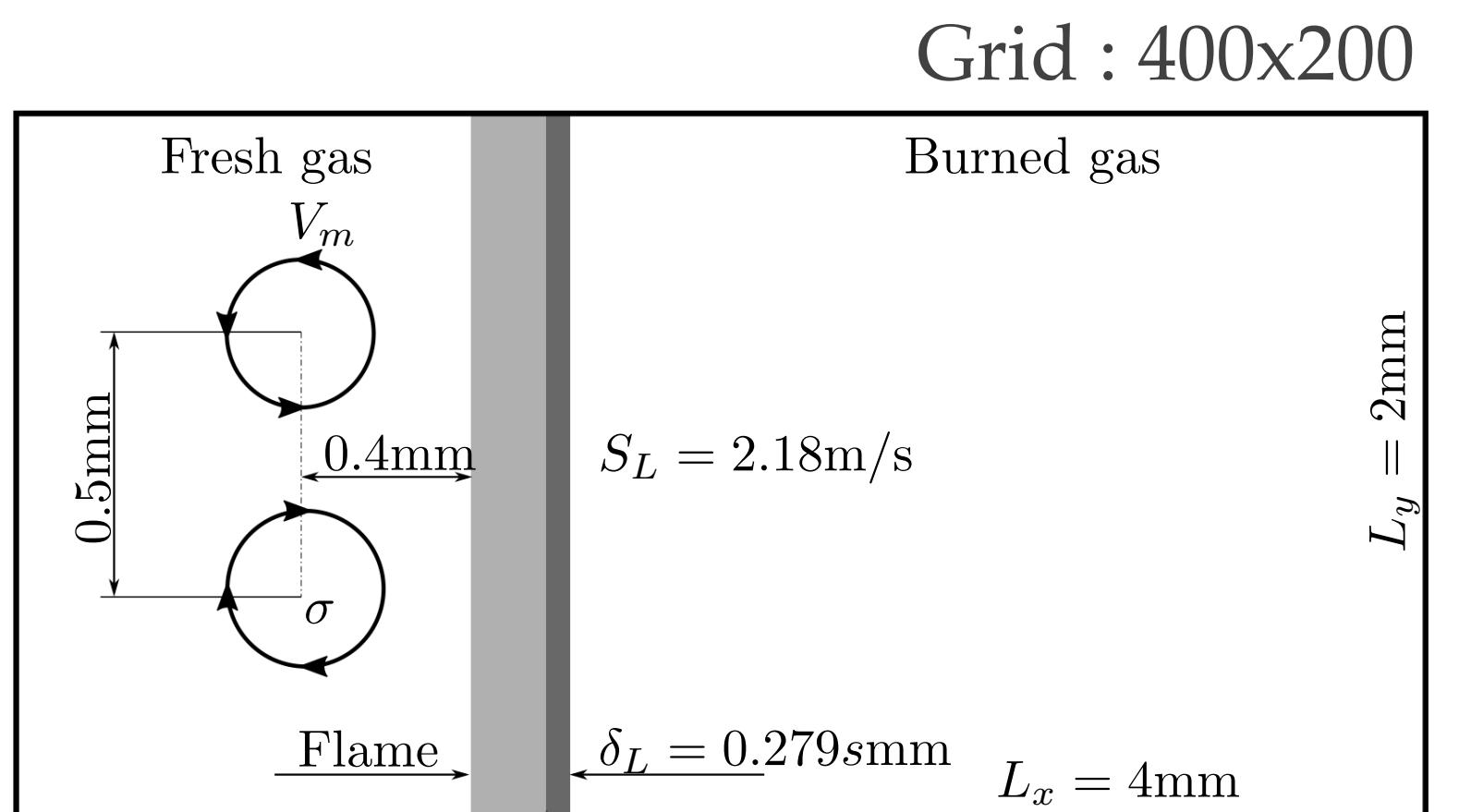


Spherical premixed flame

- ❖ Isotropy & stability test
- ❖ ~3 pts in flame thickness
- ❖ Excellent isotropy
- ❖ Non-reflecting outlets OK



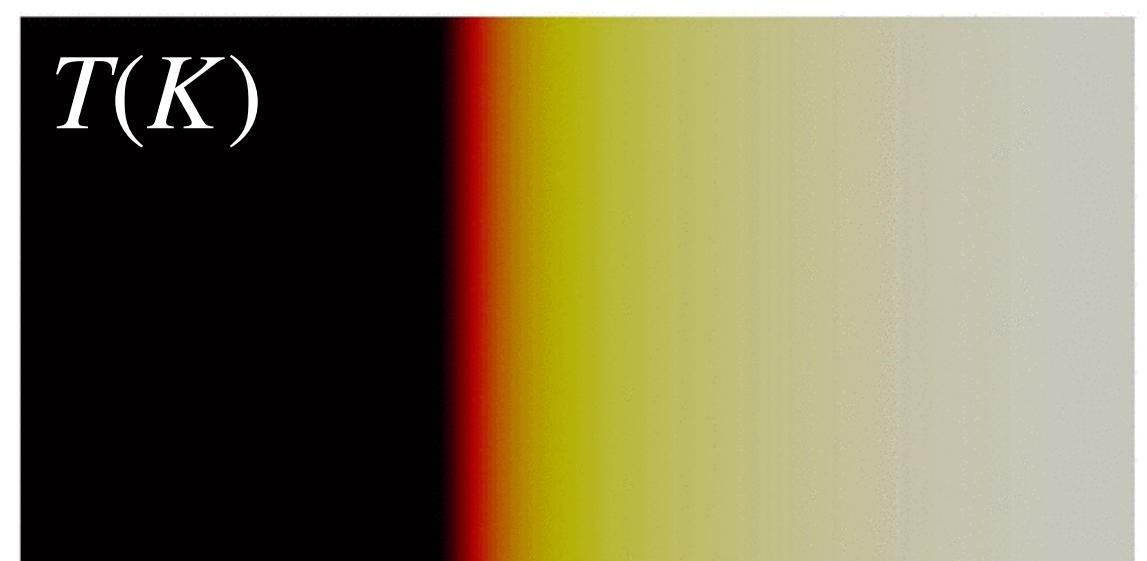
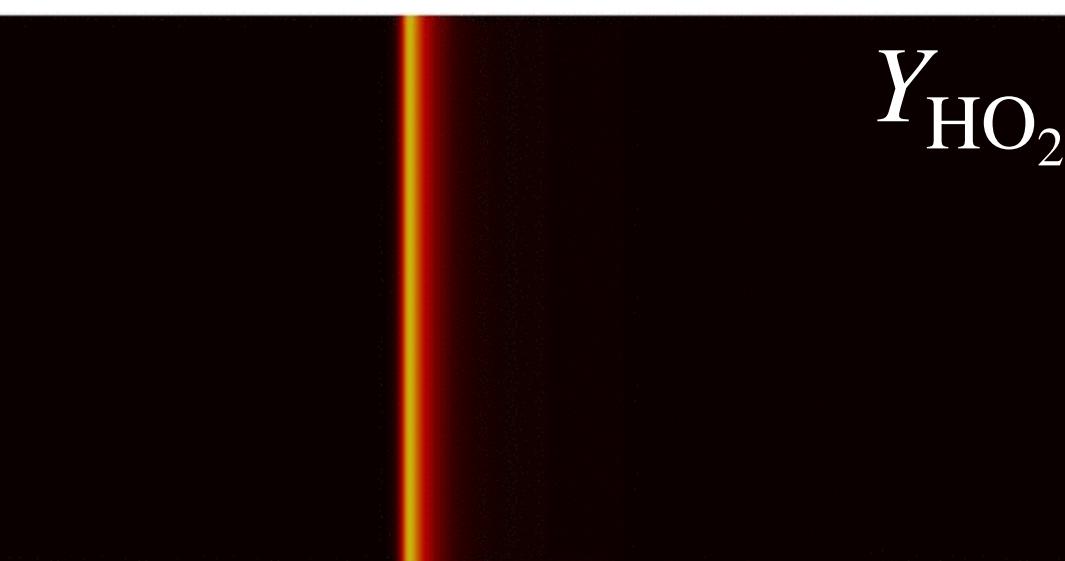
Vortex-Flame interaction



	V_m/s_L	σ/δ_L	Ka
Case A	2.24	1.18	1.89
Case B	16.18	0.93	17.39
Case C	32.68	0.92	35.52

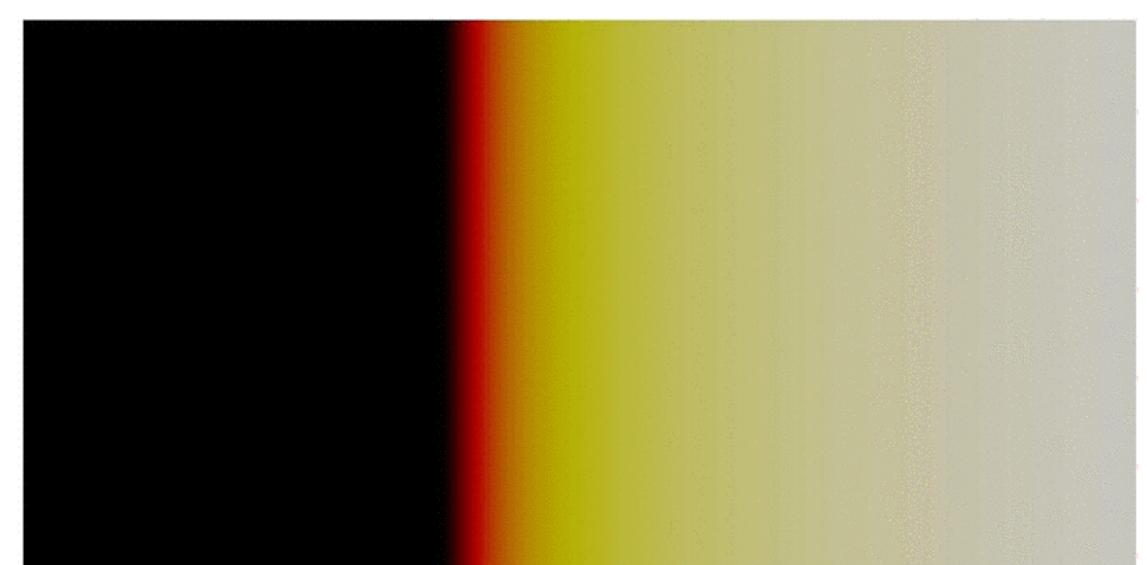
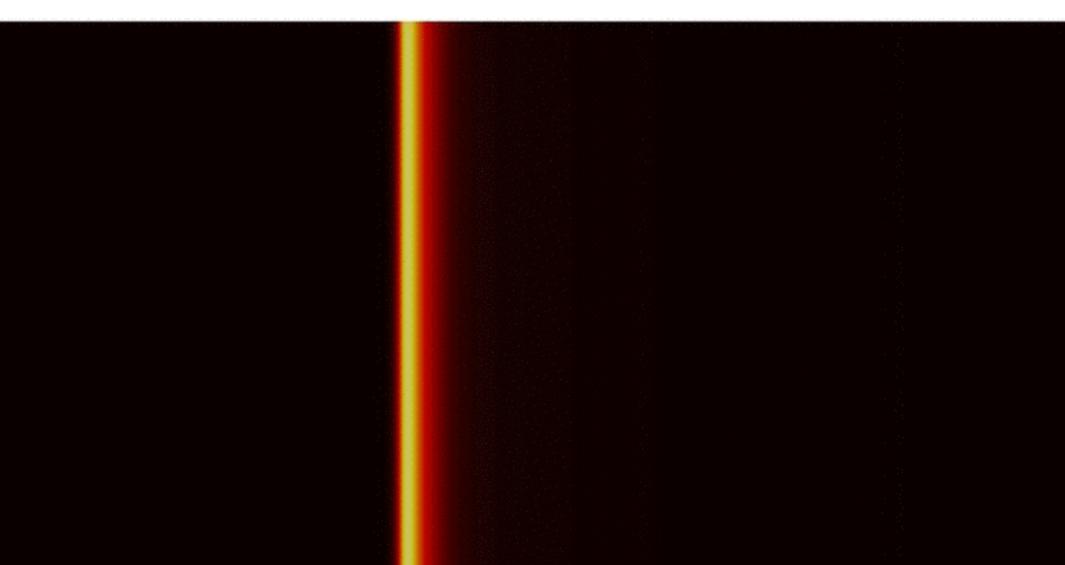
Case A:

weak



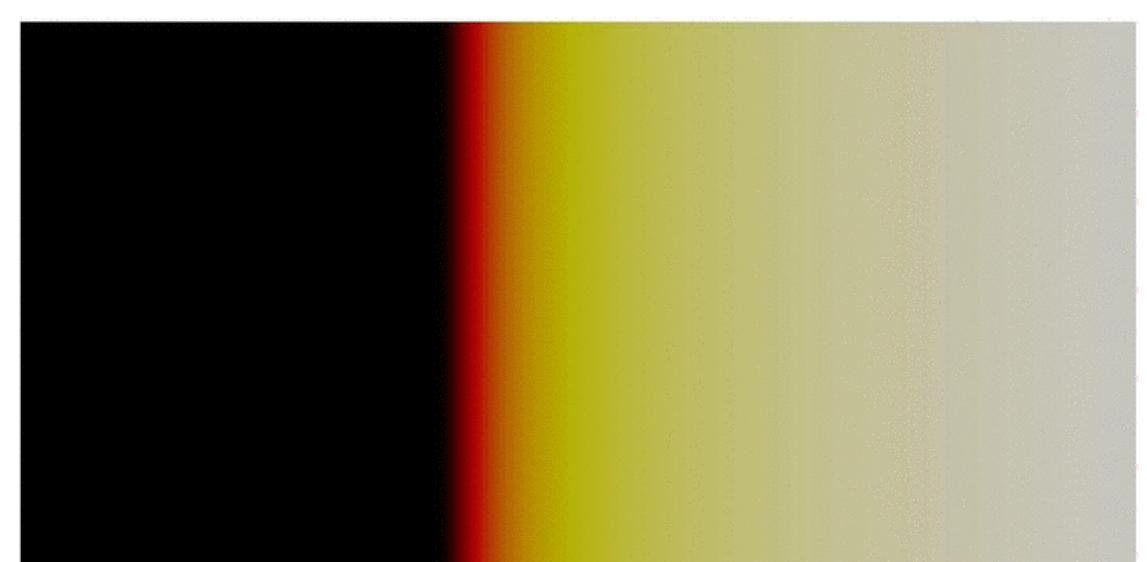
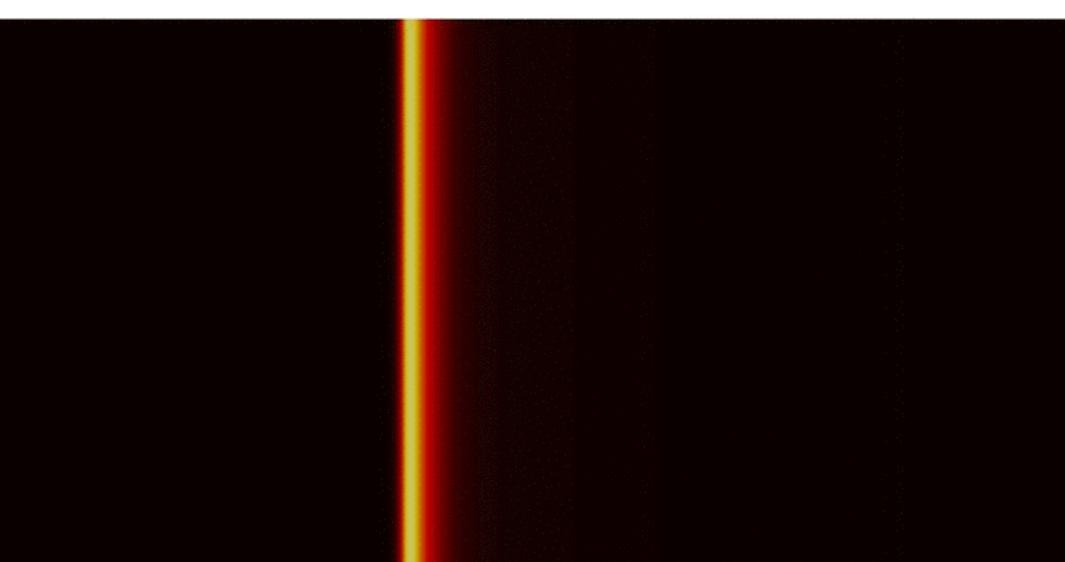
Case B:

Moderate

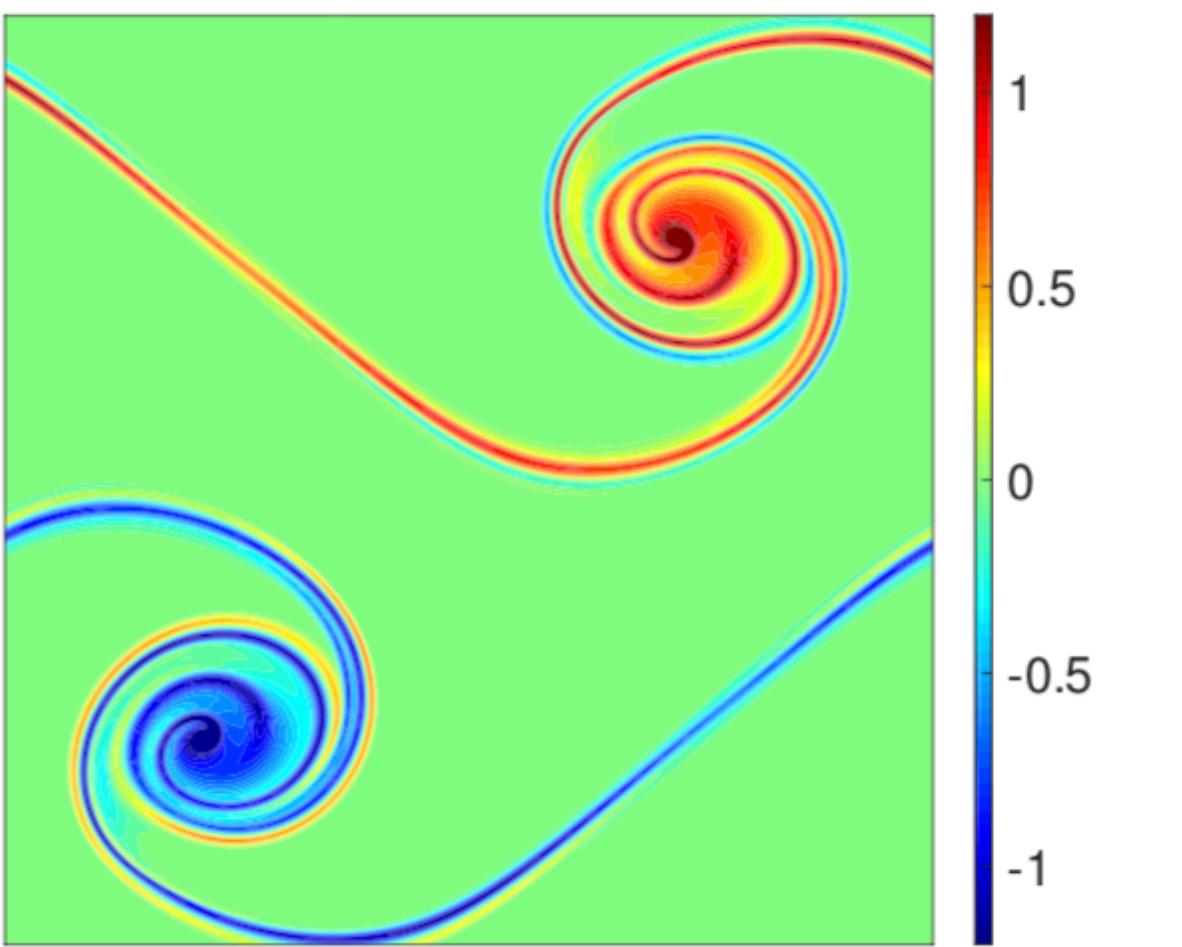
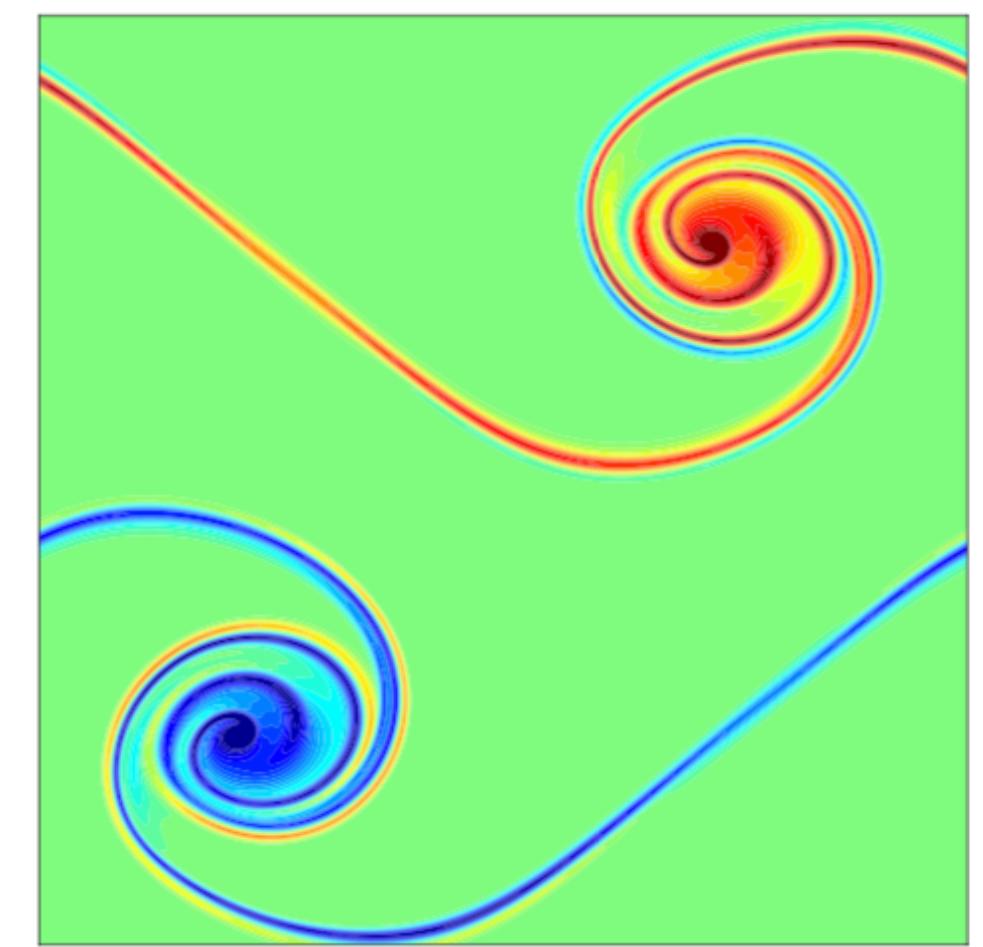
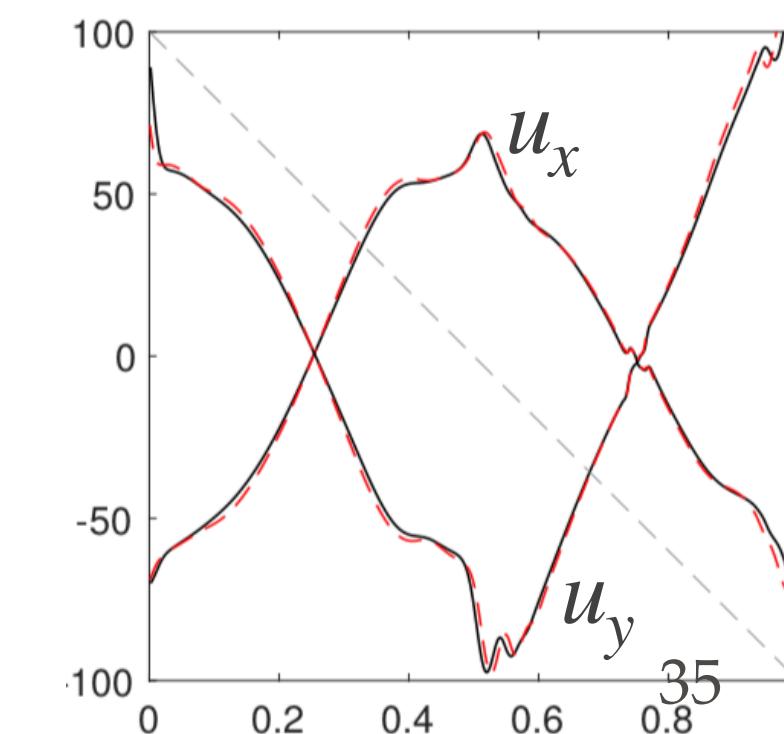
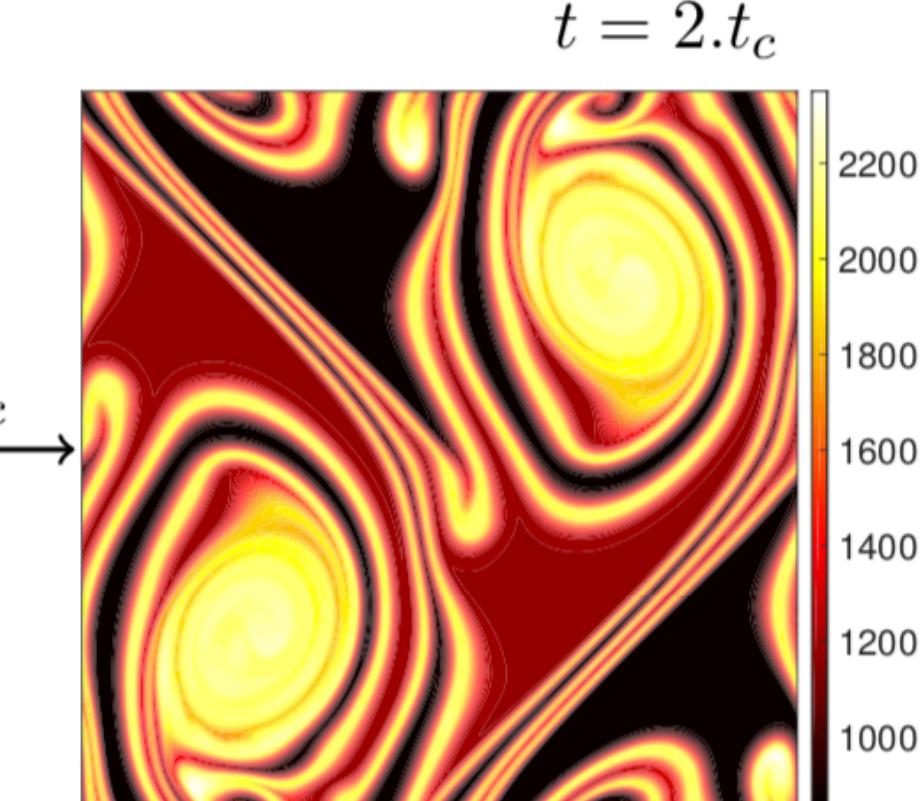
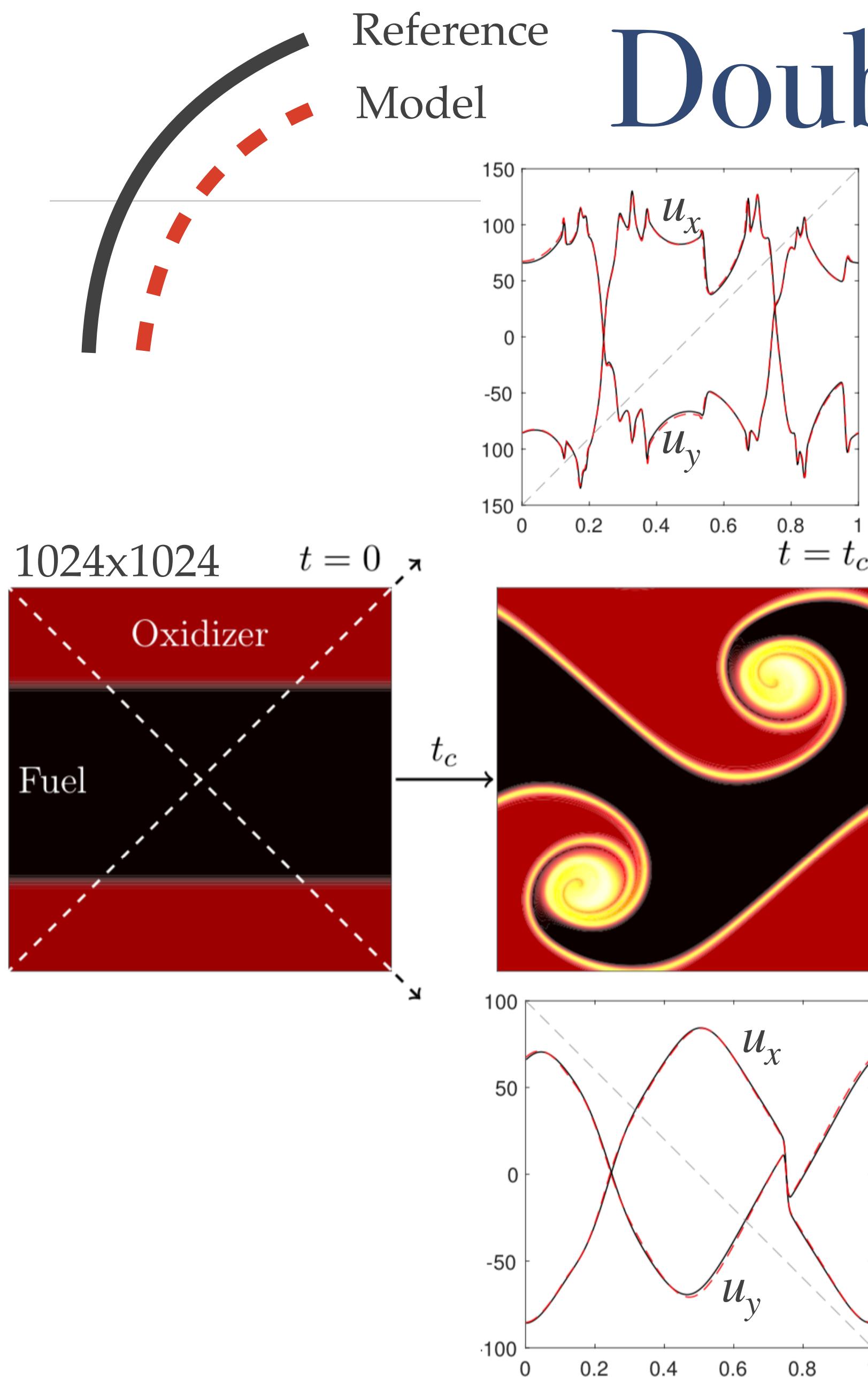


Case C:

Strong

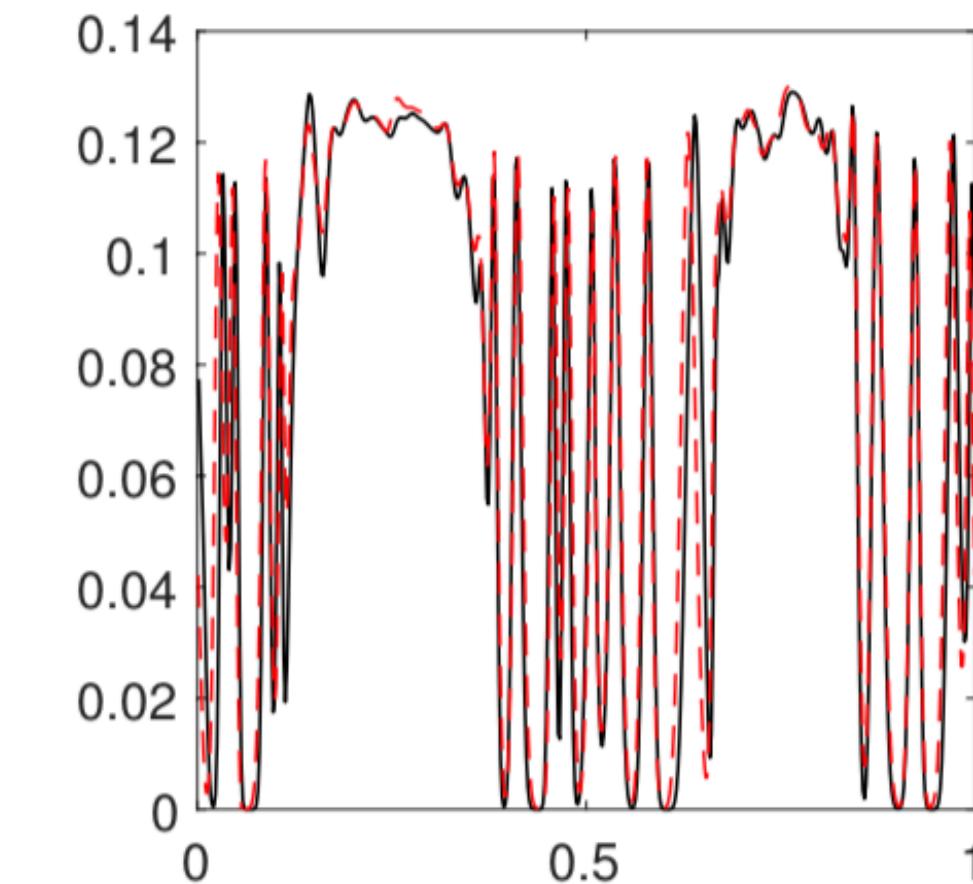
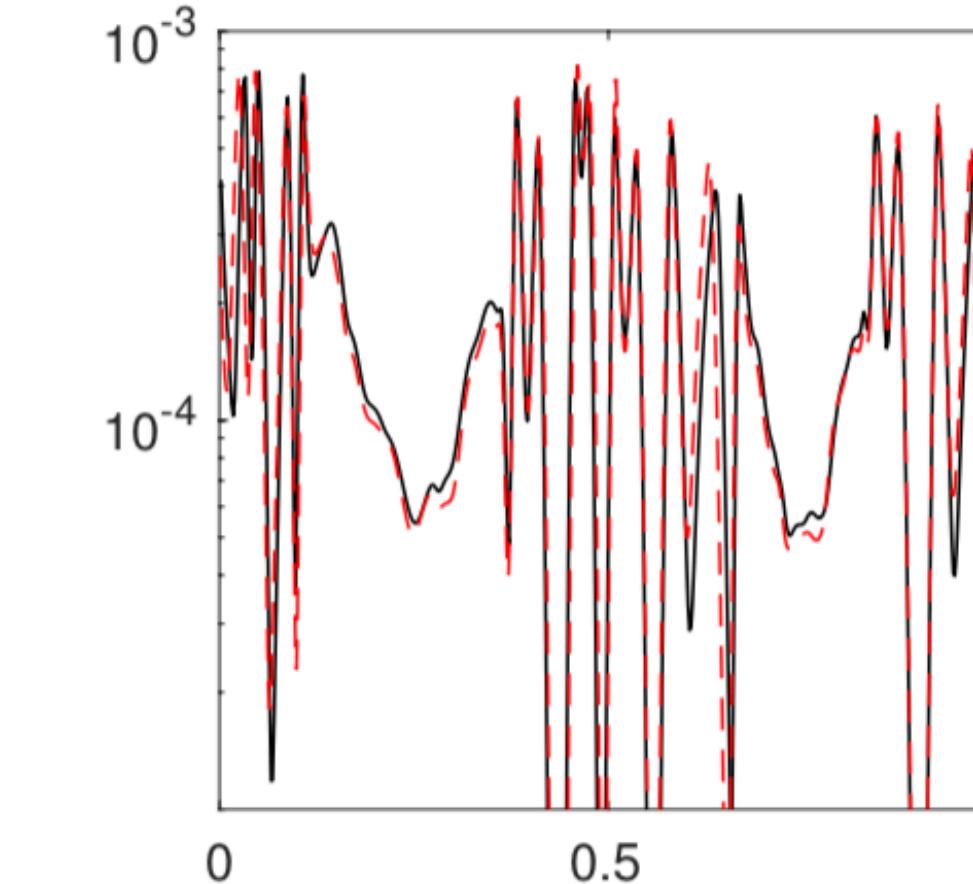
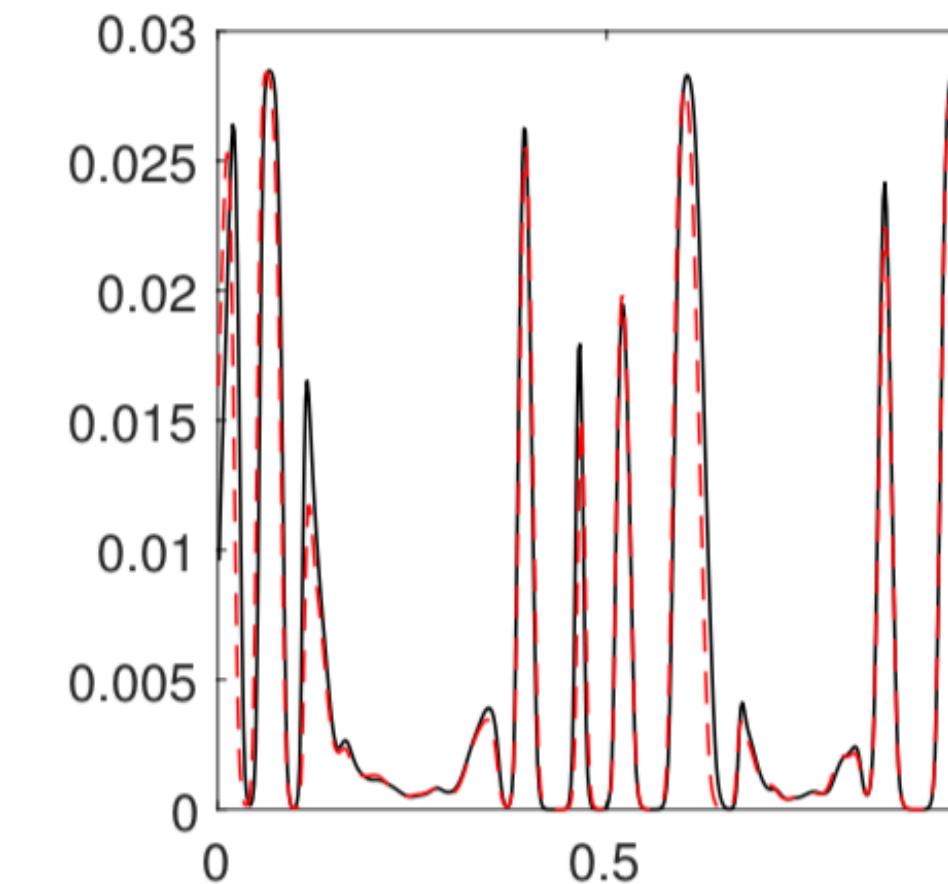
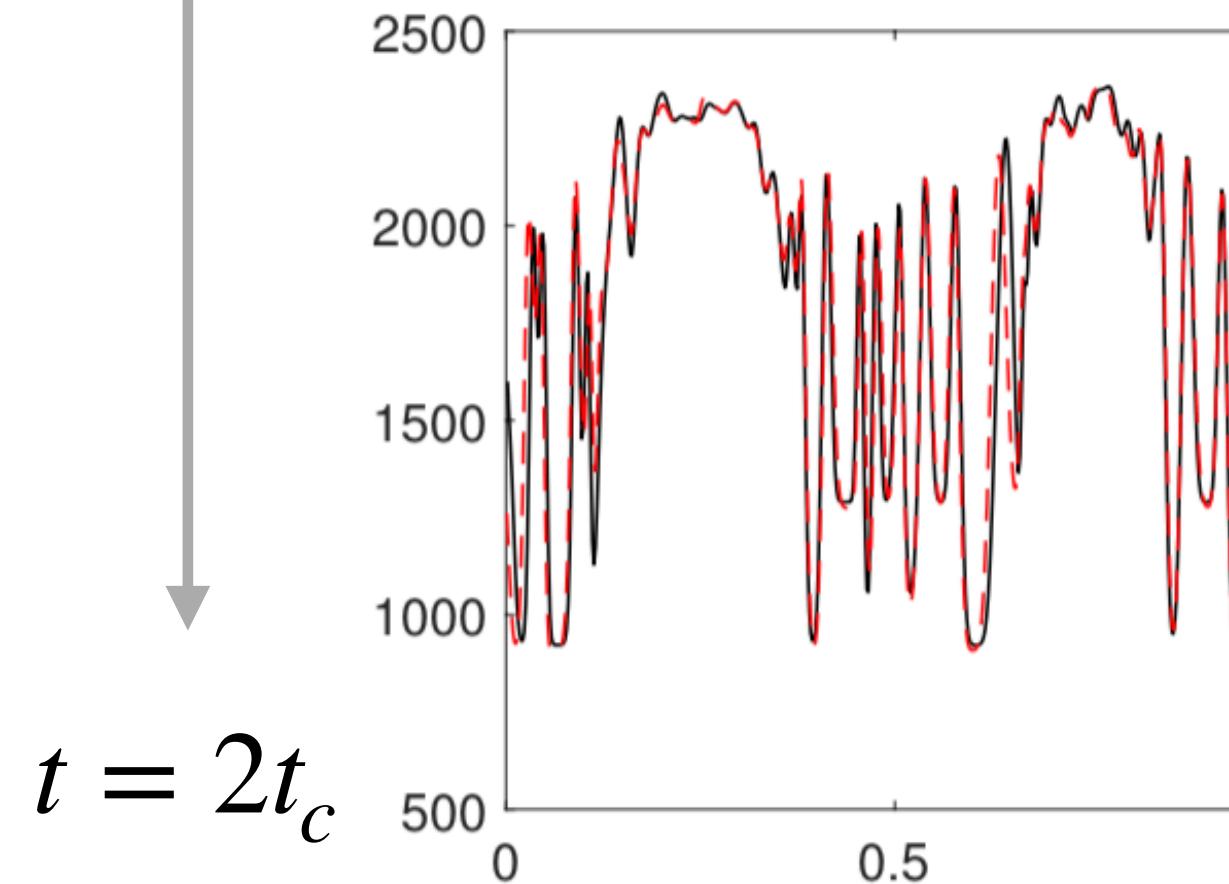
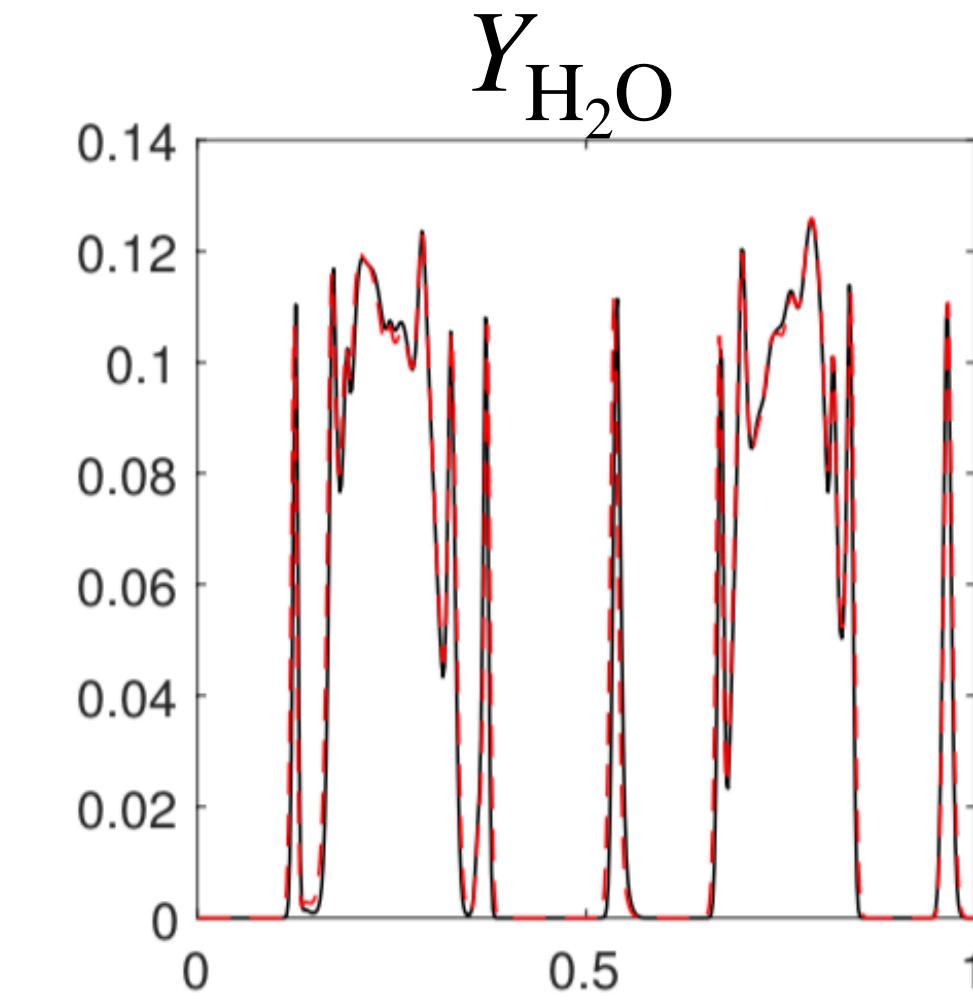
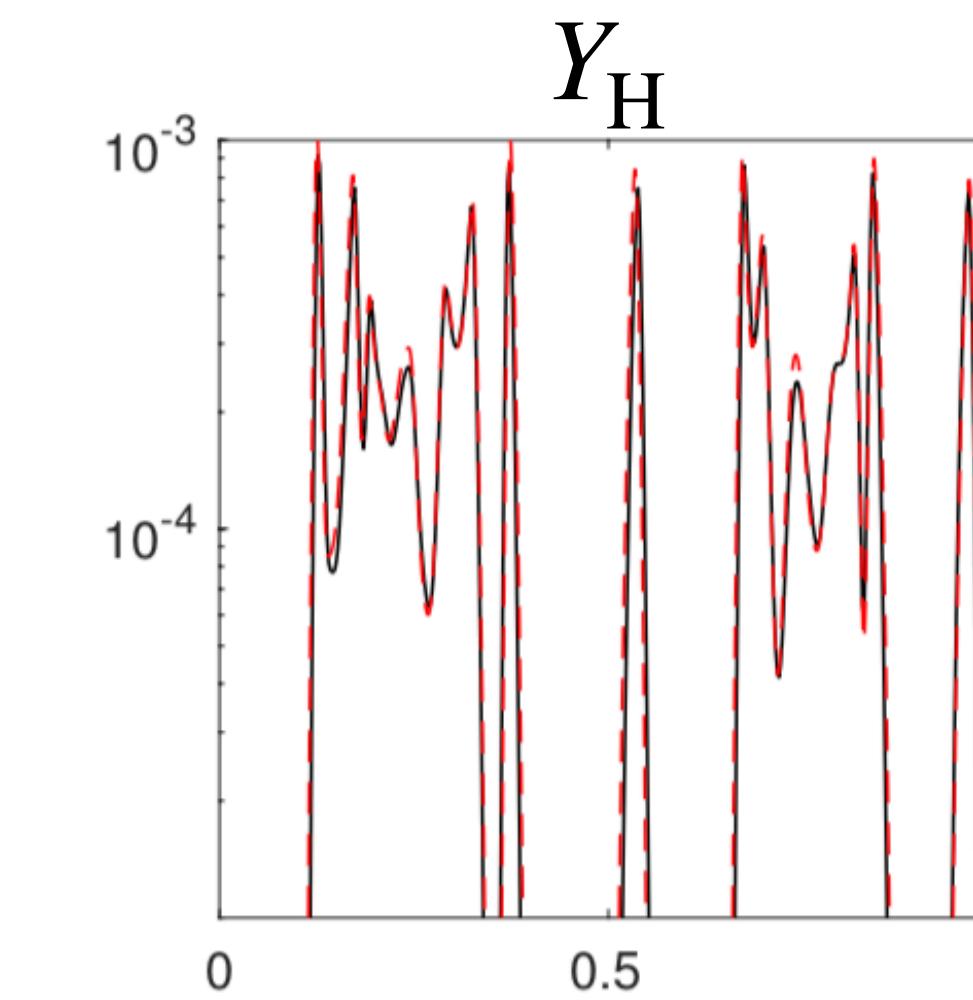
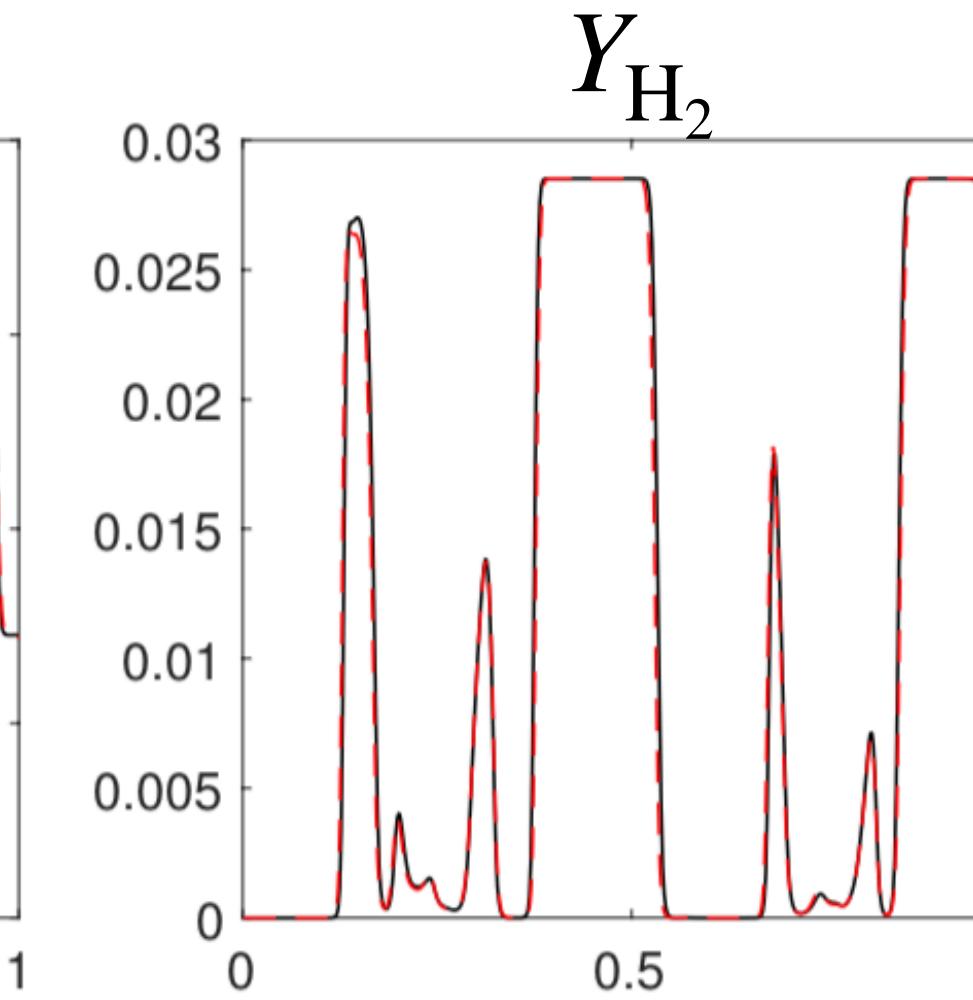
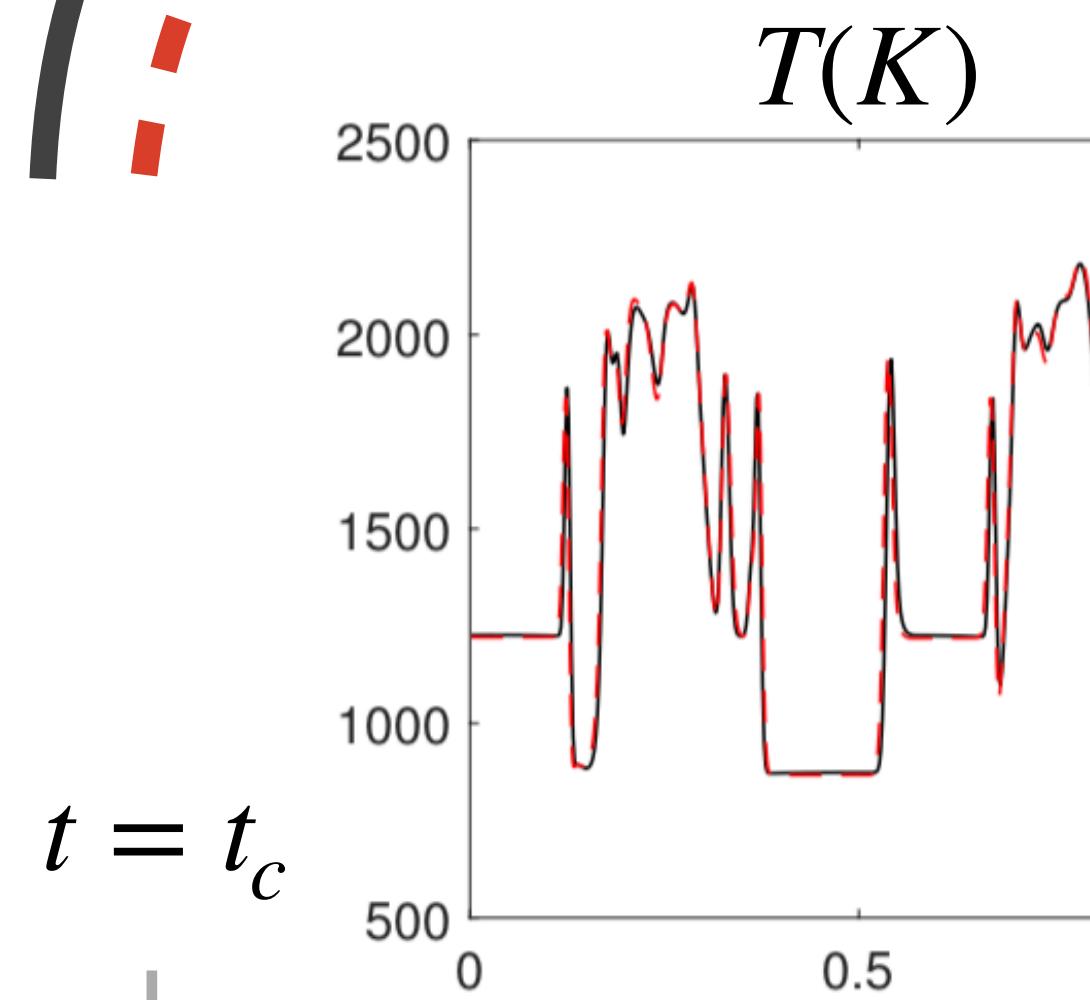


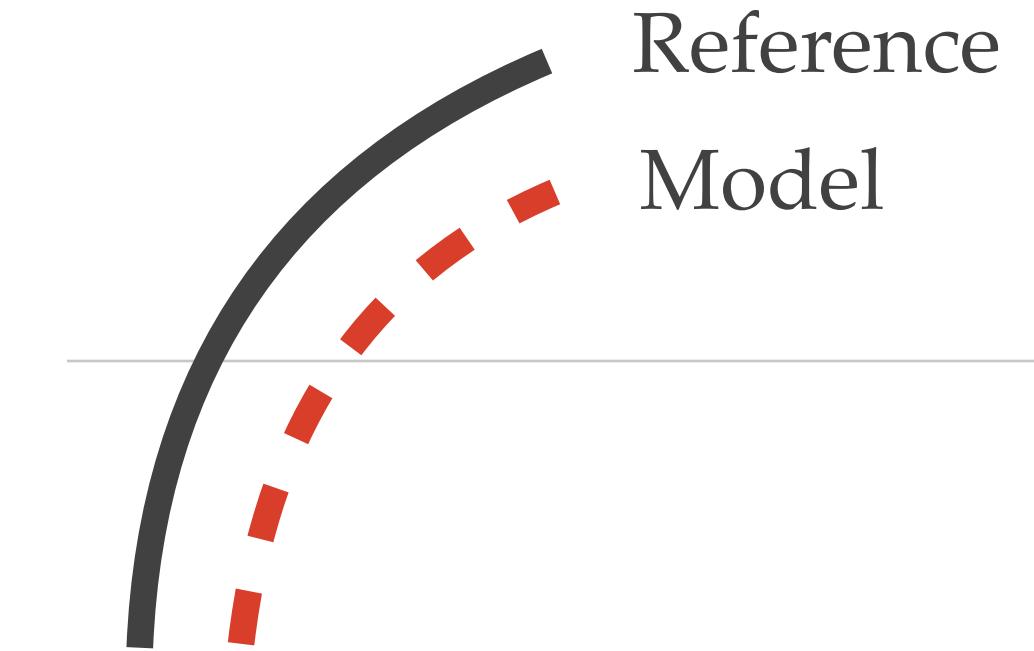
Double shear layer



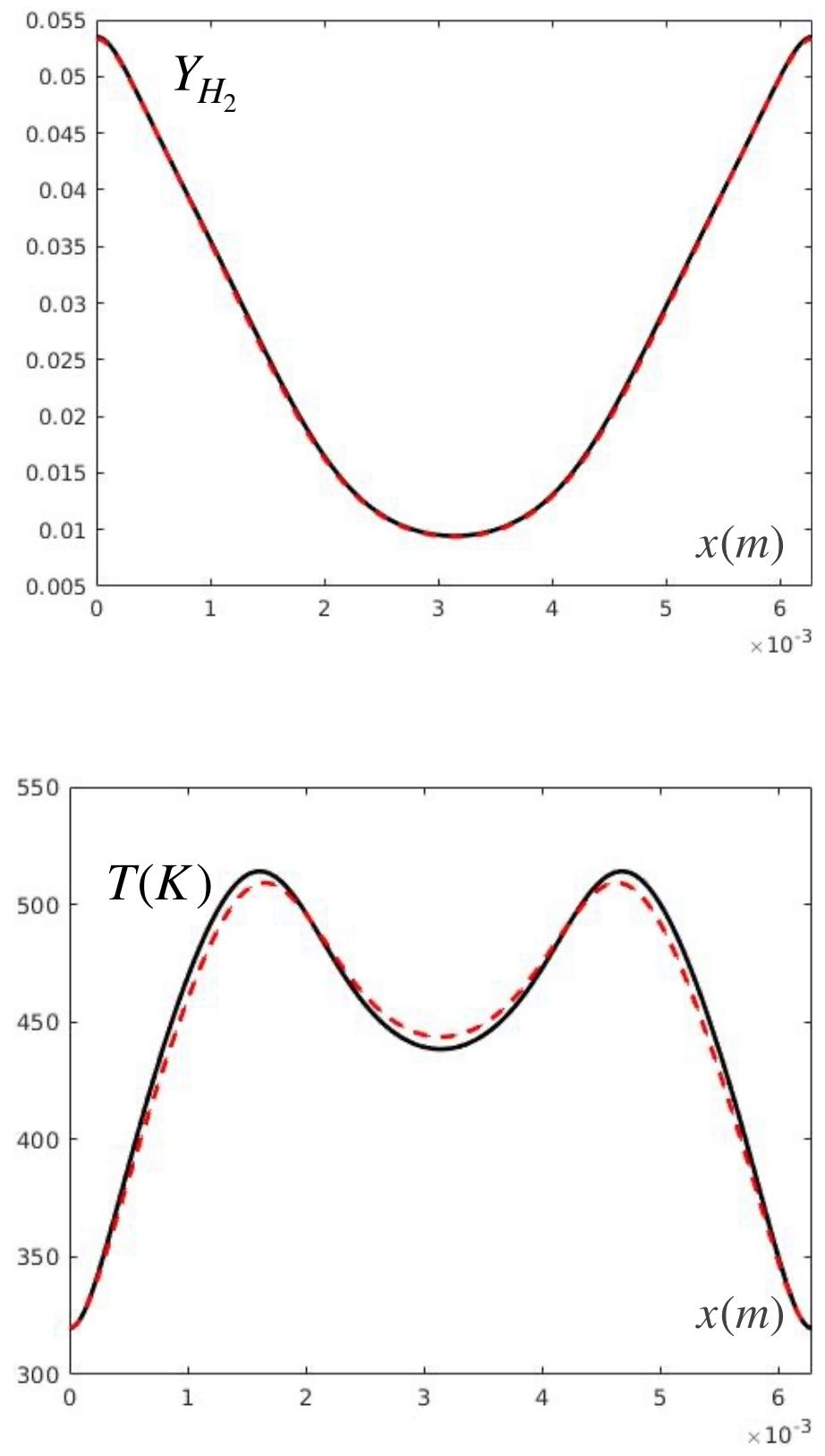
Double shear layer

Reference
Model

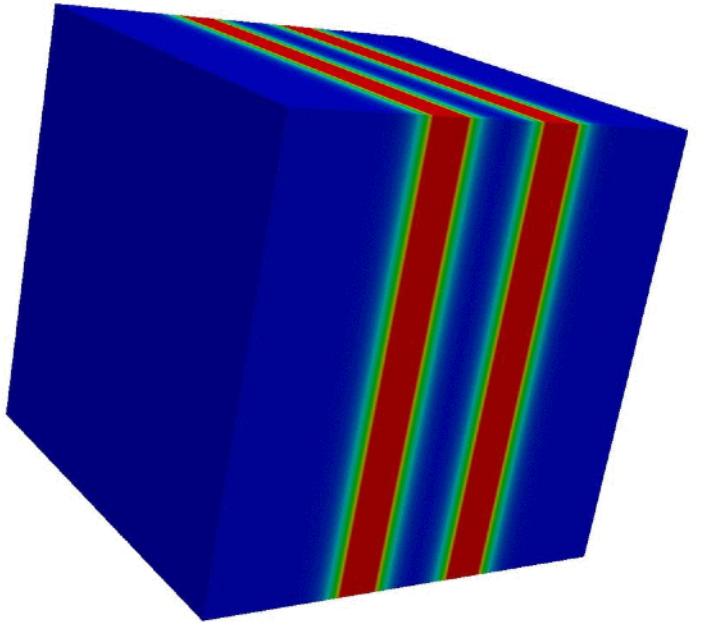




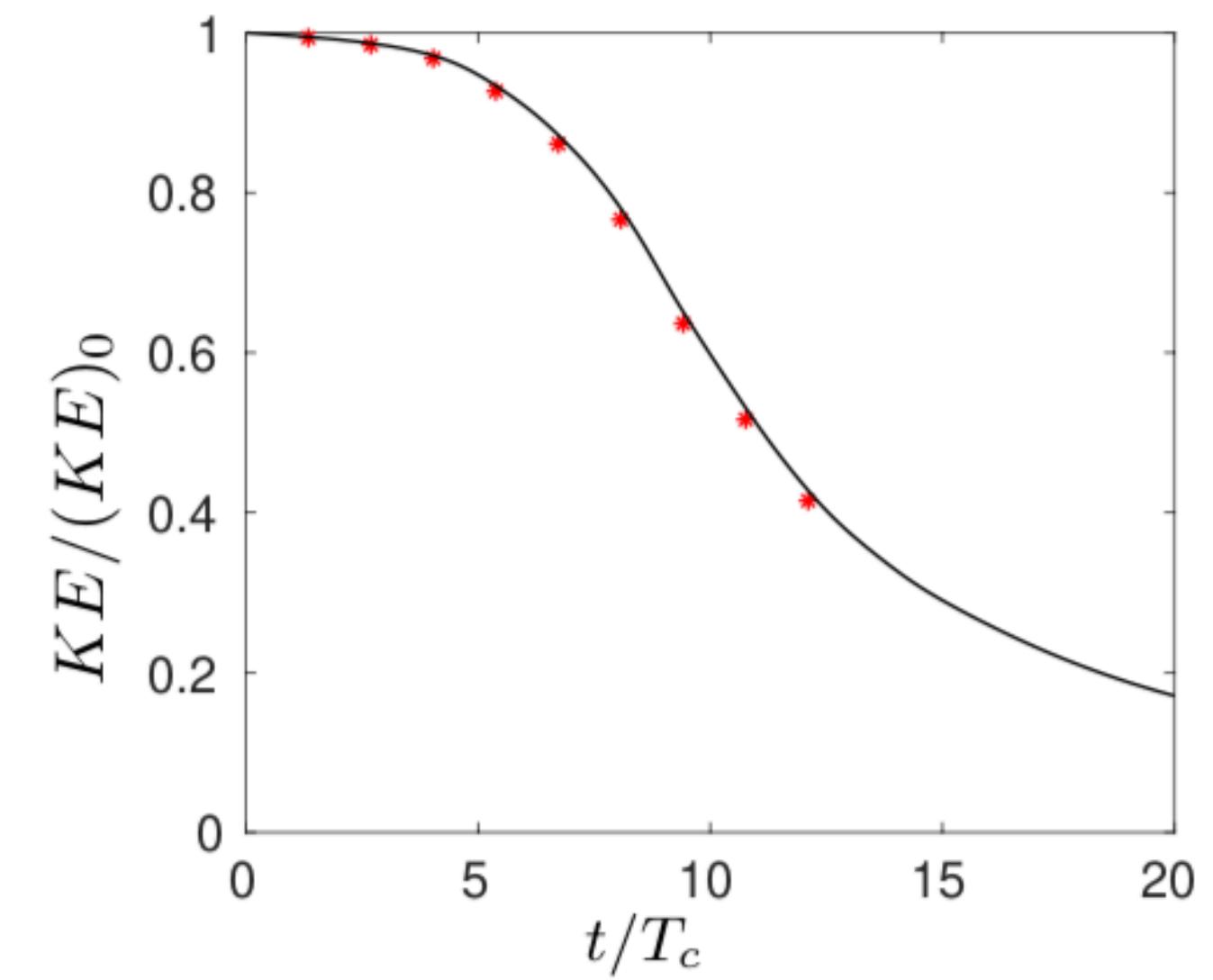
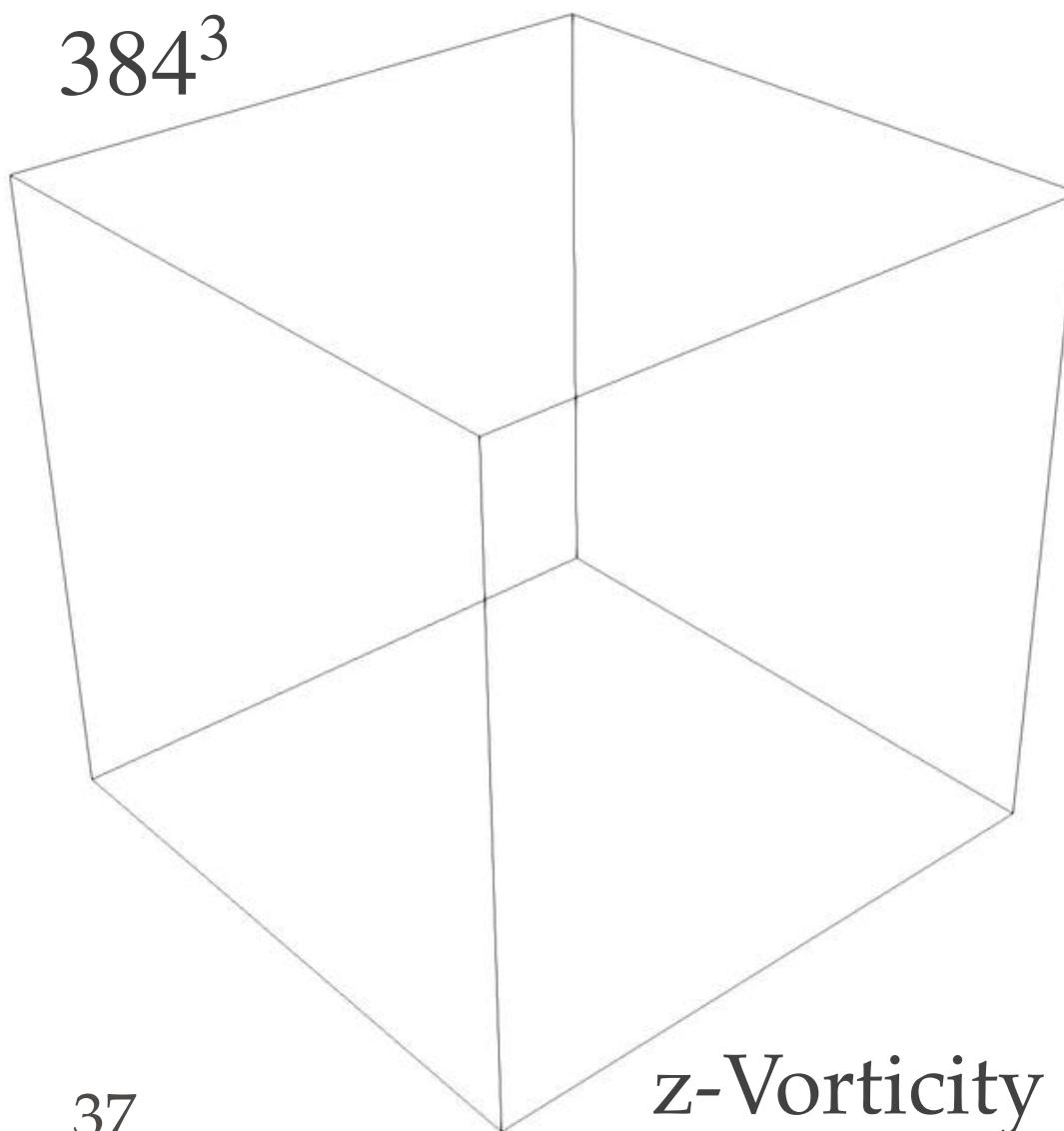
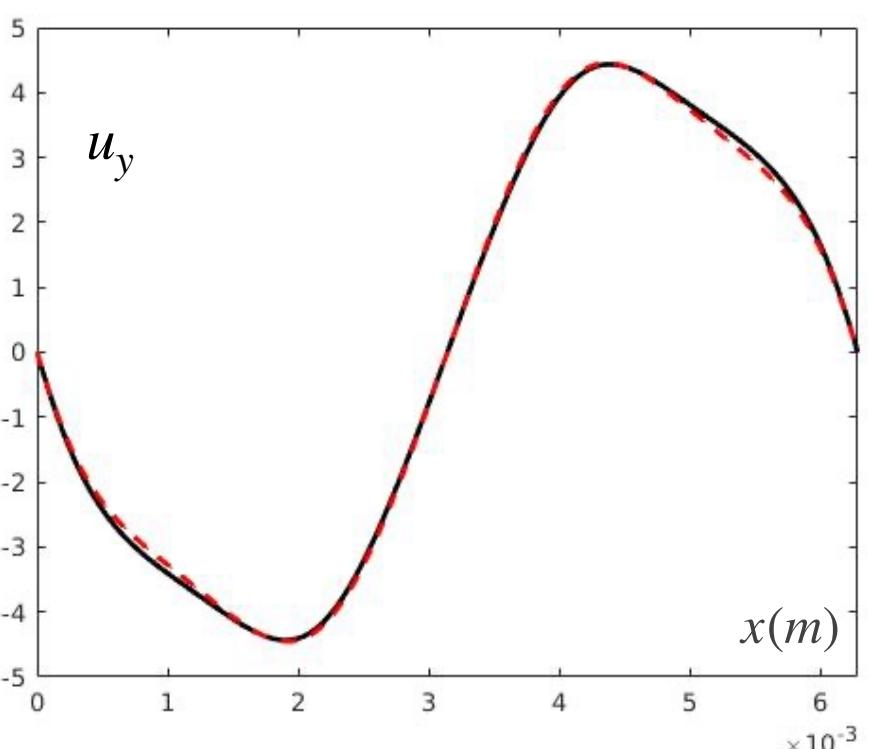
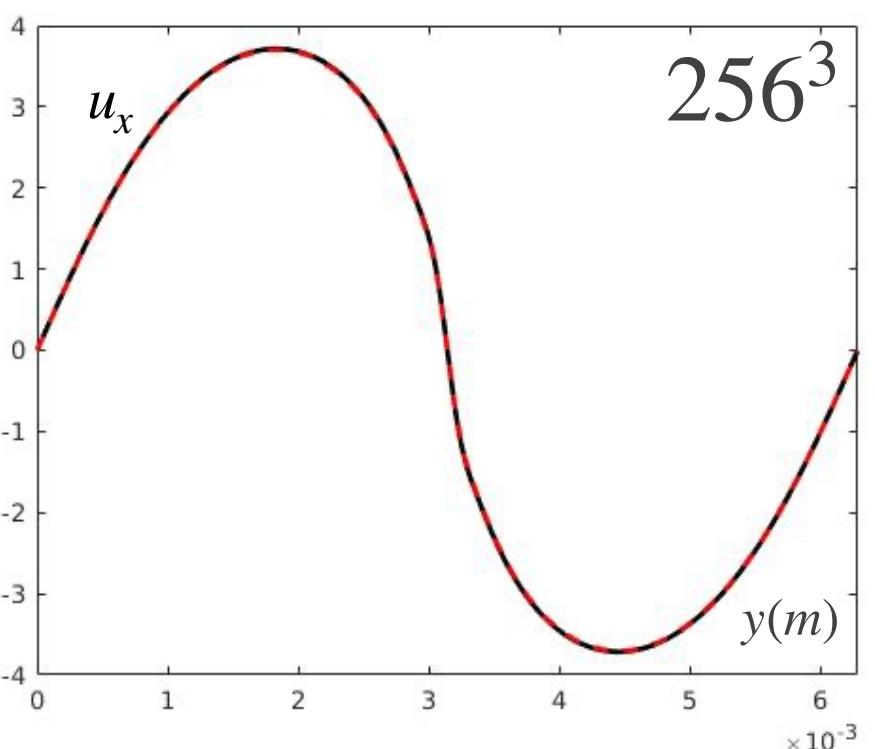
<< Cold case >>



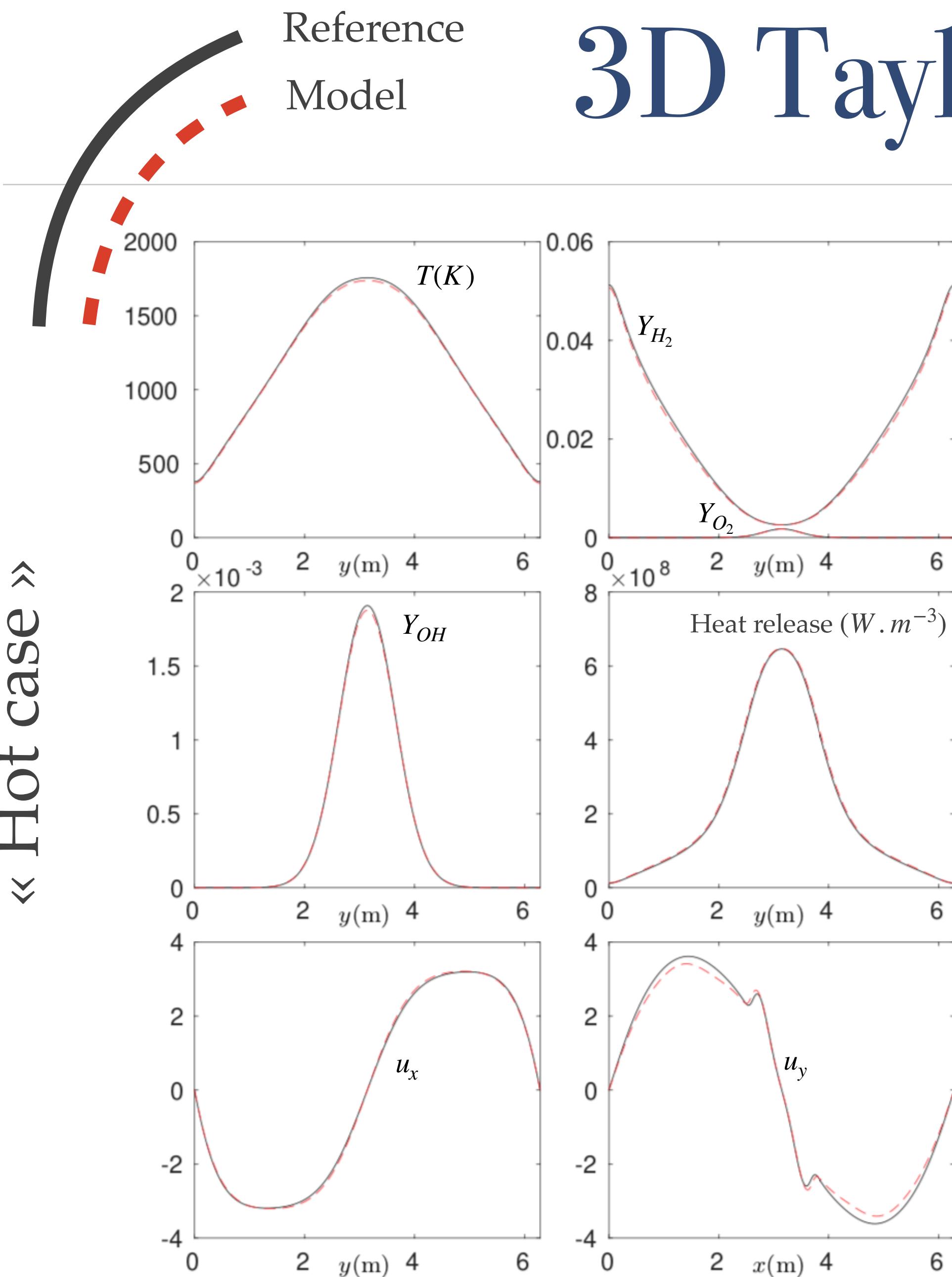
3D Taylor-Green Vortex



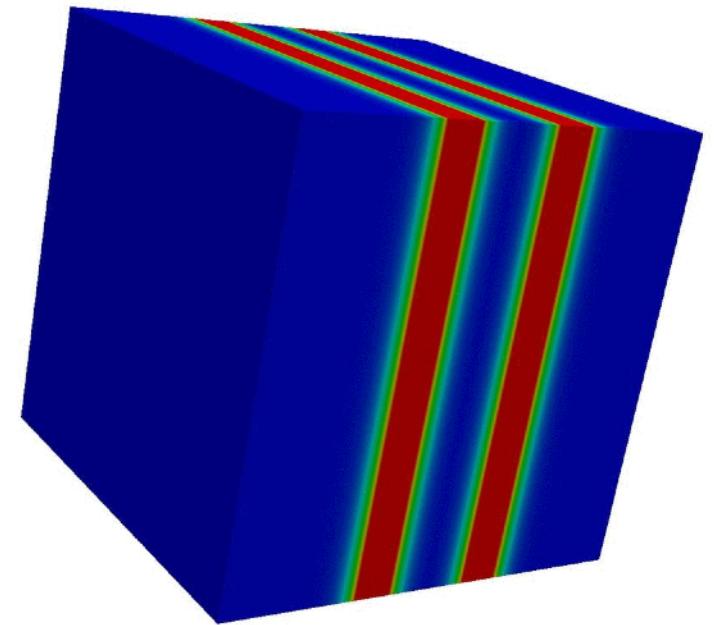
- ❖ Benchmark DNS for reactive flow
- ❖ Grids: 256^3 , 384^3 , 512^3 (mesocentre)
- ❖ ~10 codes participated (ICNC 2019)



Hot case »



3D Taylor-Green Vortex

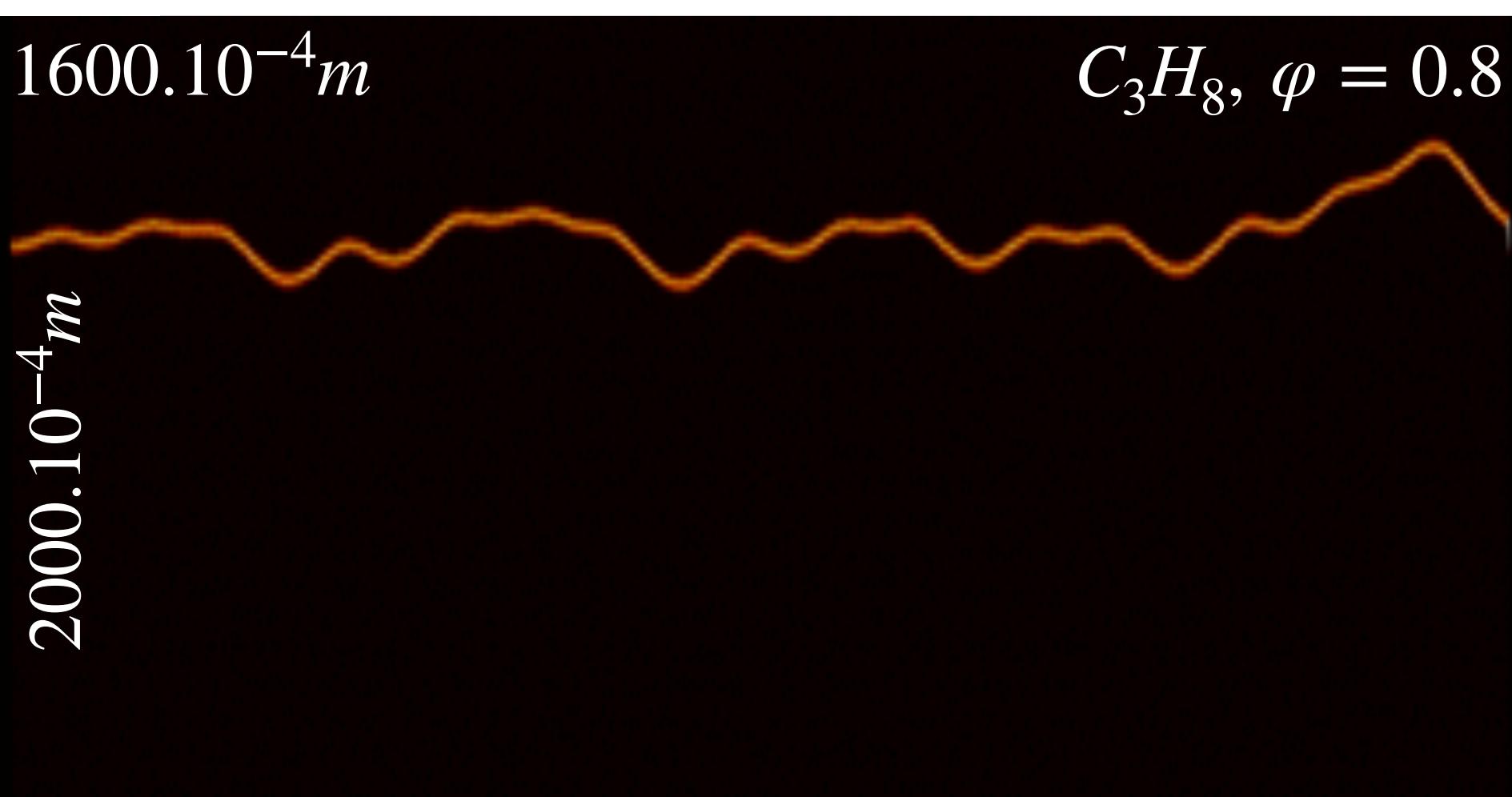


- ❖ Benchmark DNS for reactive flow
 - ❖ Grids: 256^3 , 384^3 , 512^3 (mesocentre)
 - ❖ ~ 10 codes participated (ICNC 2019)
- ❖ Comparisons are very good
- ❖ LBM is very (very) fast!

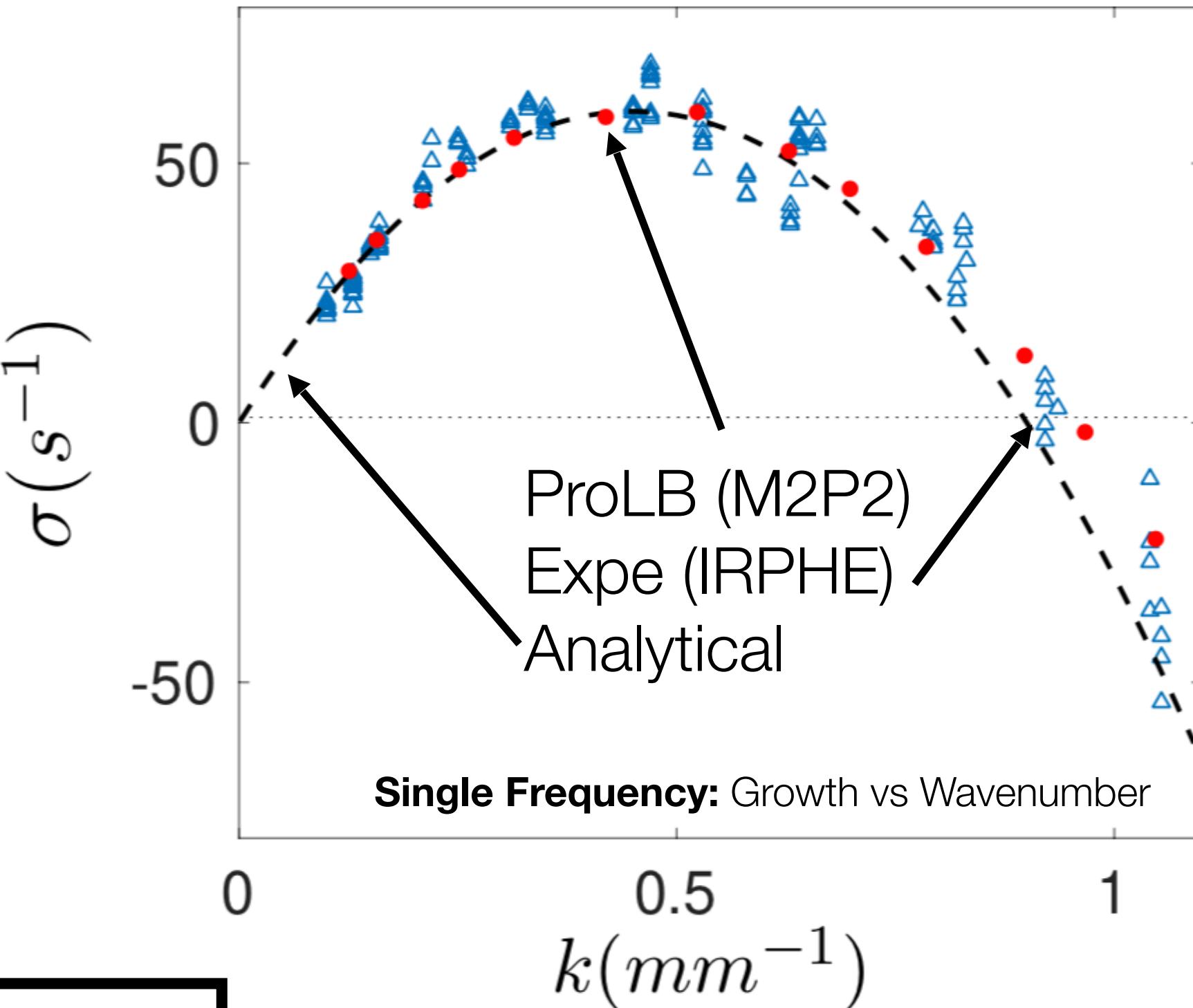
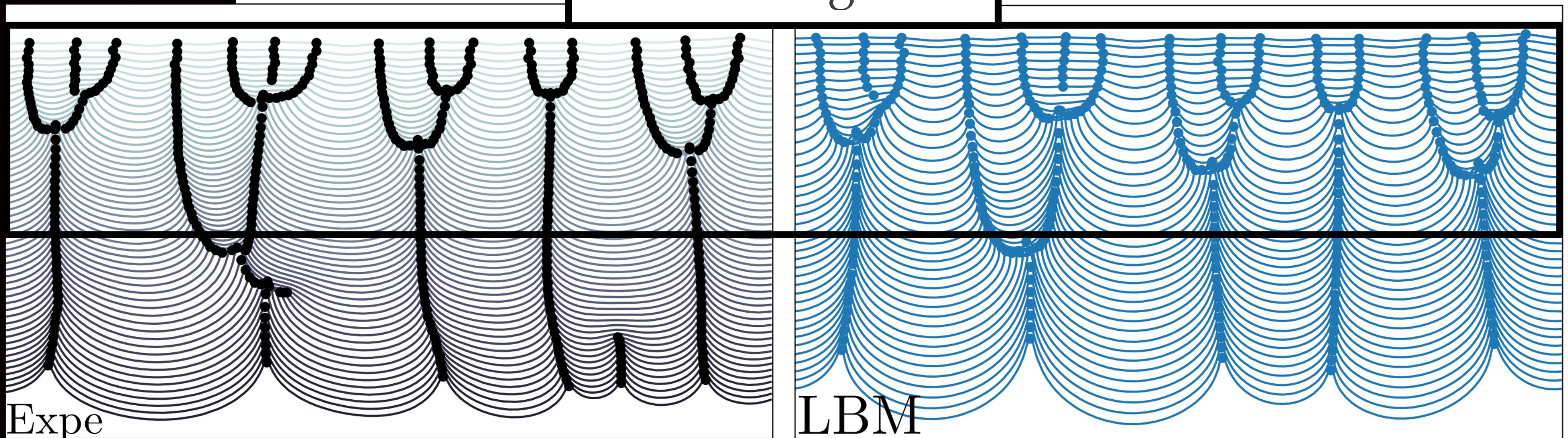
Outline

- ❖ Part I : M2P2 & me...
- ❖ Part II : LBM : price & prejudices
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Combustion instabilities



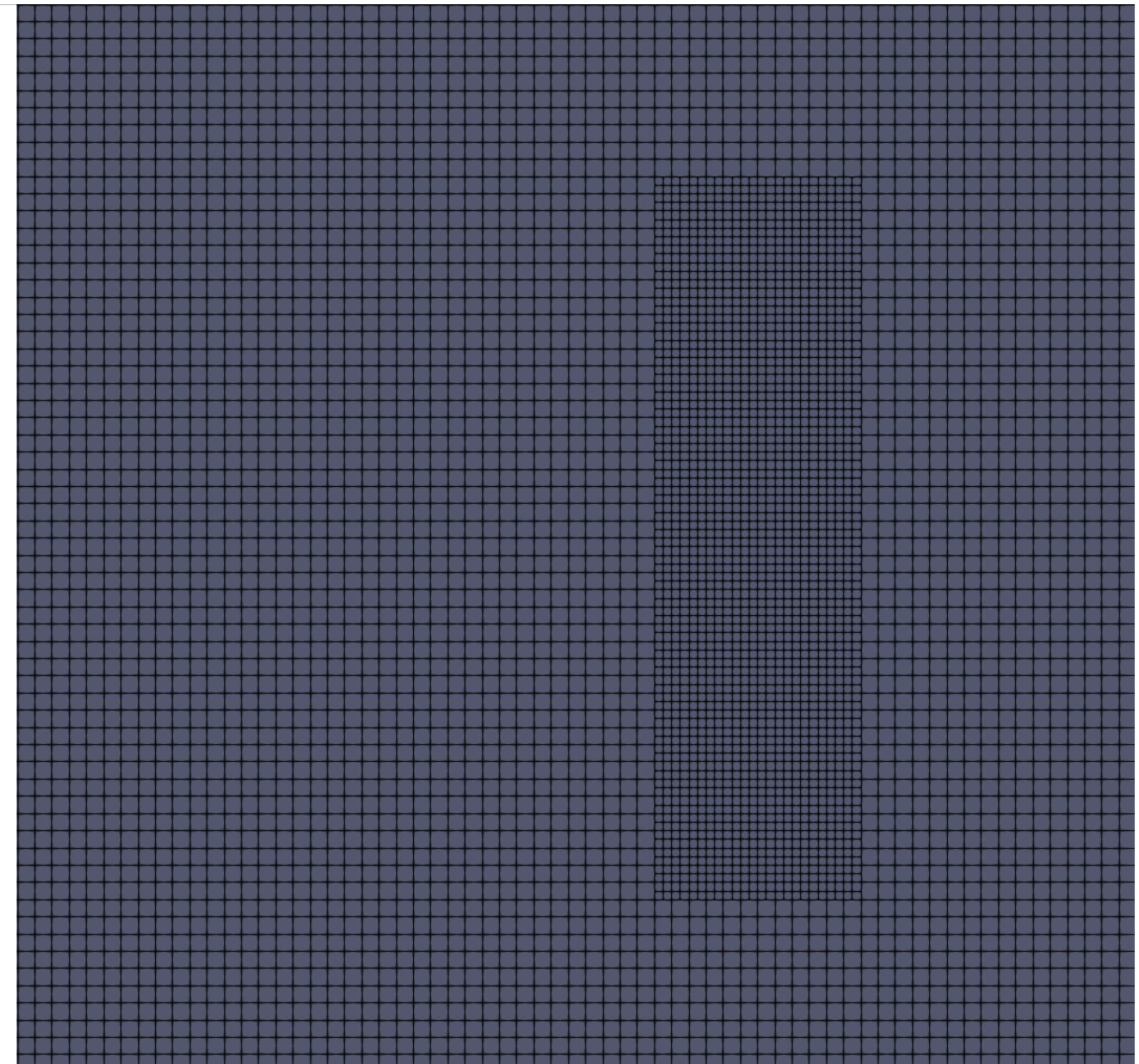
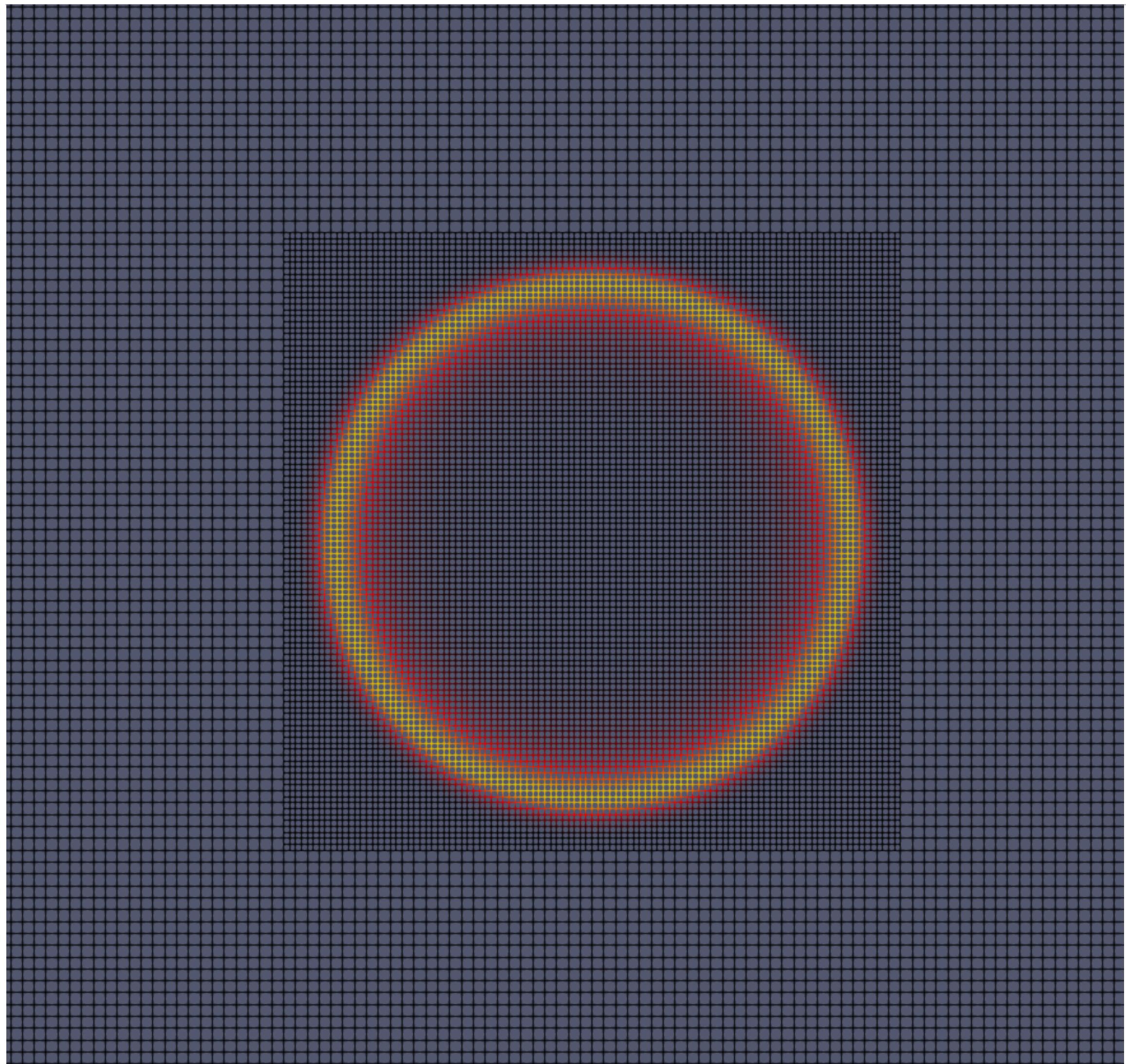
Thermo-diffusive
instabilities (propane / air)



❖ Hele-Shaw cell

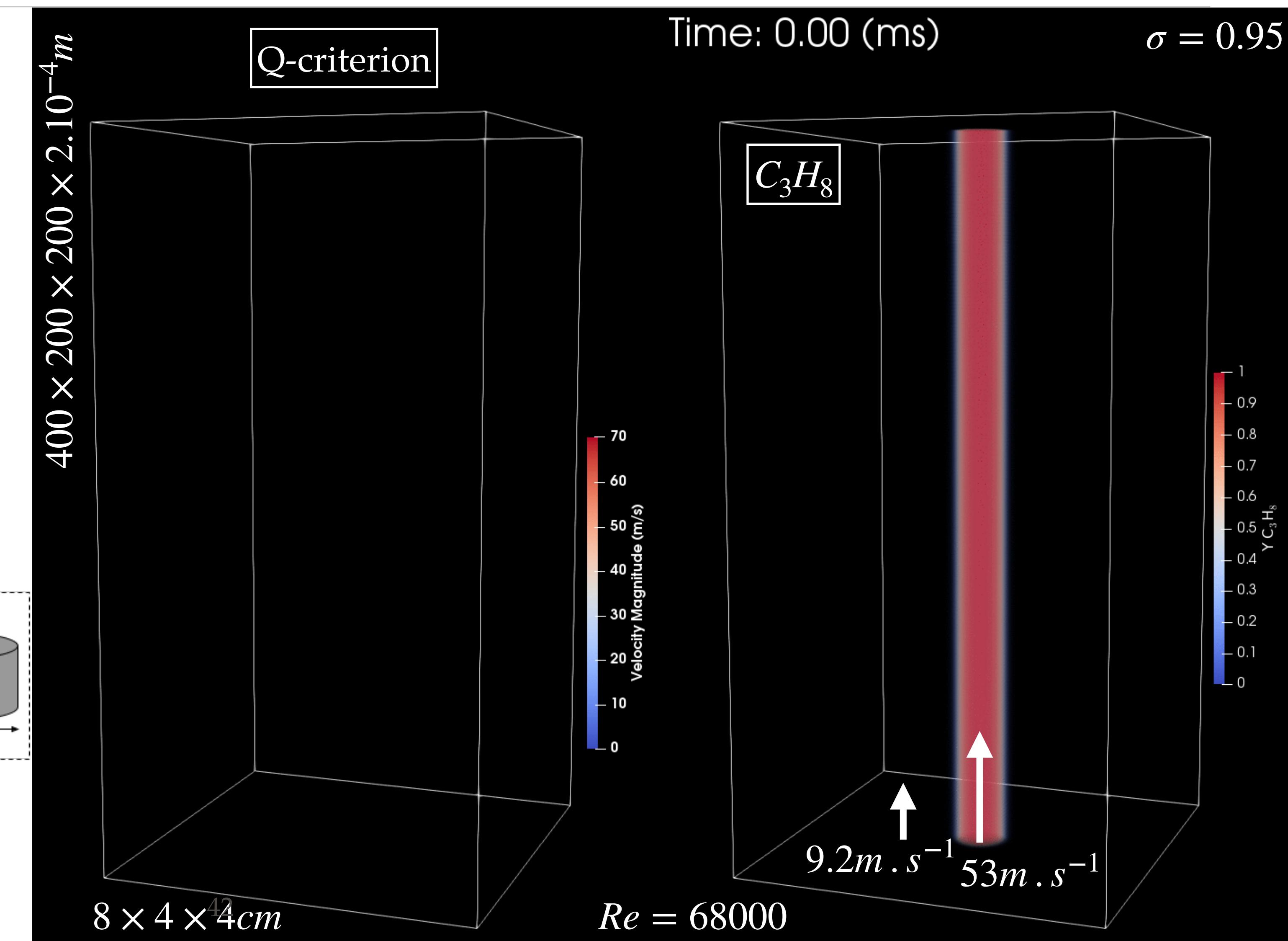
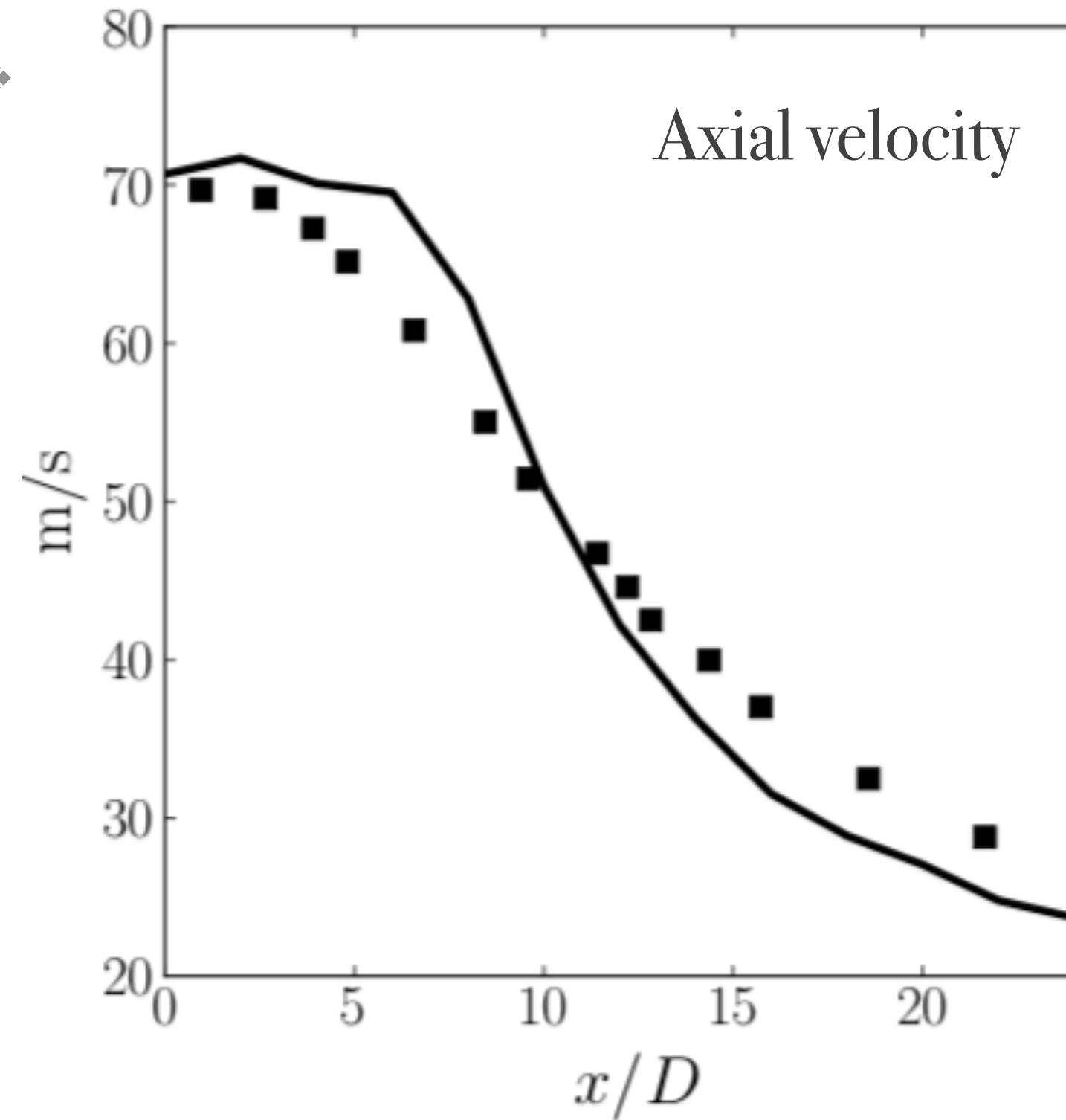
[1] M. Tayyab, B. Radisson, C. Almarcha, B. Denet, and P. Boivin, "Experimental and numerical lattice-boltzmann investigation of the Darrieus-Landau instability," Combustion and Flame, 2020.

Mesh transitions



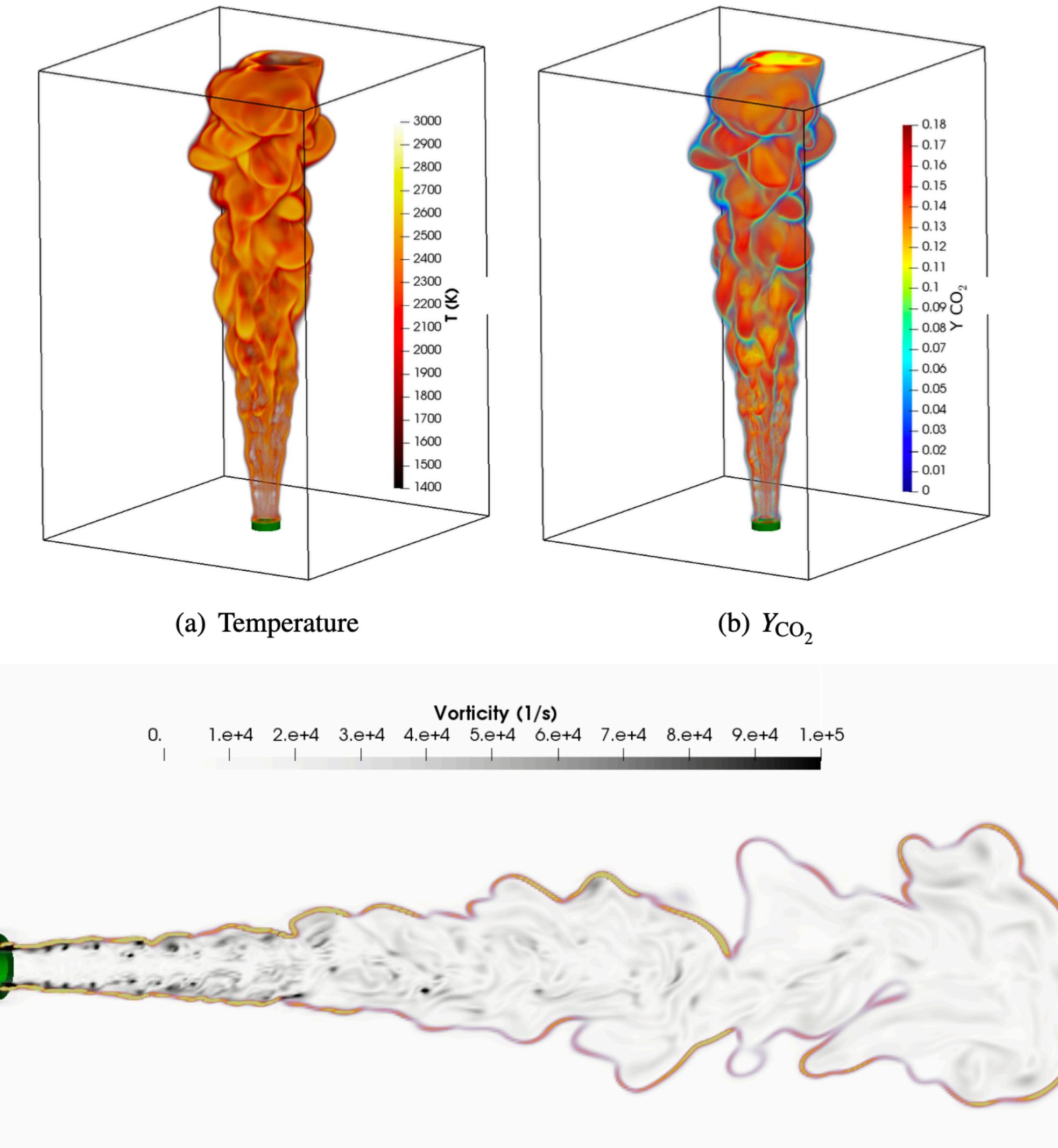
3D turbulent jet

- ❖ Propane non-premixed jet flow (variable density) - Sandia
- ❖ $300 \times 200 \times 200 + \text{refinement}$



3D turbulent jet

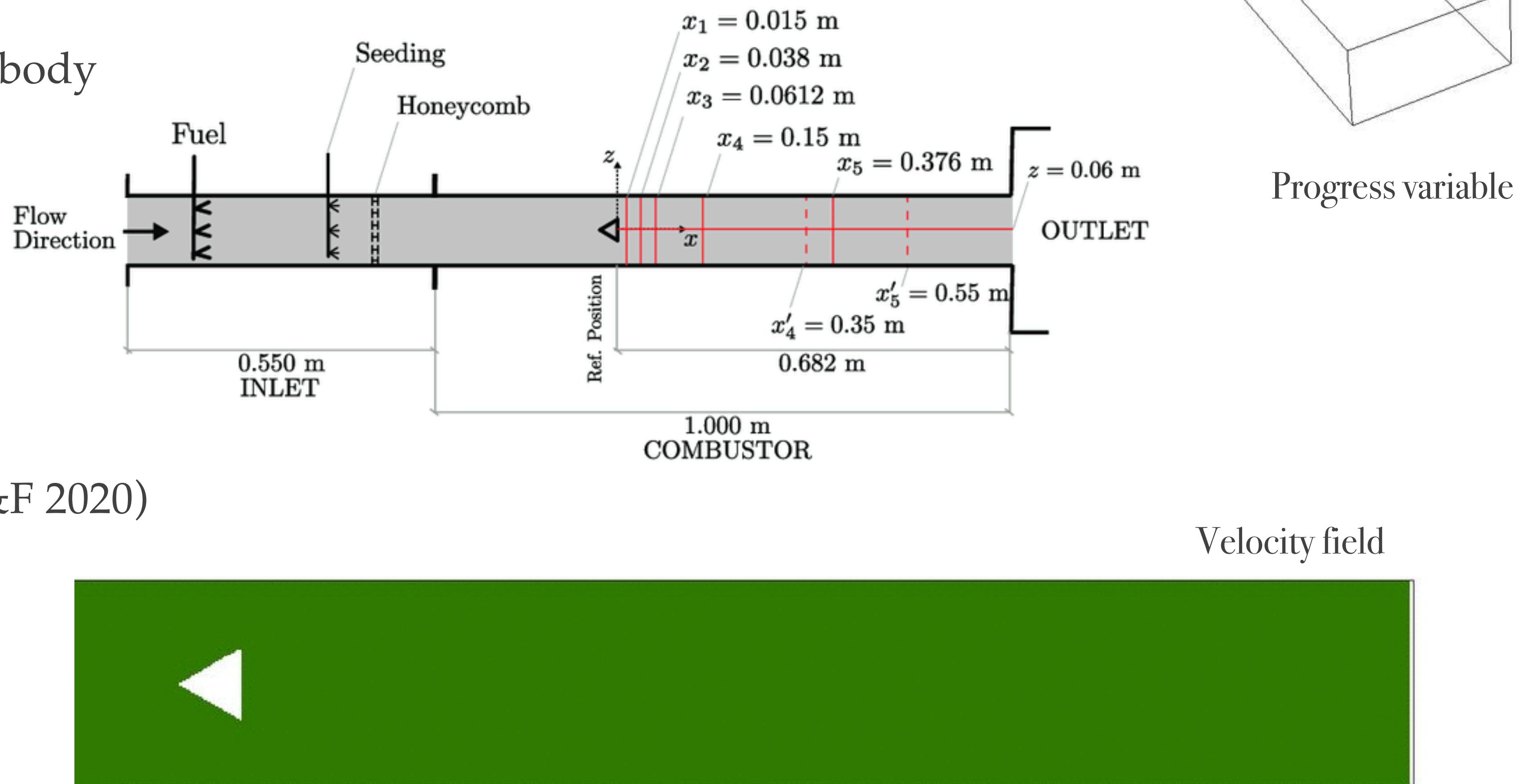
- ❖ Propane non-premixed jet flow (variable density) - Sandia
- ❖ 300x200x200 + refinement
- ❖ The same, reactive
 - ❖ No subgrid model (flow)
 - ❖ no subgrid model (combustion)
 - ❖ = Highly robust !
- ❖ Future work - rerun on an experimental jet using a turbulent combustion model





Volvo Burner

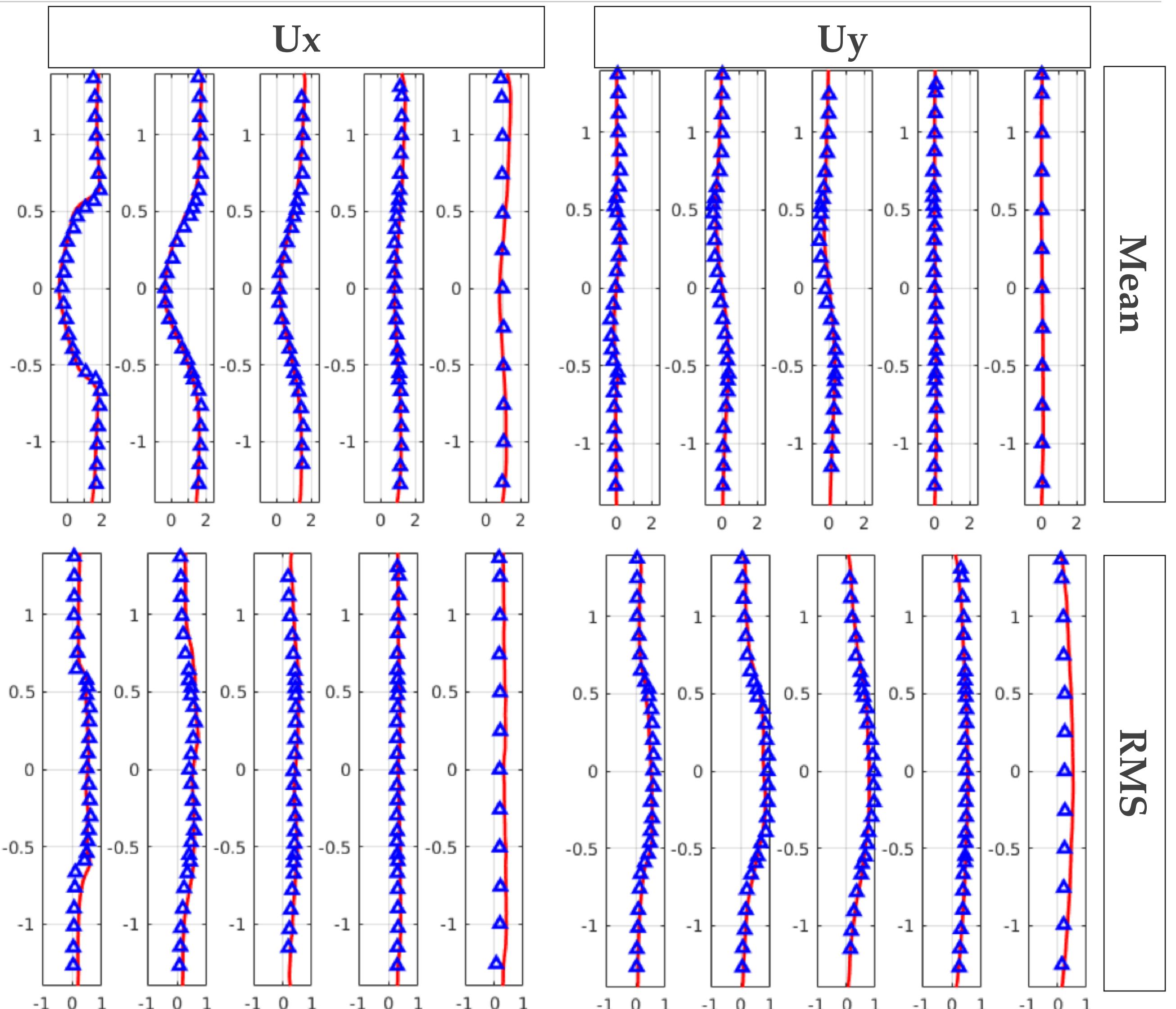
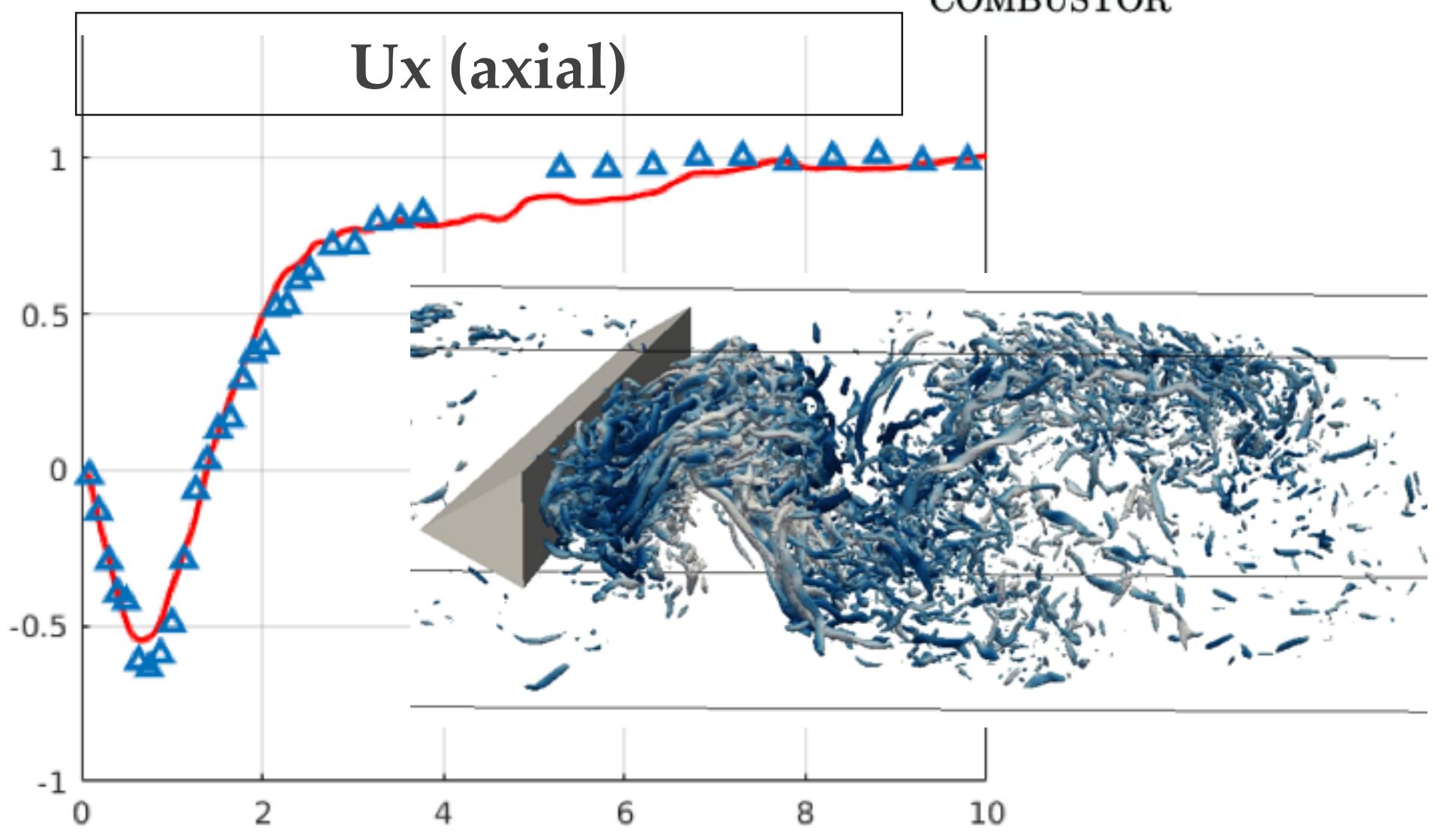
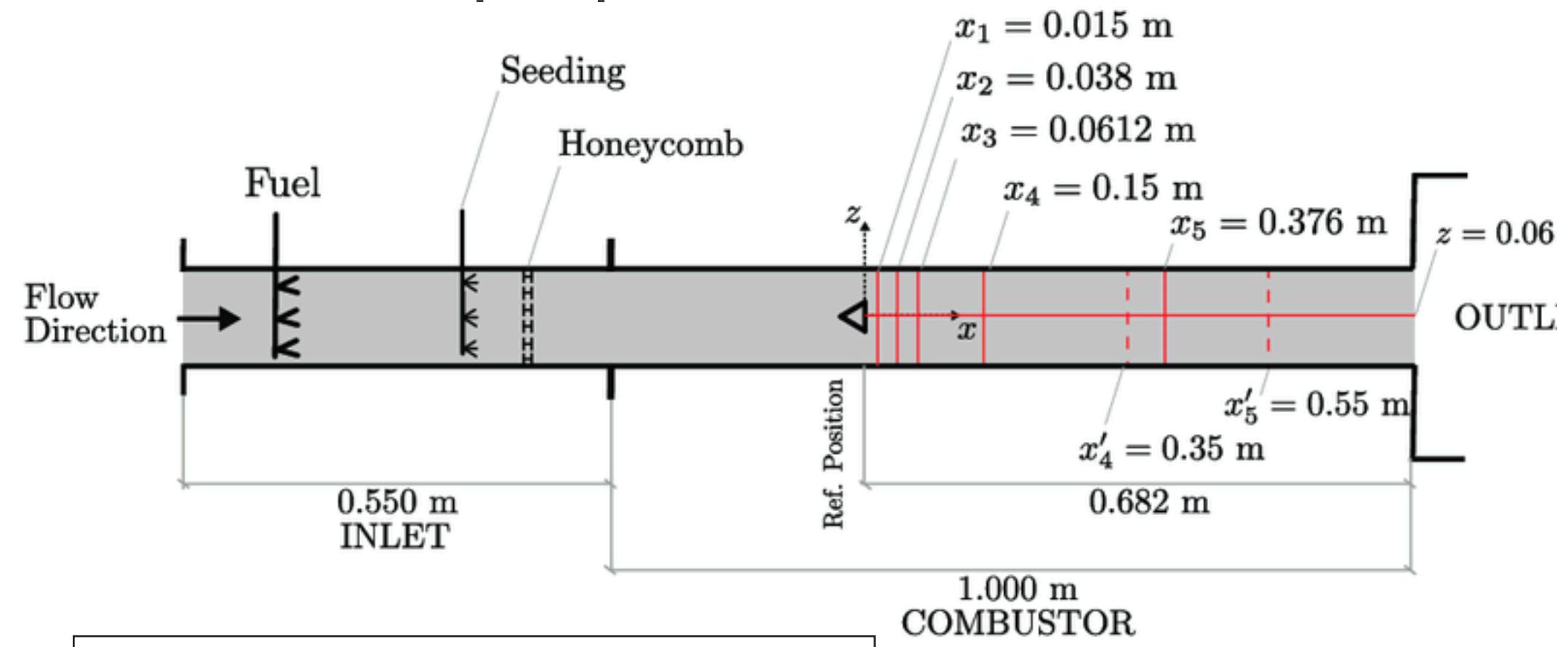
- ❖ Common to validate premixed turbulent combustion model
- ❖ Flame stabilized behind bluff body
- ❖ Numerical set-up
 - ❖ Min grid size: 2mm, 1mm
 - ❖ 2 step propane chemistry
 - ❖ TFLES model (Rochette C&F 2020)





Volvo burner

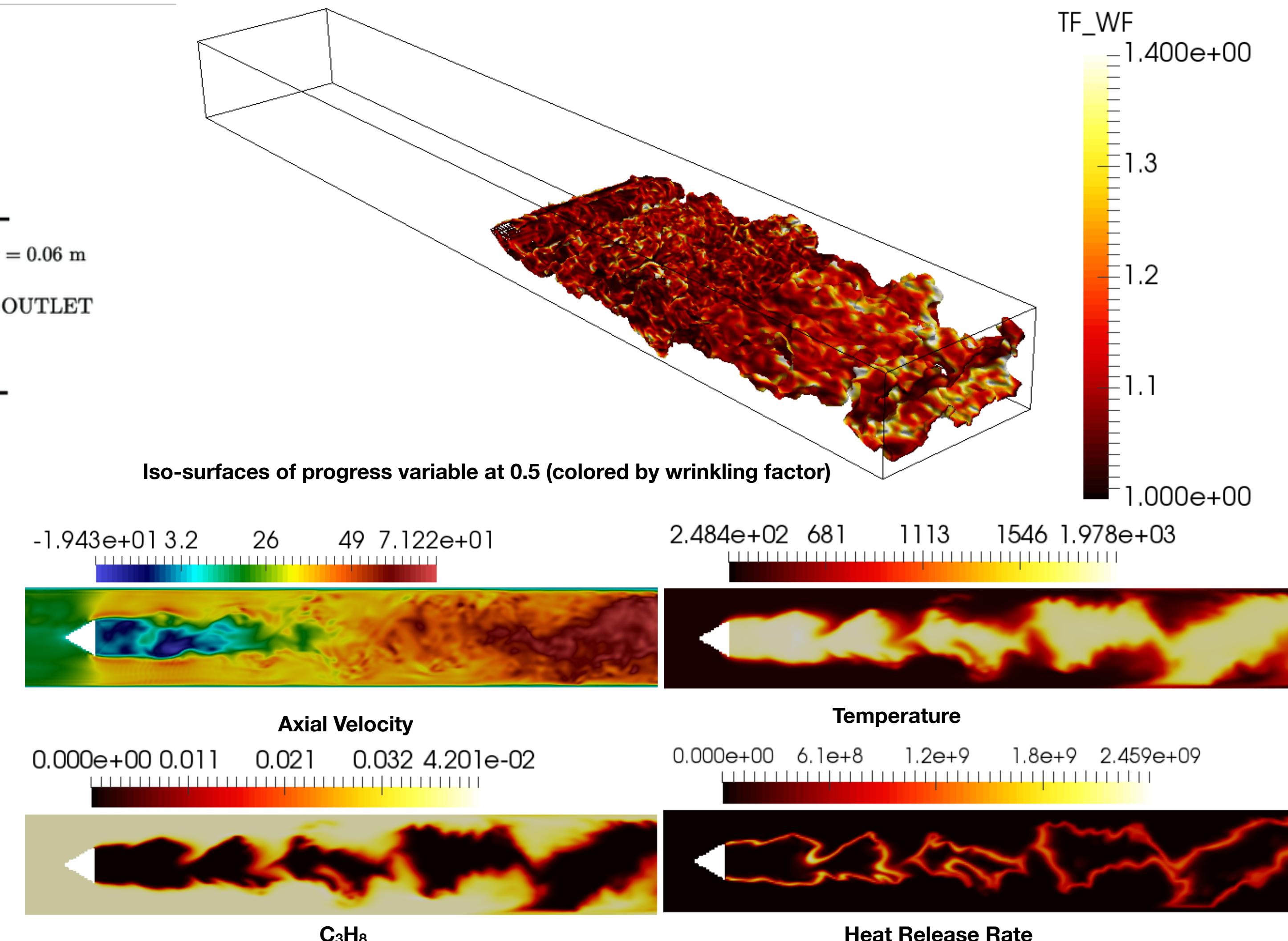
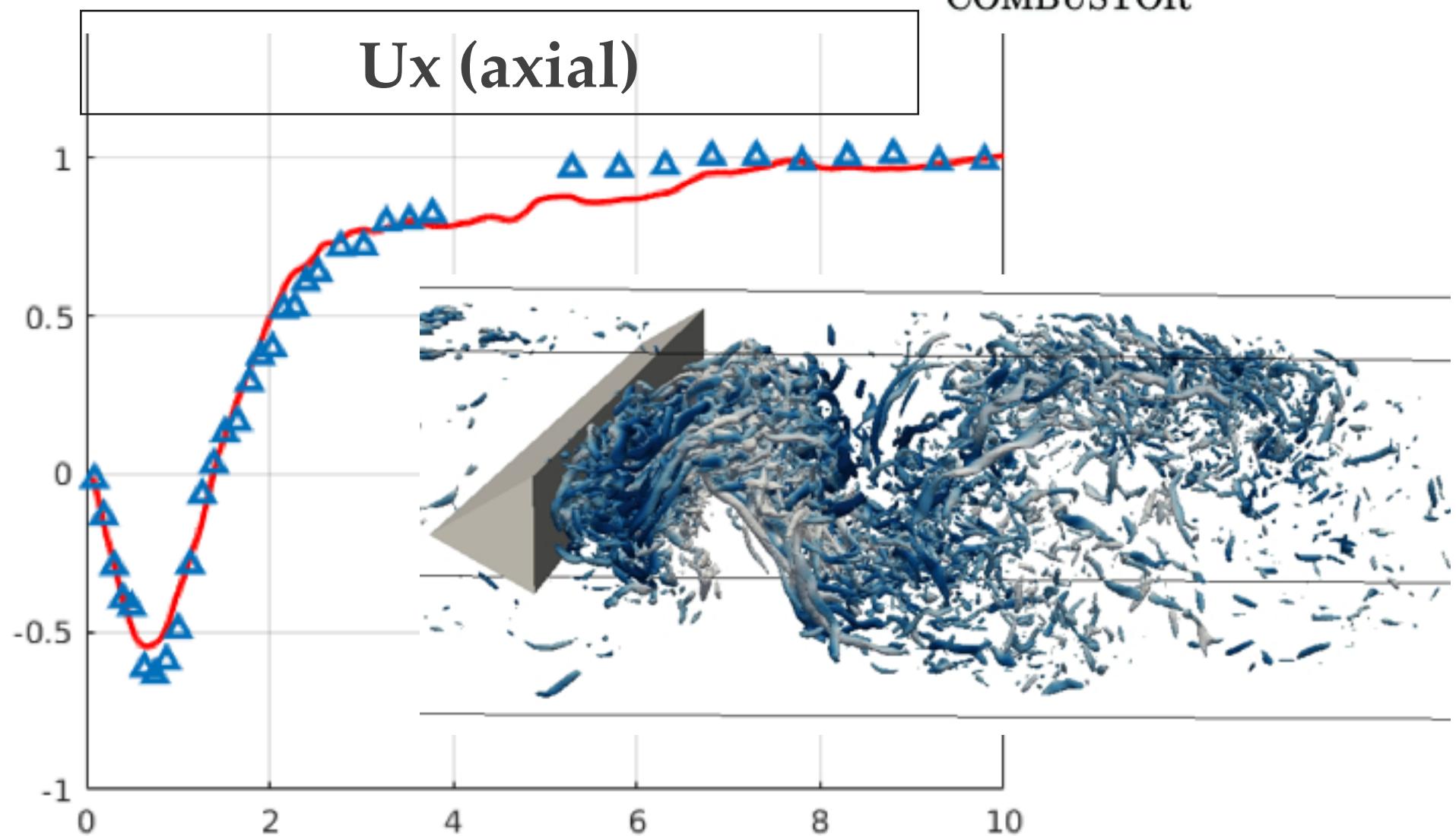
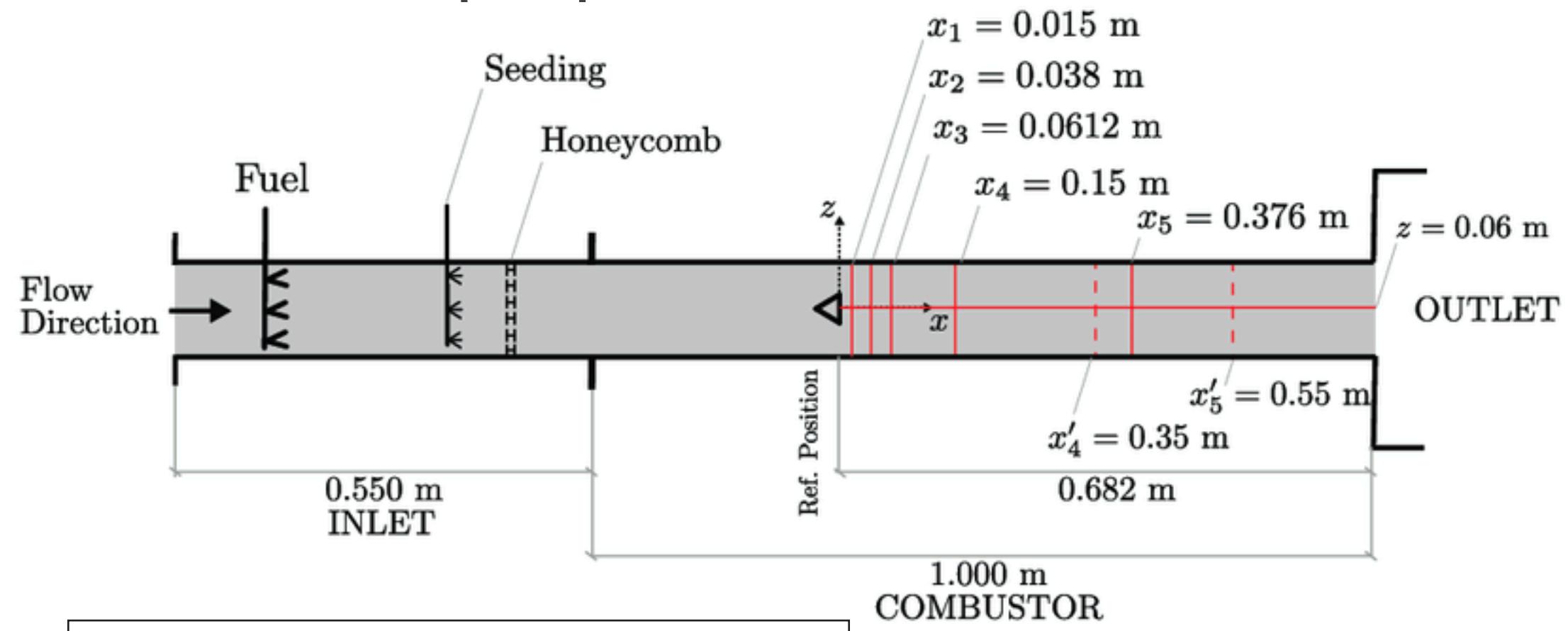
❖ Premixed propane-air





Volvo burner

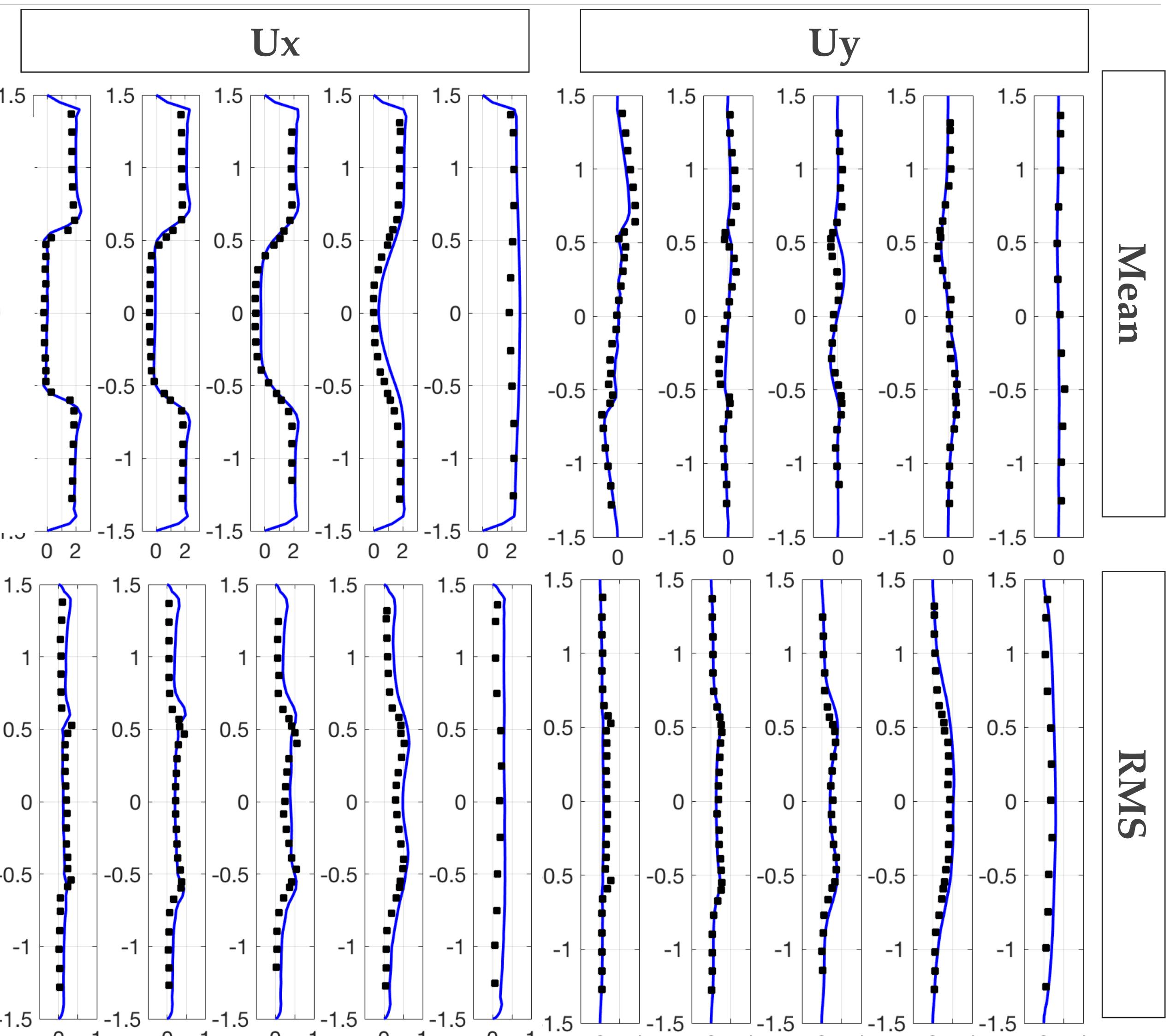
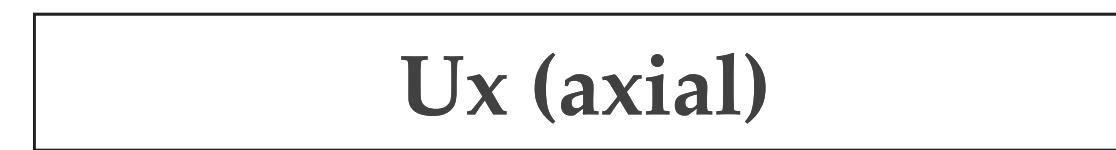
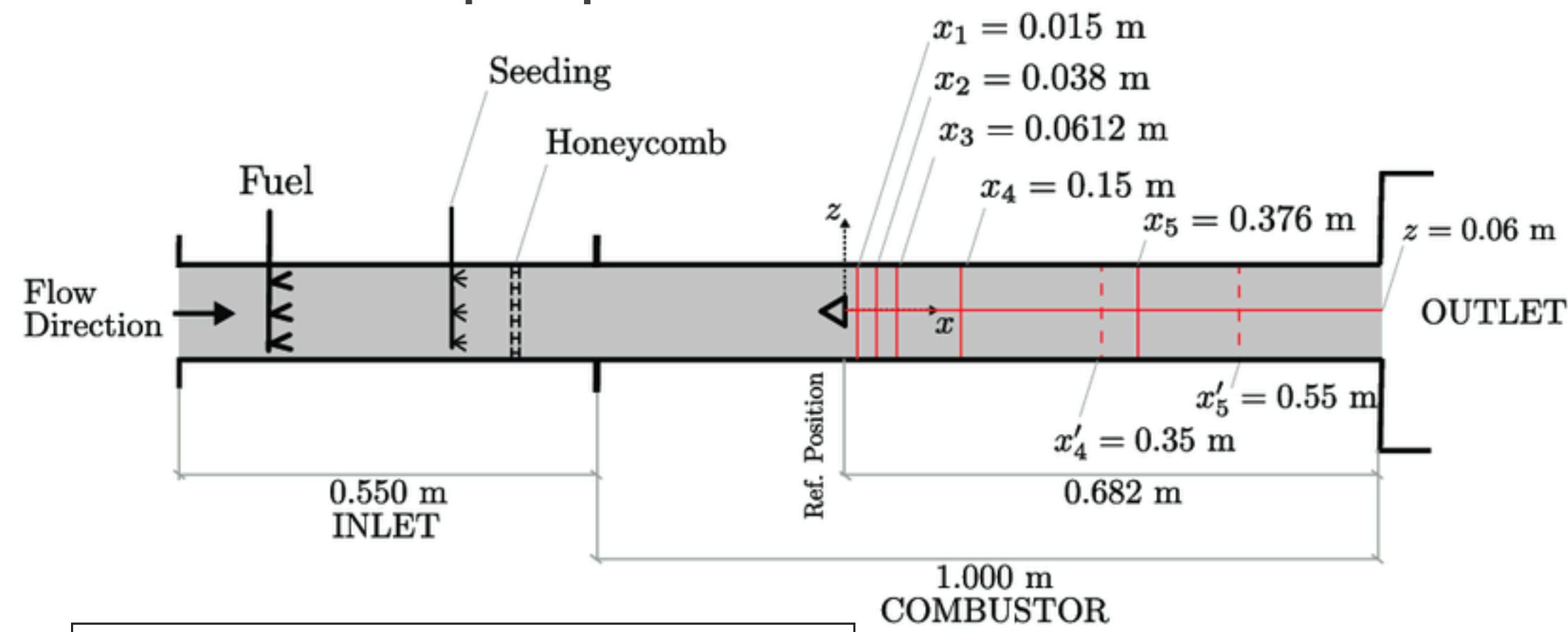
❖ Premixed propane-air





Volvo burner

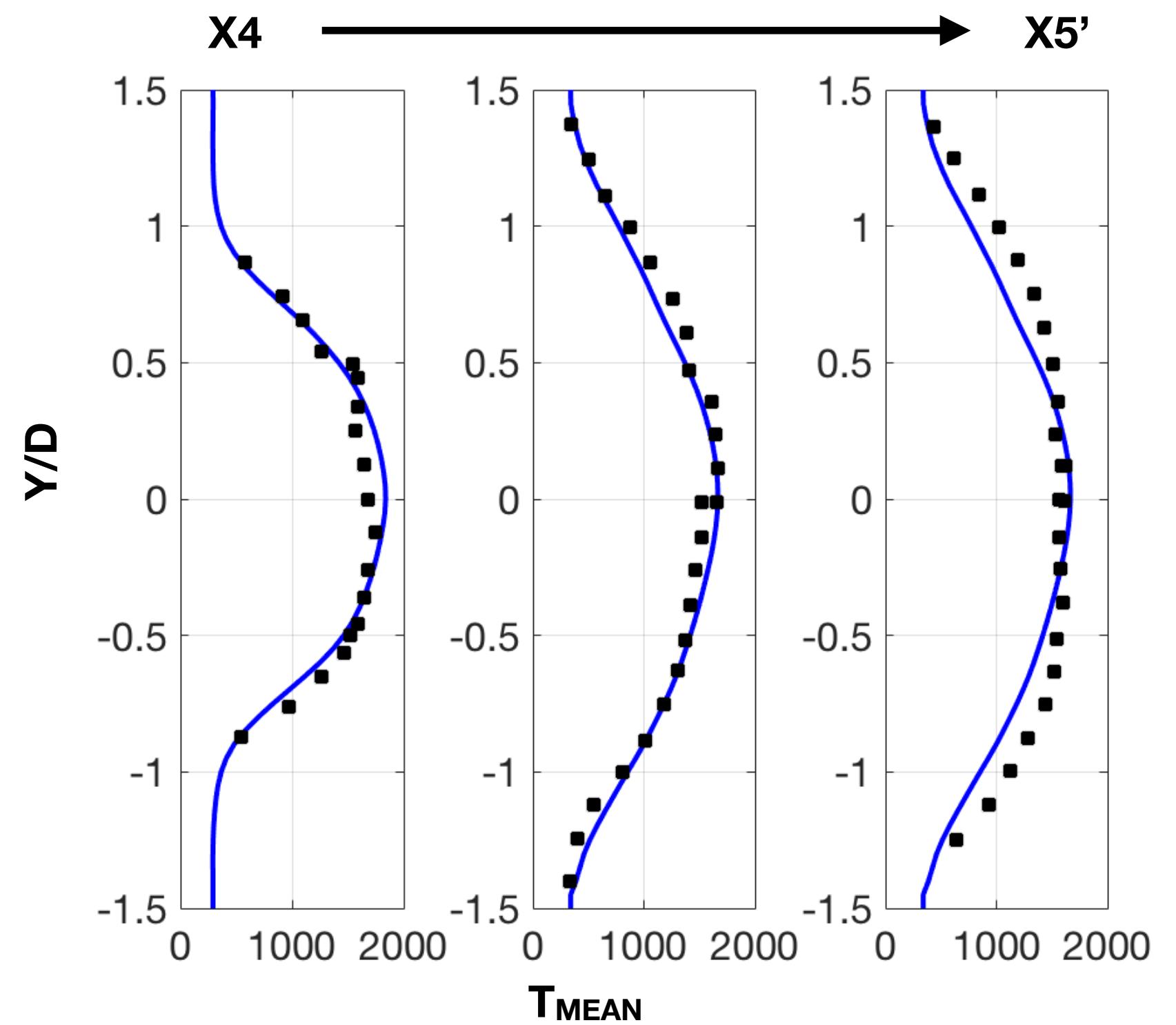
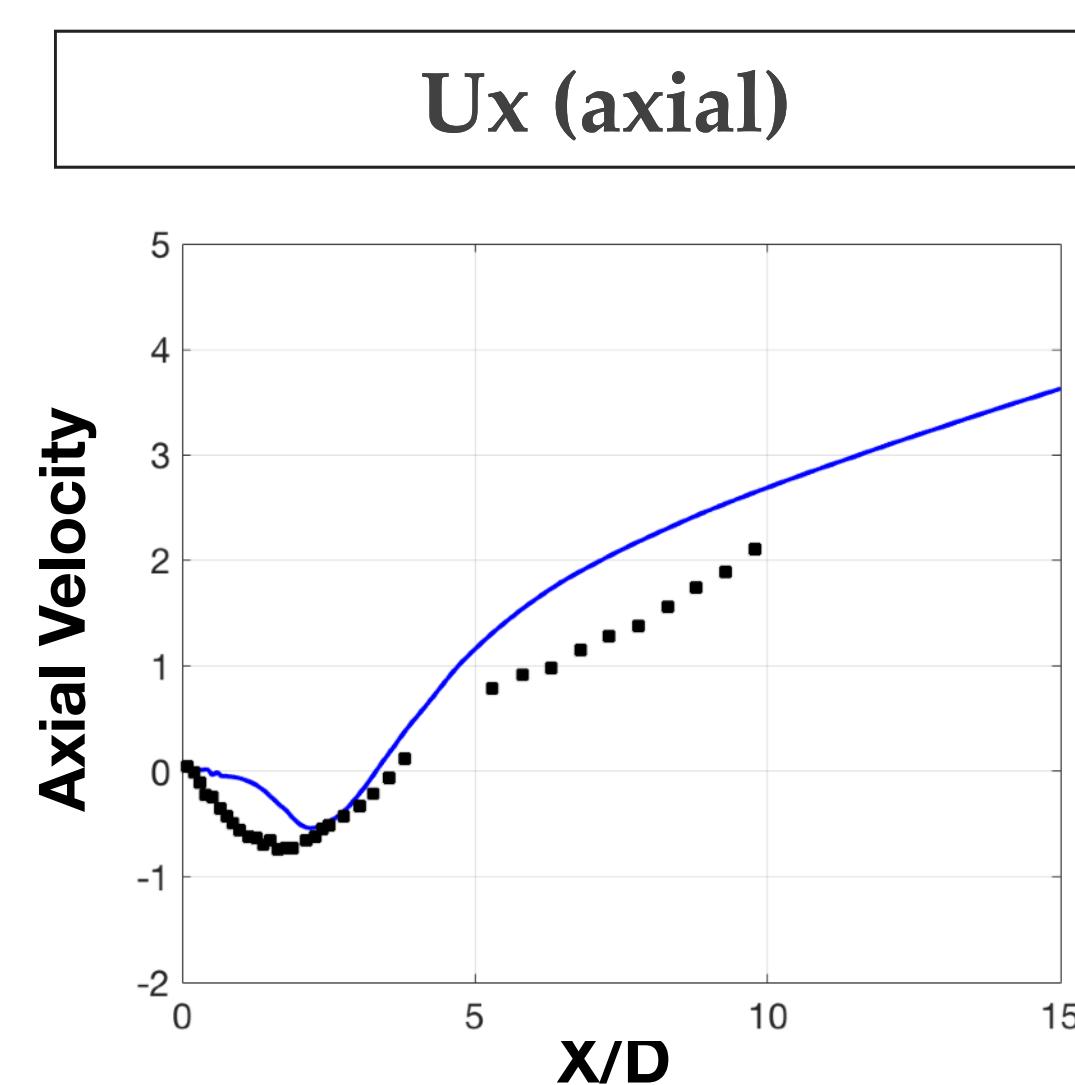
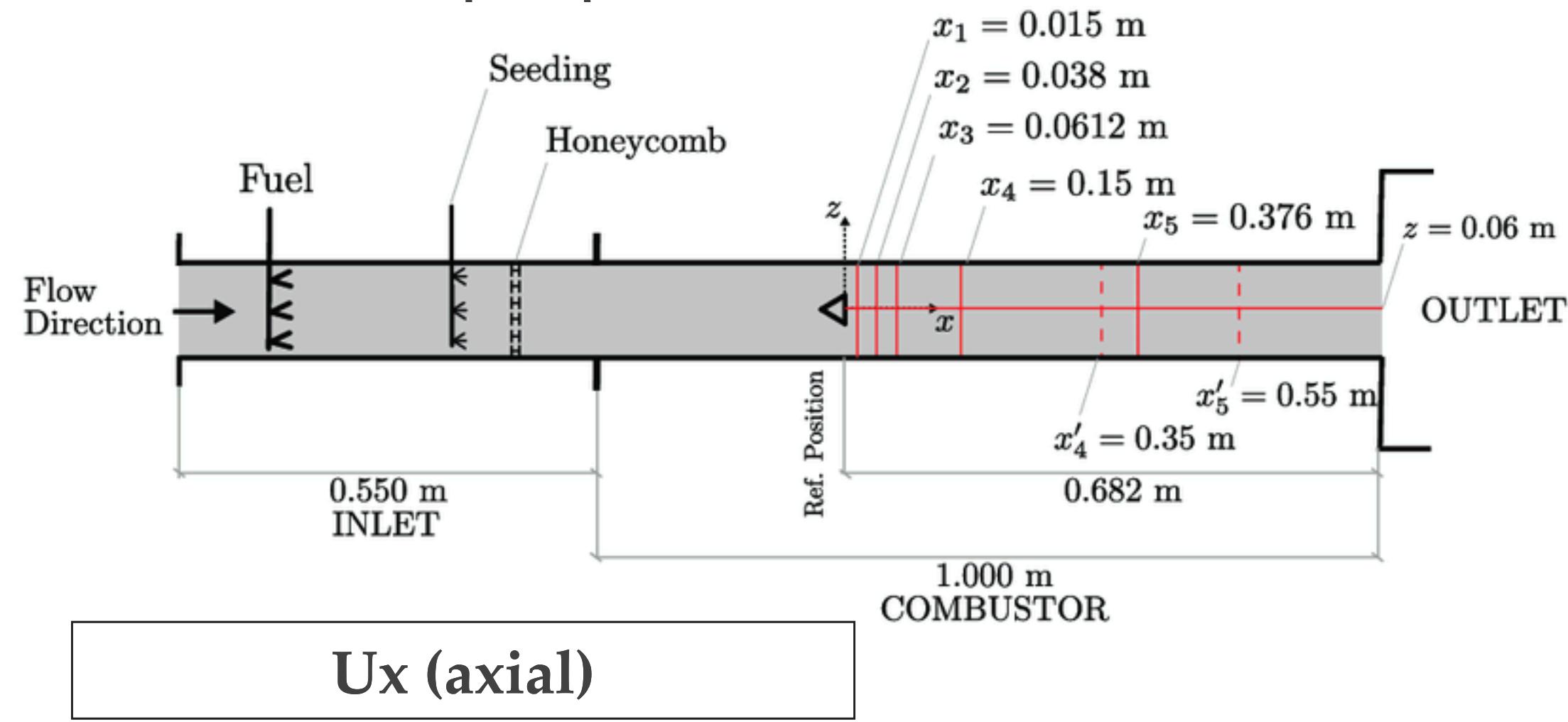
❖ Premixed propane-air





Volvo burner

- ❖ Premixed propane-air



Cost: 1000 cpu.h per flow-through-time (5.5M points)

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Conclusions

- ❖ A Hybrid LB model suitable for combustion application
- ❖ Acoustic solver for less the cost of a LMNA code (on uniform grid)
- ❖ Local time-stepping (multi-level grid) => **even cheaper**
- ❖ Keeps the low-dissipative LB features (aeroacoustics)

Merci à...

- ❖ Muhammad Tayyab (PhD 2017-2020 - LBM combustion)
- ❖ Song Zhao (Post-Doc CNES 2018-2020, now IR - LBM combustion)
- ❖ Gabriel Farag (PhD 2018-2021 - LBM compressible)
- ❖ Thomas Coratger (PhD 2019-2022 - LBM compressible, chaire ALBUMS)
- ❖ Camille Sarotte (Post-Doc 2019-2020 - LBM compressible, chaire ALBUMS)
- ❖ Mostafa Taha (PhD 2019-2022 - LBM fire / plumes)
- ❖ Karthik Guruprasad (PhD 2020-2023 - LBM combustion)
- ❖ Yongliang Feng
- ❖ Jérôme Jacob (IR, ProLB, M2P2)
- ❖ Pierre Sagaut (PR, ProLB, M2P2)
- ❖ Et pour les discussions et l'aide: les collègues du Cerfacs, de l'Irphe, du Coria
- ❖ Ceux que j'oublie...

... Questions ?