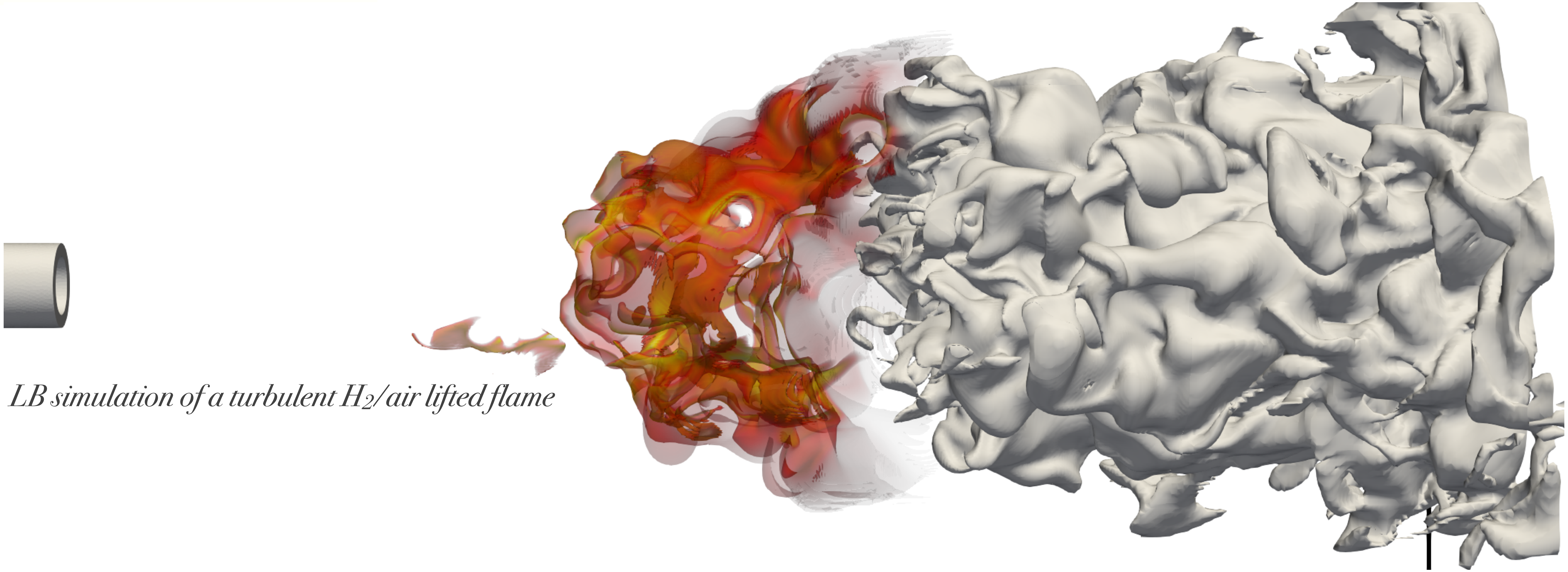
Manchester, 27 sept. 2024



LB simulation of a turbulent H_2/air lifted flame

Hybrid Lattice-Boltzmann methods

applied to H_2 Combustion and Safety

P. Boivin

Price & prejudice

LBM for combustion

- LBM is for rarefied gases and the Chapman Enskog expansion is dubious, so why bother ?
- Extending LBM to multicomponent flows 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 /…), LBM is worthless
- I do not understand LBM, it’s black magic (Hopefully not relevant anymore).
- Hybrid LBM is not true LBM, so what’s the point.

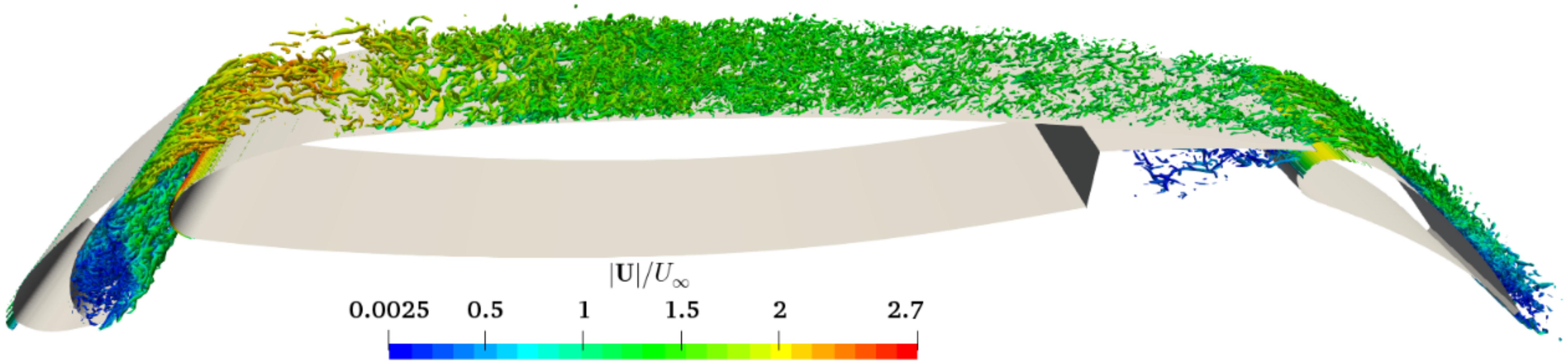
Outline

- **Part I : Problem statement**
- Part II : Additional scalar equations (weak coupling, non conservative)
- Part III : Conservativity of scalar equations
- Part IV : Application to hydrogen combustion & safety
- Part V: Discussion, perspectives

Starting point

ProLB & M2P2

- Member of the ProLB consortium
- Staff @M2P2
  - 4 Profs: P. Boivin, J. Favier, P. Sagaut, E. Serre.
  - 4 research engineers.
  - ~30 PhD/PostD

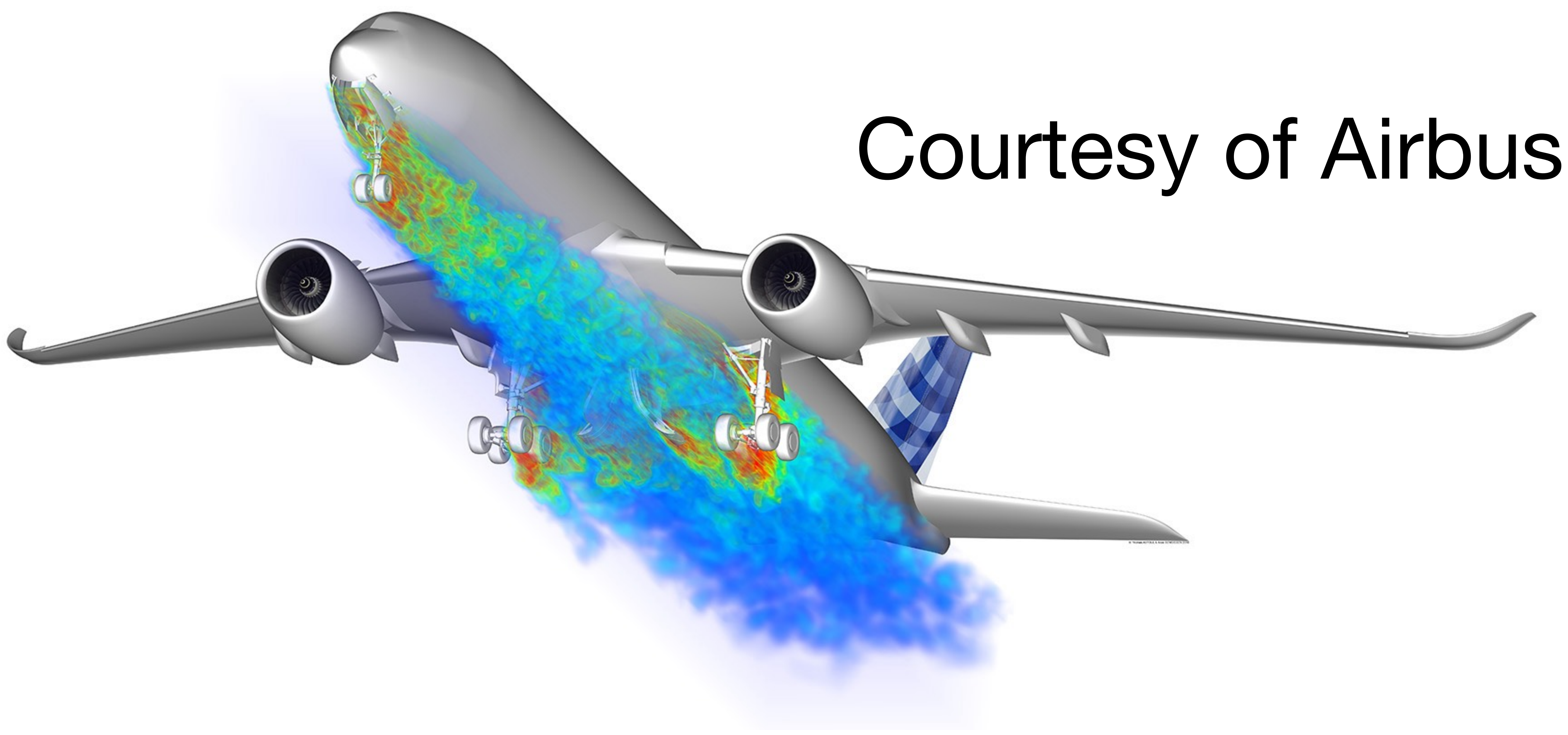


Academic/private consortium

Starting point

Isothermal model

- **<u>D3Q19</u>** code, cpu.
- Equilibrium expanded to order 2, 3 or 4.
- (Hybrid) - recursive - regularised collision kernel

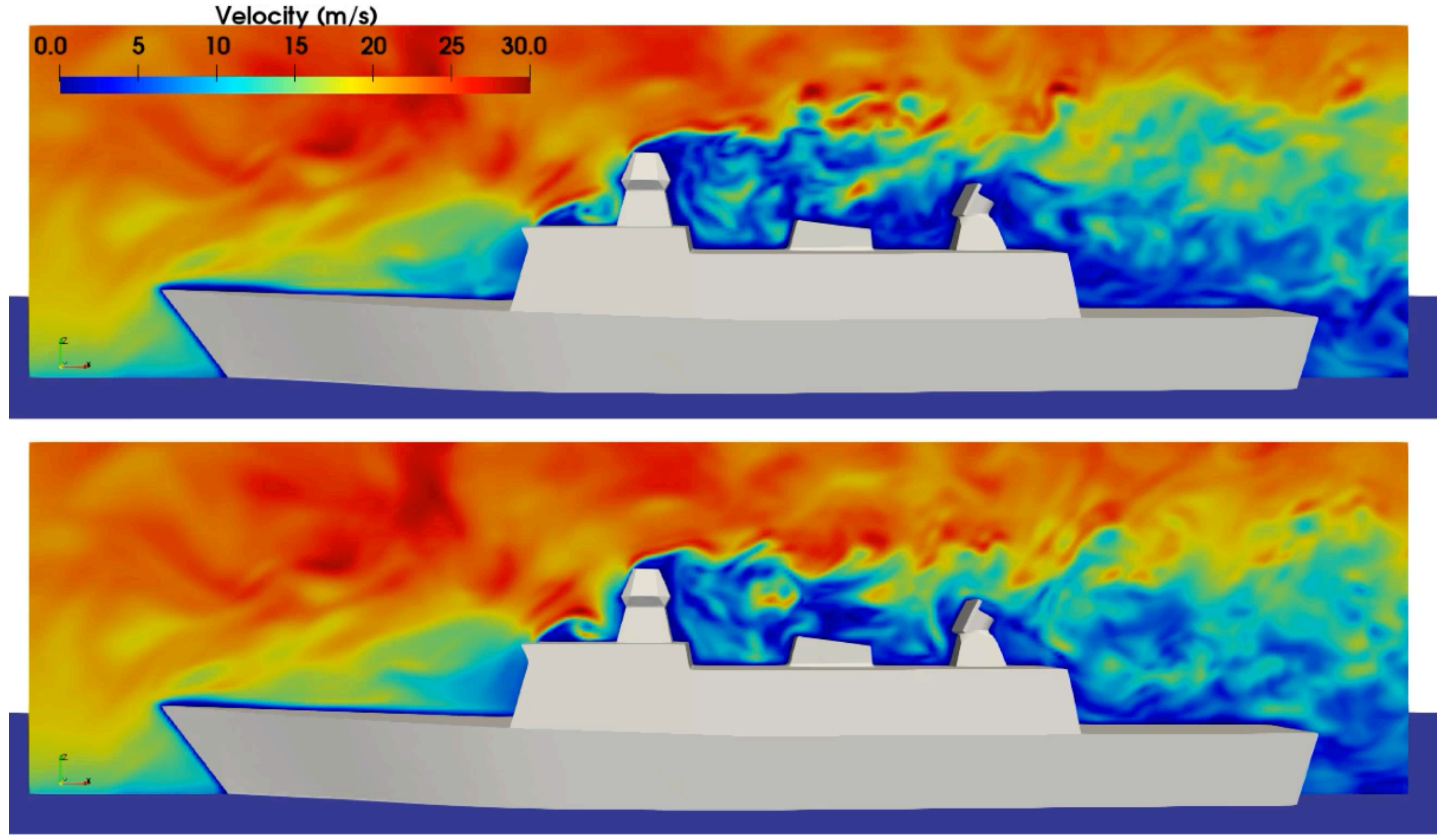


Courtesy of Airbus

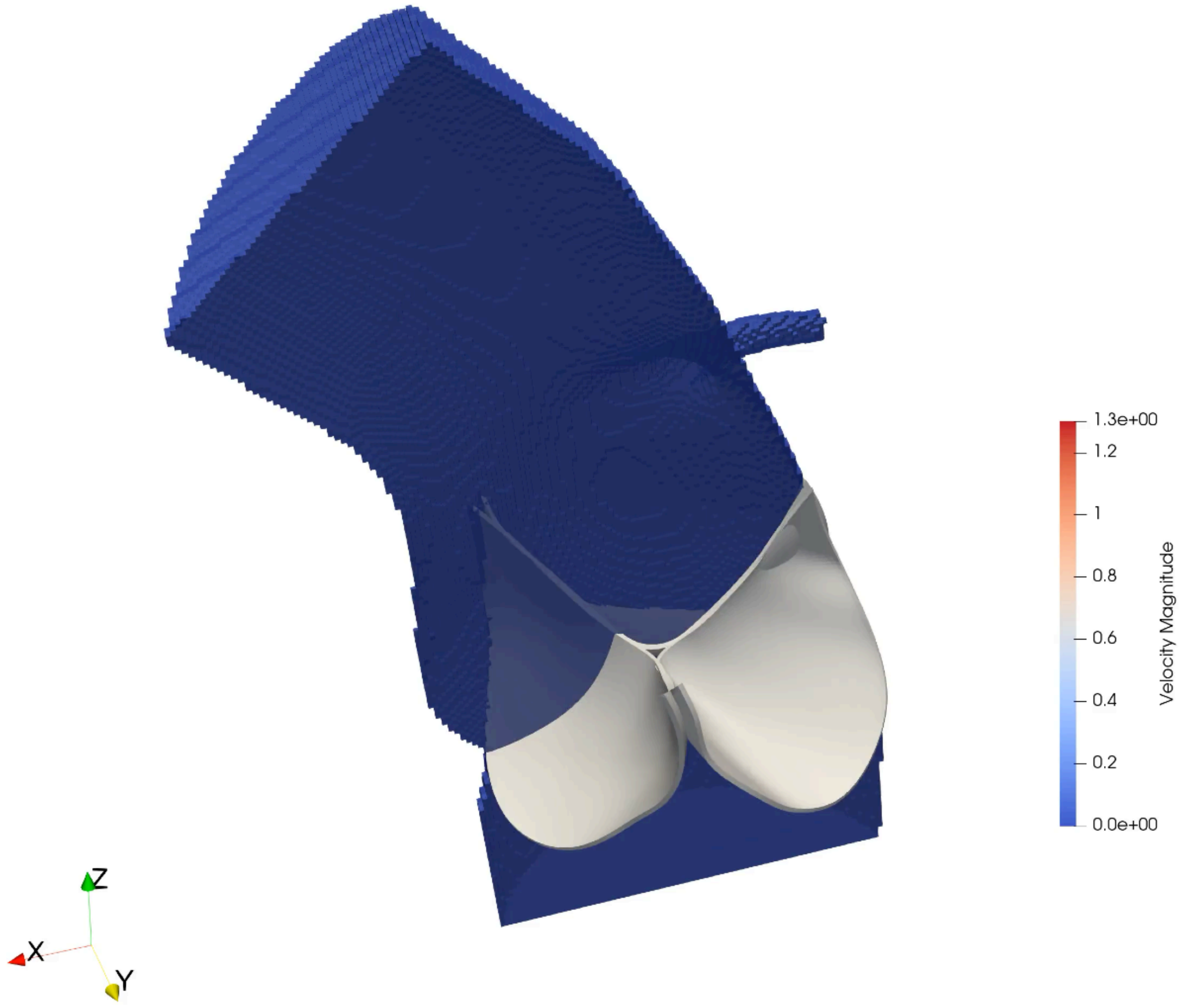
Academic/private consortium

Elsewhere

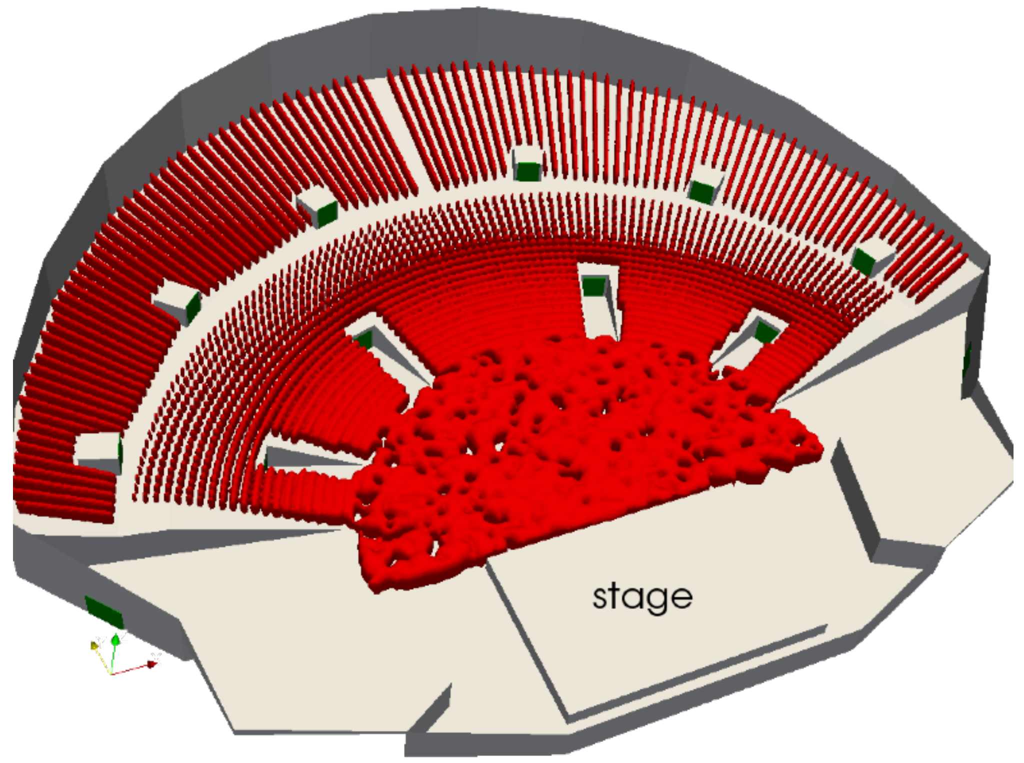
But still at M2P2

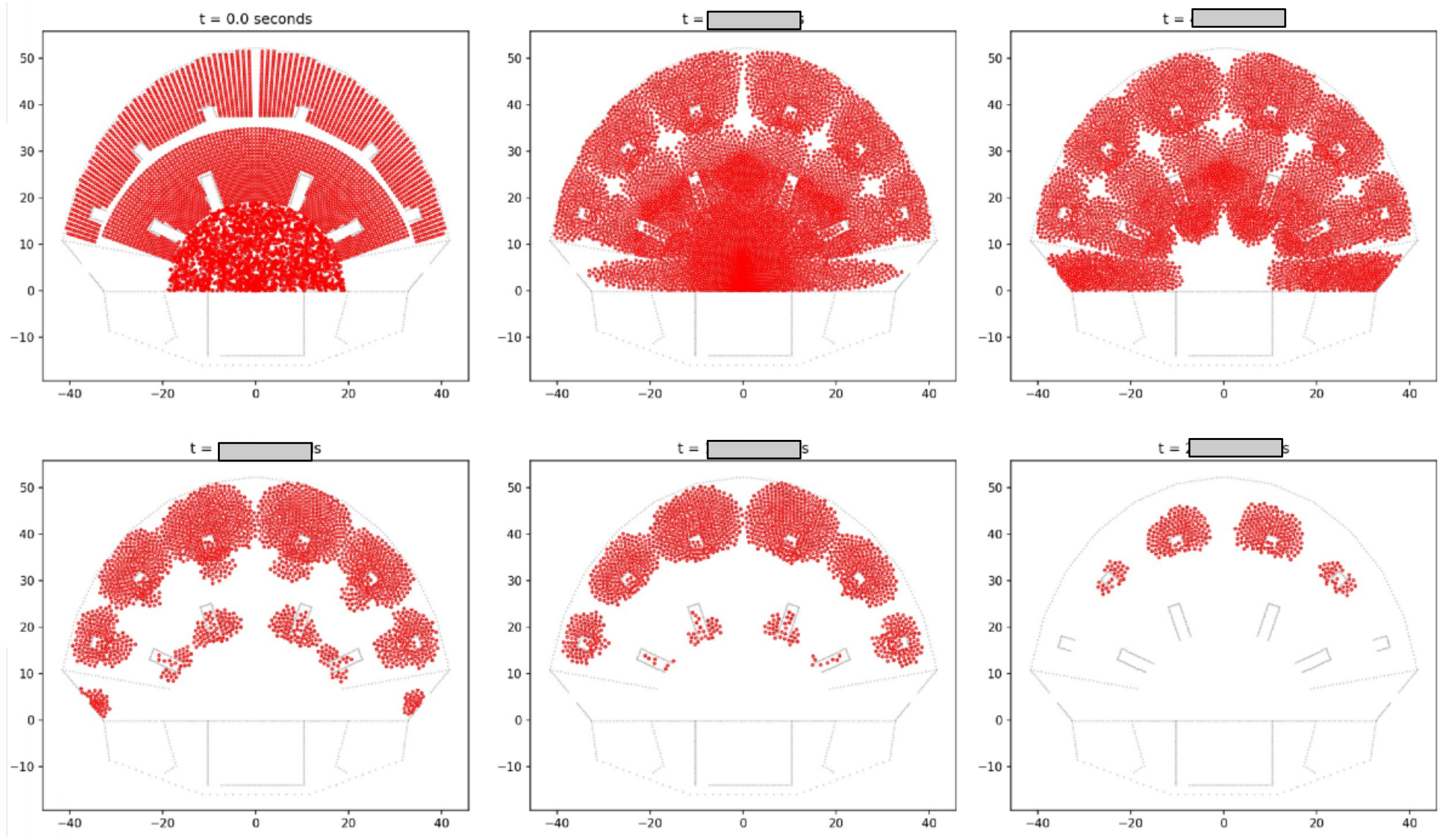


NATO ship



Heart valve studies

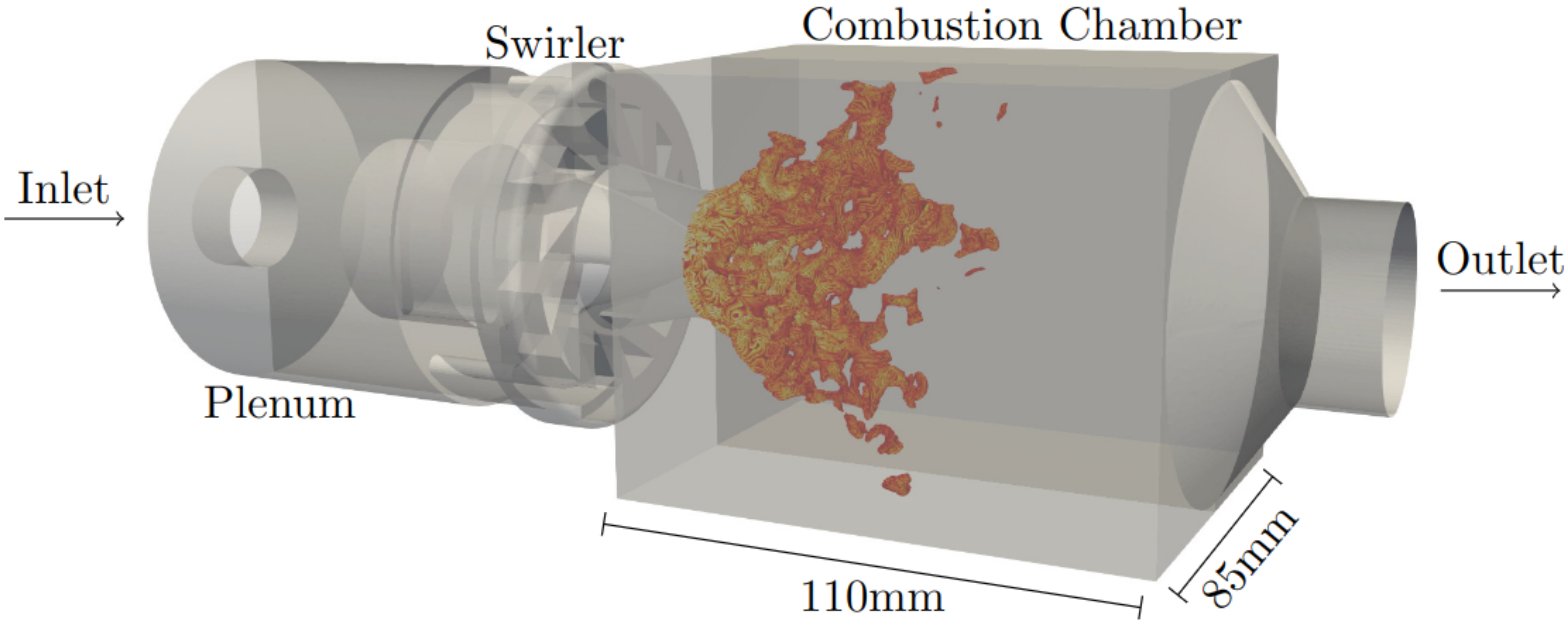




Evacuation (6000p.)

Multicomponent/reactive flows

Problem statement



Remember: **standard LBM** is valid for isothermal, weakly compressible flows.

Combustion 101

Target macroscopic equations

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

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta + p\delta_{\alpha\beta}}{\partial x_\beta} = \frac{\partial \tau_{\alpha\beta}}{\partial x_\beta}$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_\beta (E + p/\rho)}{\partial x_\beta} = \frac{\partial \tau_{\alpha\beta} u_\alpha}{\partial x_\beta} - \frac{\partial q_\beta}{\partial x_\beta}$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_\beta Y_k}{\partial x_\beta} = \frac{\partial \rho V_{k,\beta} Y_k}{\partial x_\beta} + \dot{\omega}_k$$

$5 + N_k$ conservation equations

$\dot{\omega}_k = A e^{-E_a/RT} C_m C_n$ For each reaction

Thermodynamic closure

$$p = \rho \frac{\mathcal{R}}{W} T; \qquad \frac{1}{W} = \sum_{k=1}^{N} \frac{Y_k}{W_k}$$

$$E = e + \frac{u_\alpha^2}{2}, \qquad h = e + \frac{p}{\rho}$$

$$h = \sum_{k=1}^{N_k} h_k Y_k = \sum_{k=1}^{N_k} Y_k \left(\int_{T_0}^{T} c_{p,k}(\theta) d\theta + \Delta h_k^0 \right)$$

Transport $= f(Pr, Le_k)$

$$\tau_{\alpha\beta} = (\mu + \mu_t) \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3} \delta_{\alpha\beta} \frac{\partial u_\gamma}{\partial x_\gamma} \right)$$

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

$$V_{k,\alpha} = -\frac{\mathcal{D}_k}{X_k} \frac{\partial X_k}{\partial x_\alpha} + V_\alpha^c; \qquad V_\alpha^c = \sum_{k=1}^{N} Y_k \frac{\mathcal{D}_k}{X_k} \frac{\partial X_k}{\partial x_\alpha}$$

$$\mu = f(T), \qquad \lambda = \mu C_p / \mathrm{Pr}, \qquad \mathcal{D}_k = \lambda / (\rho C_p \mathrm{Le}_k)$$

Notations from Poinsot & Veynante combustion textbook

Combustion 101

Difficulties for LBM

$5 + N_k$ conservation equations

For Hydrogen, typically $N_k = 9$

Large temperature/density variations

> dilatable / compressible

> Variable sound speed

$\dot{\omega}_k$ ~ 20-100 (detailed), 1-3 (reduced)
Very stiff term

Thermodynamic closure

Variable Cp, NASA polynomials

Variable $\gamma = \frac{c_p}{c_v}$

Large molecular weight differences
H_2 > 2, O_2 > 32.

Transport $= f(Pr, Le_k)$

Variable μ

Arbitrary Prandtl & Lewis numbers

Notations from Poinsot & Veynante combustion textbook

Outline

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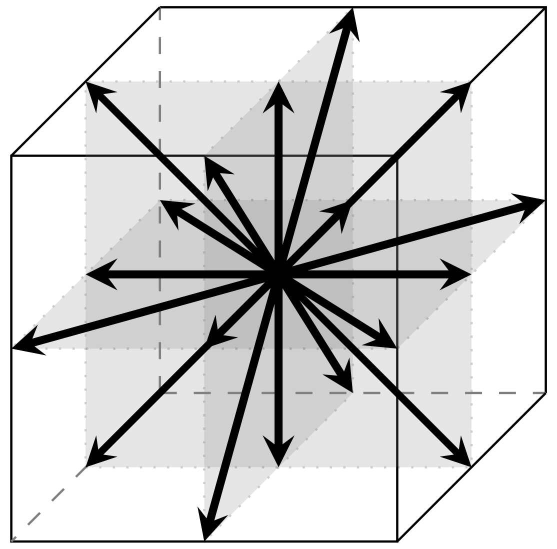
Compressible LBM: possible approaches

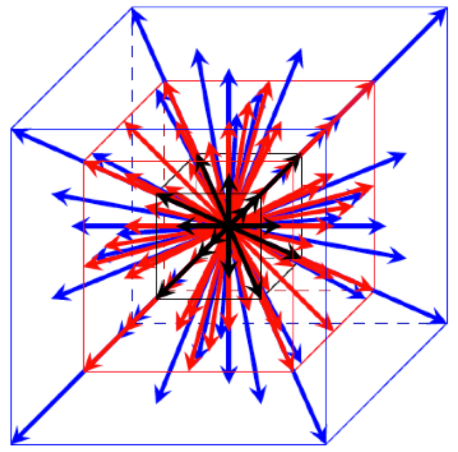
Remember: **standard LBM** is valid for isothermal, weakly compressible flows.



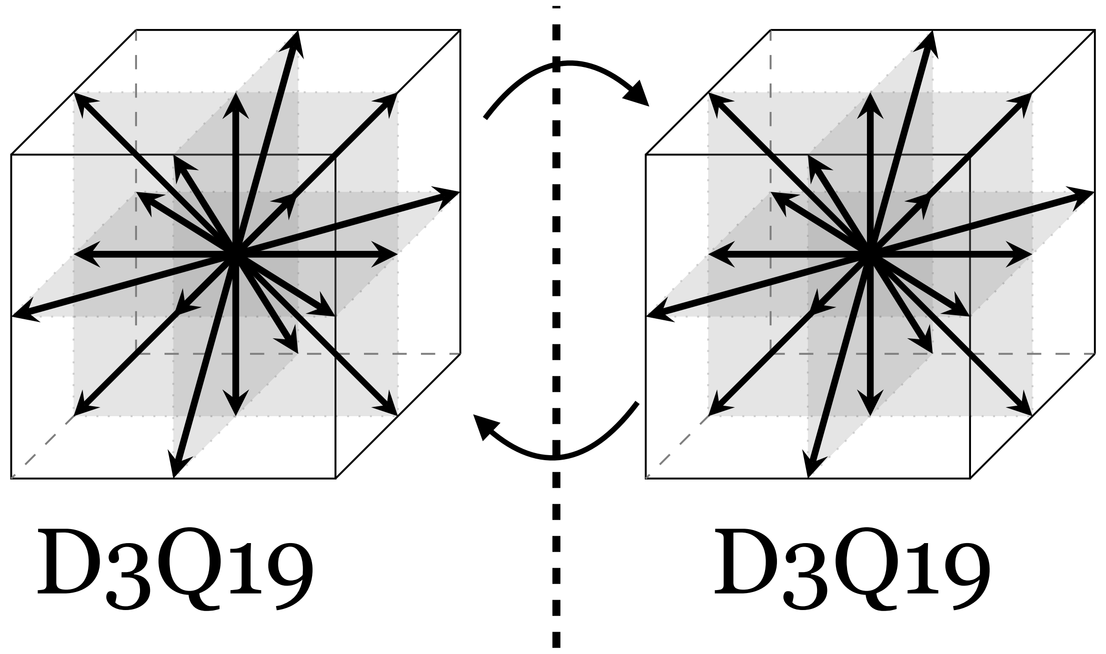
D3Q19

LBM compressible

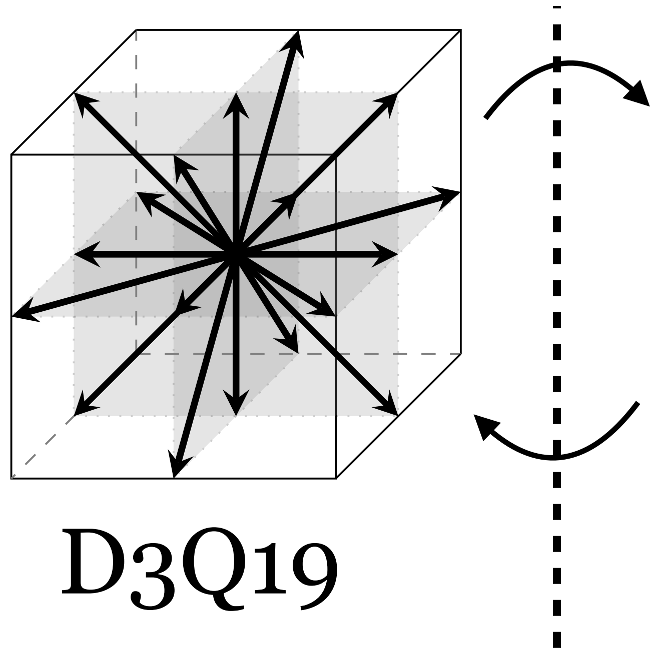
- **Single Distribution**
  - **Multi-Speed**
- **Segregated Methods**
  - **Double Distribution Function**
  - **Hybrid**



D3Q103



D3Q19 D3Q19

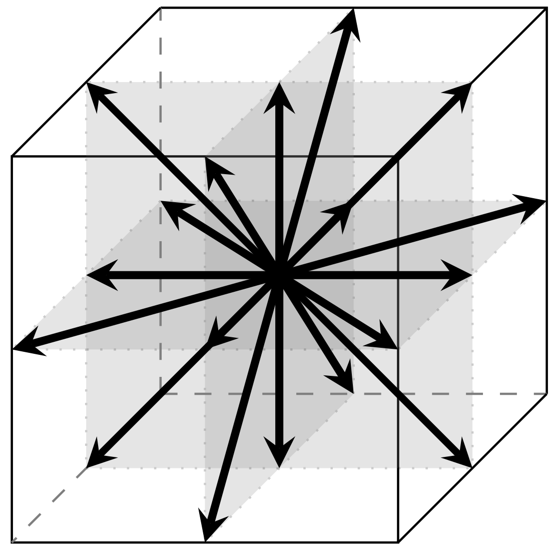


D3Q19

FV/FD scheme for energy

Compressible LBM: possible approaches

Remember: **standard LBM** is valid for isothermal, weakly compressible flows.



D3Q19

LBM compressible

Single Distribution

Segregated Methods

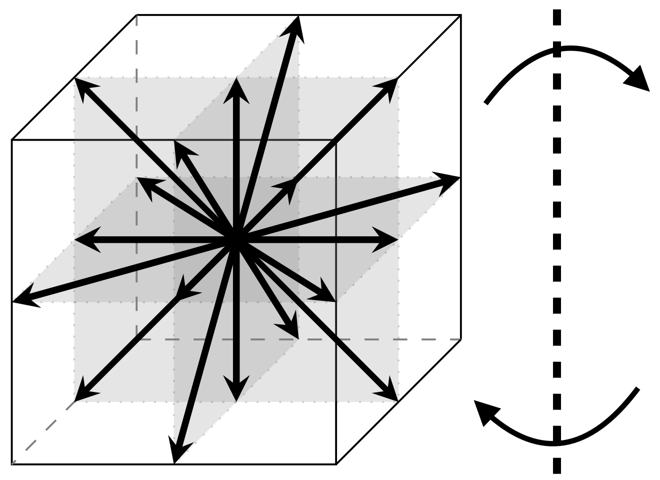
Multi-Speed

D3Q103

Double Distribution Function

D3Q19 D3Q19

Hybrid



D3Q19

FV/FD scheme for energy

Notations

Generic LBM core & notations

- **Streaming step**

$$f_i(t+\delta t, \boldsymbol{x}+\boldsymbol{c}_i\delta t) = f_i^{\mathrm{col}}(t, \boldsymbol{x})$$

- **Collision step**

$$f_i^{\mathrm{col}} = f_i^{\mathrm{eq}} + \left(1 - \frac{\delta t}{\overline{\tau}}\right) f_i^{\mathrm{neq}} + \frac{\delta t}{2} F_i^{\mathrm{E}}$$

- f_i^{neq} is the only term collision kernel dependent.
  At the lab: Recursive regularized (+ hybrid for most applications)

[1] O. Malaspinas, “Increasing stability and accuracy of the lattice boltzmann scheme: recursivity and regularization,” arXiv preprint arXiv:1505.06900, 2015.
[2] J. Jacob, O. Malaspinas, and P. Sagaut, “A new hybrid recursive regularised bhatnagar–gross–krook collision model for lattice boltzmann method-based large eddy simulation,” Journal of Turbulence, pp. 1– 26, 2018.

Equilibrium definition

Compressible core

[1] 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.
[2] 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.
[3] G. Farag, T. Coratger, G. Wissocq, S. Zhao, P. Boivin, and P. Sagaut, "A unified hybrid lattice-boltzmann method for compressible flows: bridging between pressure-based and density-based methods," Physics of Fluids, vol. 33, no. 8, 2021

Let's introduce $\theta = p/\rho c_s^2$

The equilibrium distribution that generalizes ProLB models is

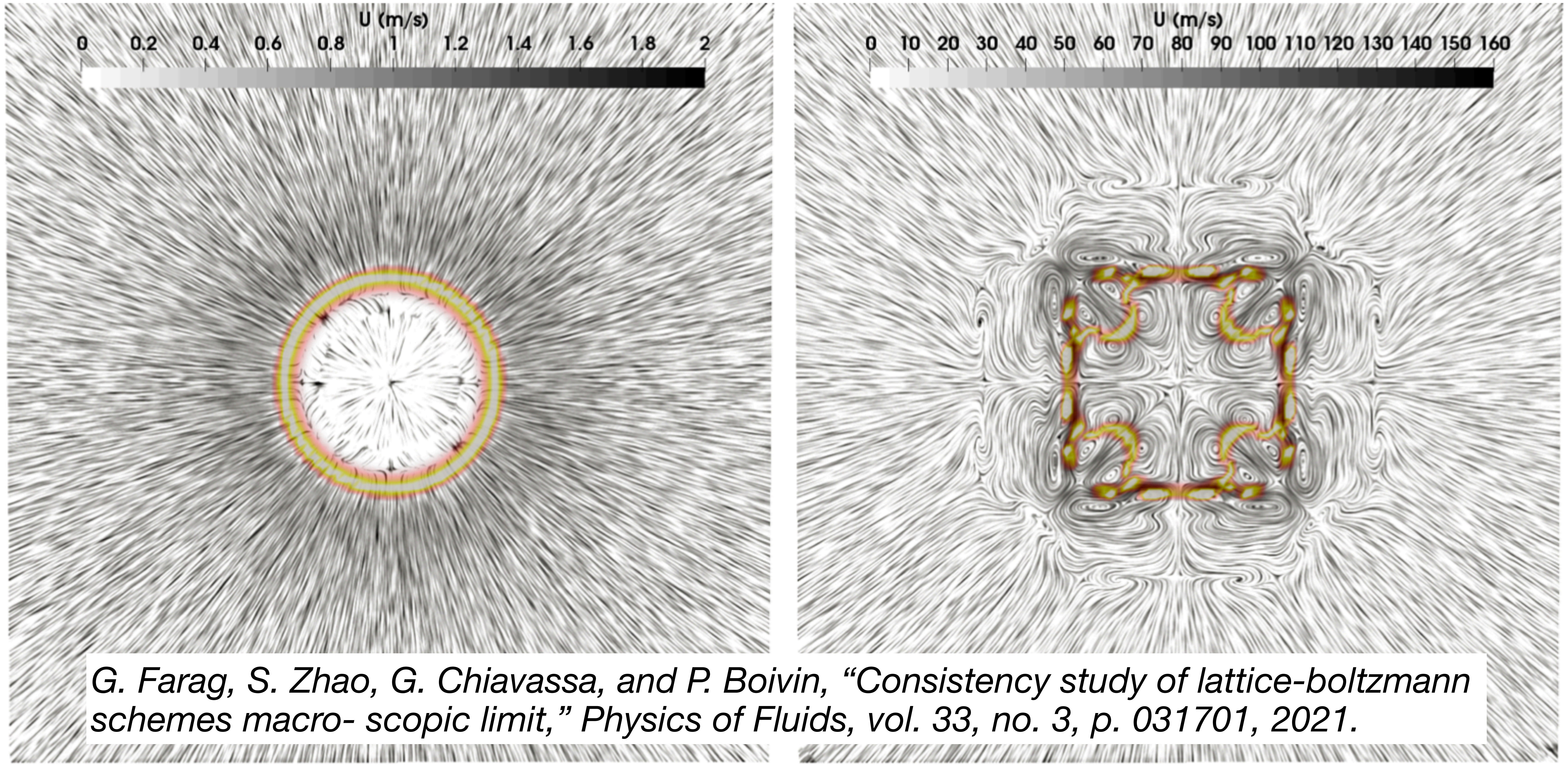
$$f_i^{eq} = \omega_i \Big\{ \mathcal{H}^{(0)}\rho + \frac{\mathcal{H}^{(1)}_{i\alpha}}{c_s^2}\rho u_\alpha + \frac{\mathcal{H}^{(2)}_{i\alpha\beta}}{2c_s^4}\left[\rho u_\alpha u_\beta + \delta_{\alpha\beta}\rho c_s^2(\theta-1)\right] + \frac{\mathcal{H}^{(3)}_{i\alpha\beta\gamma}}{6c_s^6}\Big[\rho u_\alpha u_\beta u_\gamma - \kappa \rho c_s^2\left(u_\alpha\delta_{\beta\gamma} + u_\beta\delta_{\gamma\alpha} + u_\gamma\delta_{\alpha\beta}\right)\Big] - \frac{\mathcal{A}_i + \mathcal{B}_i + \mathcal{C}_i}{12c_s^4}\rho[\theta-1](1-\zeta)\Big\} \quad (49)$$

- $\zeta = 1$ and $\kappa = 1-\theta$ is the classical ρ-based.
- $\zeta = 0$ and $\kappa = 0$ is for p-based and $i\rho$-based. Same core model !

➔ Differences between models are inside 3^{rd} and 4^{th}-order moments ⬅

Effect of 4th order

Compressibility errors / spurious currents



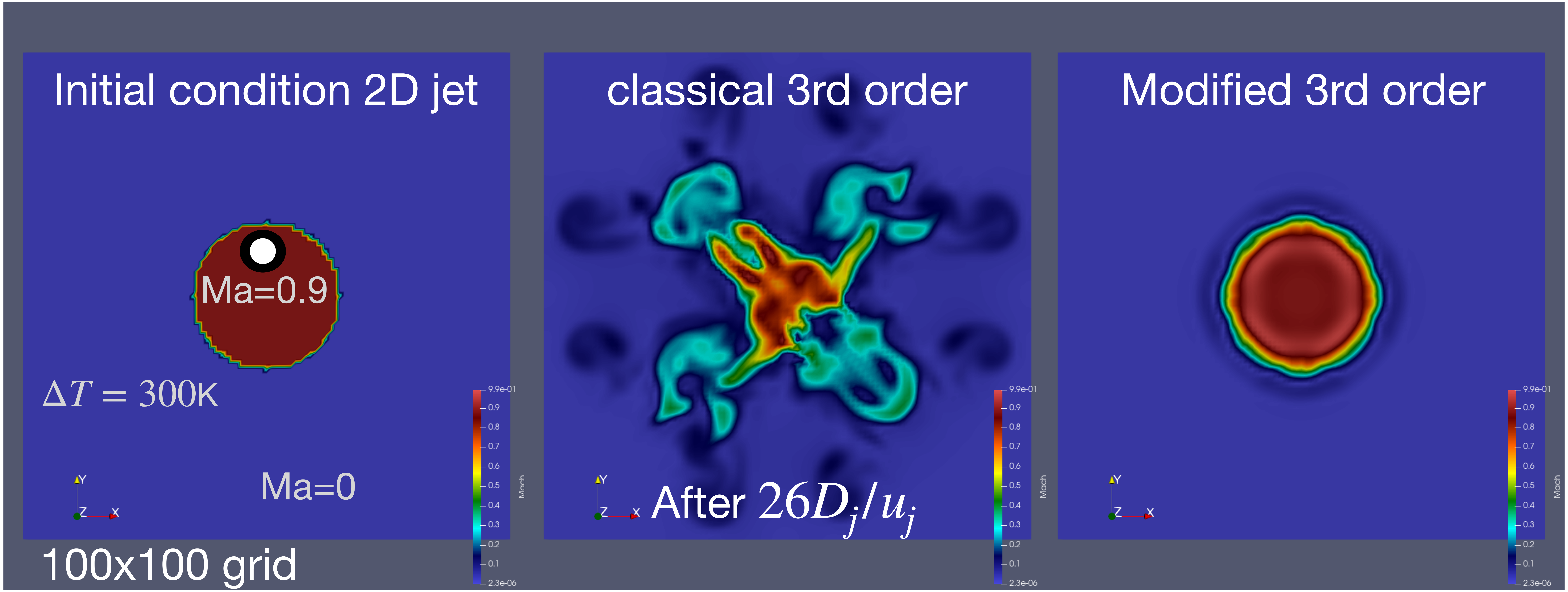
G. Farag, S. Zhao, G. Chiavassa, and P. Boivin, "Consistency study of lattice-boltzmann schemes macro- scopic limit," Physics of Fluids, vol. 33, no. 3, p. 031701, 2021.

(b) $t=4.0\times10^{-2}$ms

Spherical flame. With 4th order (left) and without (right)

Effect of 3rd order

Jet isotropy



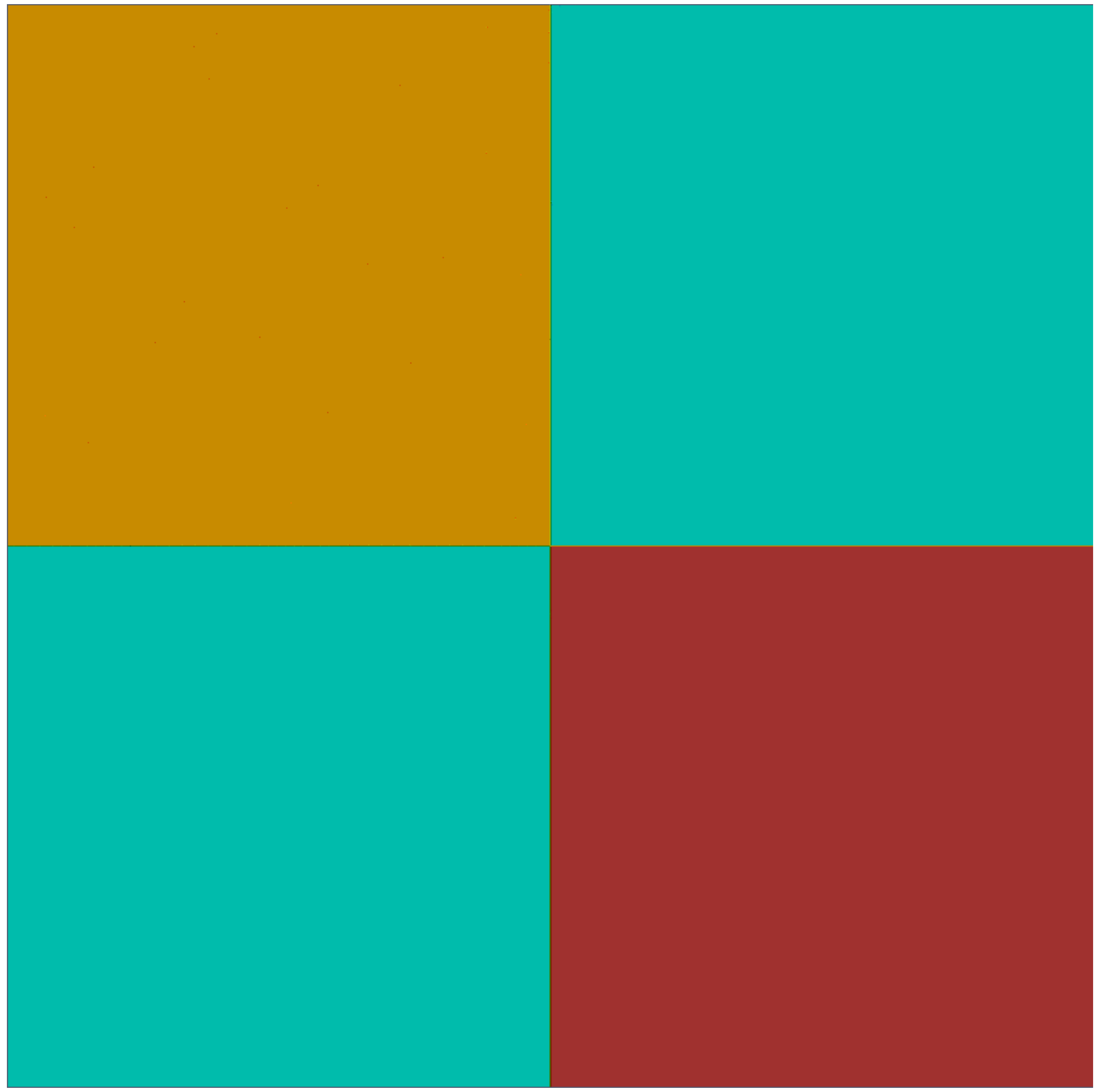
M. Bauer and U. Rude, *“An improved lattice boltzmann d3q19 method based on an alternative equilibrium discretization,” arXiv preprint arXiv:1803.04937, 2018.*

Back to scalar equations

Basic idea

Hybrid compressible core

- Scalar equations are solved on the same grid.
- Explicit time-stepping is used
  <u>same time-step as LB time-step</u>
- Finite volume methods to compute all RHS terms



Entropy equation (MUSCL)

General algorithm

[1] 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.
[2] 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.
[3] G. Farag, T. Coratger, G. Wissocq, S. Zhao, P. Boivin, and P. Sagaut, "A unified hybrid lattice-boltzmann method for compressible flows: bridging between pressure-based and density-based methods," Physics of Fluids, vol. 33, no. 8, 2021

- Initial solution, $\rho(t, \boldsymbol{x})$, $u_\alpha(t, \boldsymbol{x})$, $T(t, \boldsymbol{x})$ and $\Pi^{f^{neq},(2)}_{\alpha\beta}(t, \boldsymbol{x})$ are known.

↓ ↓

Lattice-Boltzmann

- Compute Equilibrium $f_i^{eq}(t, \boldsymbol{x})$ and Non-Equilibrium $\overline{f}_i^{neq}(t, \boldsymbol{x})$.
- Collide & Stream provides the updated distribution $\overline{f}_i(t + \Delta t, \boldsymbol{x})$.
- Macroscopic update provides $\rho(t + \Delta t, \boldsymbol{x})$ and $u_\alpha(t + \Delta t, \boldsymbol{x})$.

Finite Differences

- Compute the updated Entropy $s(t + \Delta t, \boldsymbol{x})$ using a one step explicit scheme. MUSCL-Hancock for advection and centered schemes for heat diffusion and viscous heat.

↓ ↓

- Temperature update $T(t + \Delta t, \boldsymbol{x})$ using $\rho(t + \Delta t, \boldsymbol{x})$ and $s(t + \Delta t, \boldsymbol{x})$.
- Stress-tensor update $\Pi^{\overline{f}^{neq}}_{\alpha\beta}(t + \Delta t, \boldsymbol{x})$ using $\left[\Pi^{\overline{f}}_{\alpha\beta}, \rho, u_\alpha, T\right](t + \Delta t, \boldsymbol{x})$.

➔ Interface Lattice-Boltzmann/Finite Differences is $\Pi^{(2)}_{\alpha\alpha}$ ⬅

Conservative or Primitive ?

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) = 0$$
$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x}\left(\left(\rho E + p\right) u\right) = 0$$
$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u}{\partial x} = 0$$

TD break

In the context of multi-component perfect gas EOS:

- **Derive the Euler equation in primitive variables** $(\rho, u, e = E - u^2/2, Y_k)$
- **Show that the energy equation can be expressed as a pressure equation using EOS** $p = (\gamma - 1)\rho e$
- **Find the eigenvalues of the associated Jacobian**
- **Deduce that the system is strictly hyperbolic…**
- **Repeat the last two questions from the conservative form.**

Euler - primitive variables

Compressible flows 101

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) = 0$$
$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x}\left(\left(\rho E + p\right) u\right) = 0$$
$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u}{\partial x} = 0$$

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial x} = 0$$
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0$$
$$\frac{\partial e}{\partial t} + u\frac{\partial e}{\partial x} + \frac{p}{\rho}\frac{\partial u}{\partial x} = 0$$
$$\frac{\partial Y_k}{\partial t} + u\frac{\partial Y_k}{\partial x} = 0$$

$$\frac{\partial e}{\partial t} = \left.\frac{\partial e}{\partial p}\right)_\rho \frac{\partial p}{\partial t} + \left.\frac{\partial e}{\partial \rho}\right)_p \frac{\partial \rho}{\partial t}$$
$$\frac{\partial e}{\partial x} = \left.\frac{\partial e}{\partial p}\right)_\rho \frac{\partial p}{\partial x} + \left.\frac{\partial e}{\partial \rho}\right)_p \frac{\partial \rho}{\partial x}$$
$$c^2 = \gamma.\bar{r}.T$$

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + \rho\frac{\partial u}{\partial x} = 0$$
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0$$
$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} + \rho c^2\frac{\partial u}{\partial x} = 0$$
$$\frac{\partial Y_k}{\partial t} + u\frac{\partial Y_k}{\partial x} = 0$$

$$\frac{\partial W}{\partial t} + A(W)\frac{\partial W}{\partial x} = 0$$

$$W = \begin{bmatrix} \rho \\ u \\ p \\ Y_k \end{bmatrix} \quad A(W) = \begin{bmatrix} u & \rho & 0 & 0 \\ 0 & u & 1/\rho & 0 \\ 0 & \rho c^2 & u & 0 \\ 0 & 0 & 0 & u \end{bmatrix}$$

$$\lambda = \begin{bmatrix} u \\ u+c \\ u-c \\ u \end{bmatrix}$$

Distinct real eigenvalues
> Hyperbolic system

System characteristics

Some characteristic equations (good)

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

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

$$\frac{\partial h}{\partial t} + u_\beta \frac{\partial h}{\partial x_\beta} = \frac{dp}{dt}$$

If dp neglected

System characteristics

Some characteristic equations (good)

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

$$\frac{\partial s}{\partial t} + u_\beta \frac{\partial s}{\partial x_\beta} = 0$$ -> Very painful for multi species

acoustics ruined, but easy <- $$\frac{\partial h}{\partial t} + u_\beta \frac{\partial h}{\partial x_\beta} = \frac{dp}{dt}$$ If dp neglected

System characteristics

Another way to look at it

Take any conservative equation $\dfrac{\partial \rho \phi}{\partial t} + \nabla \rho u \phi = 0,$

$$= \rho \left(\frac{\partial \phi}{\partial t} + u \nabla \phi \right) + \phi \left(\frac{\partial \rho}{\partial t} + \nabla \rho u \right)$$

Mass (solved by LBM) is included in any other form.

Also, pressure work (for most energy equations) is coupled with the LBM part.

System characteristics

Some characteristic equations (good)

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

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

$$\frac{\partial h}{\partial t} + u_\beta \frac{\partial h}{\partial x_\beta} = \frac{dp}{dt}$$

If dp neglected

Discretization

Main message: ~anything works

- Second order centered differences OK most of the time.
- Upwind, MUSCL, TVD, AUSM,….
- Works better with isotropic schemes, e.g.

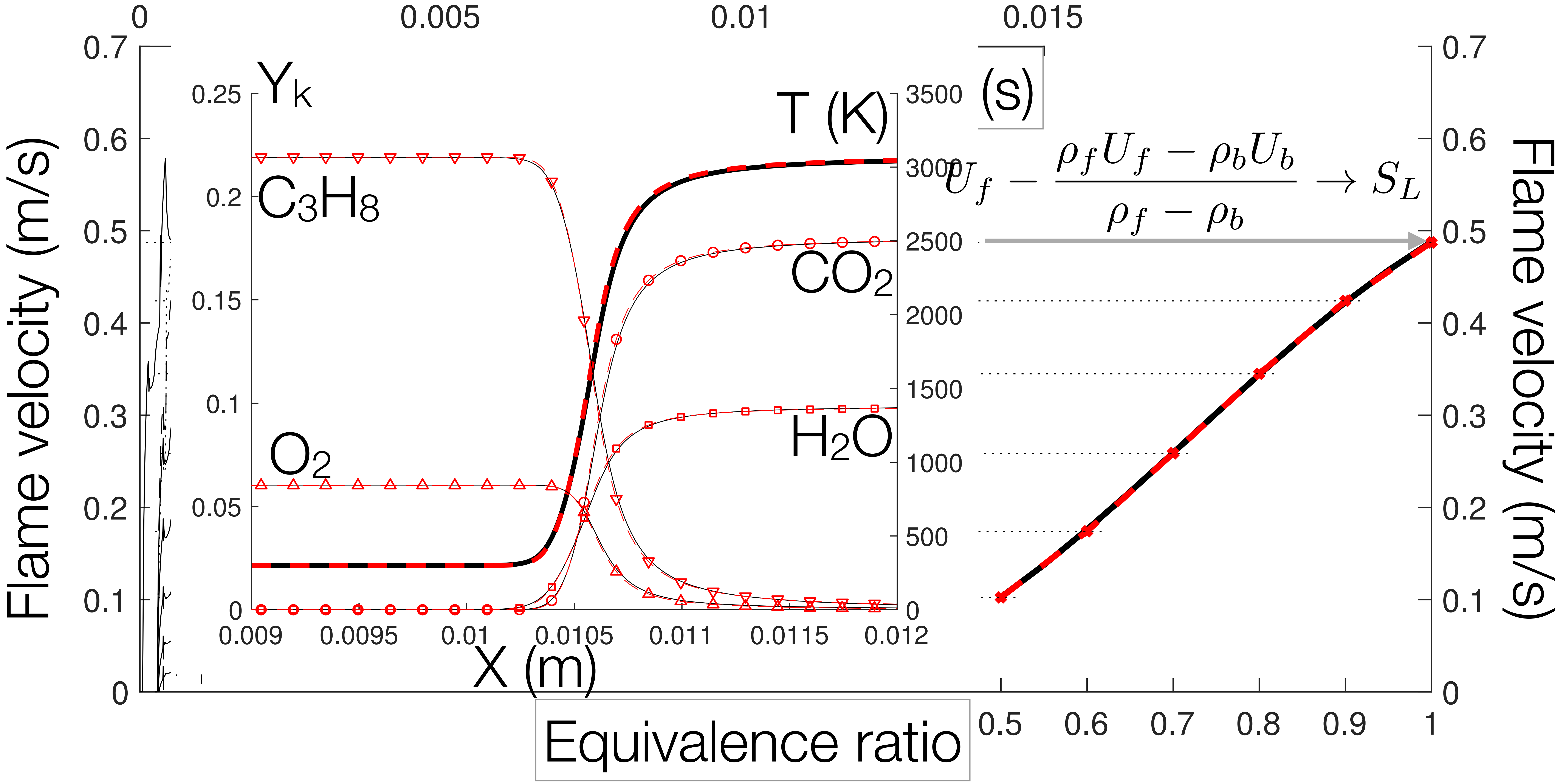
  A. Kumar, "Isotropic finite-differences," Journal of Computational Physics, vol. 201, no. 1, pp. 109 – 118, 2004.

  This is because LBM « sees » diagonal fluxes.

C3H8-air - 1s
Lewis transp.
Cp(T)

Success: premixed flame.

Enthalpy equation + species equations



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.

How to get closer to LBM ?

- Several proposals available, from very early LBM models

  [1] J. Onishi, Y. Chen, and H. Ohashi, “A lattice boltzmann model for polymeric liquids,” Progress in Computational Fluid Dynamics, an International Journal, vol. 5, no. 1-2, pp. 75–84, 2005.
  [2] F. Osmanlic and C. Korner, “Lattice boltzmann method for oldroyd-b fluids,” Computers & Fluids, vol. 124, pp. 190–196, 2016.

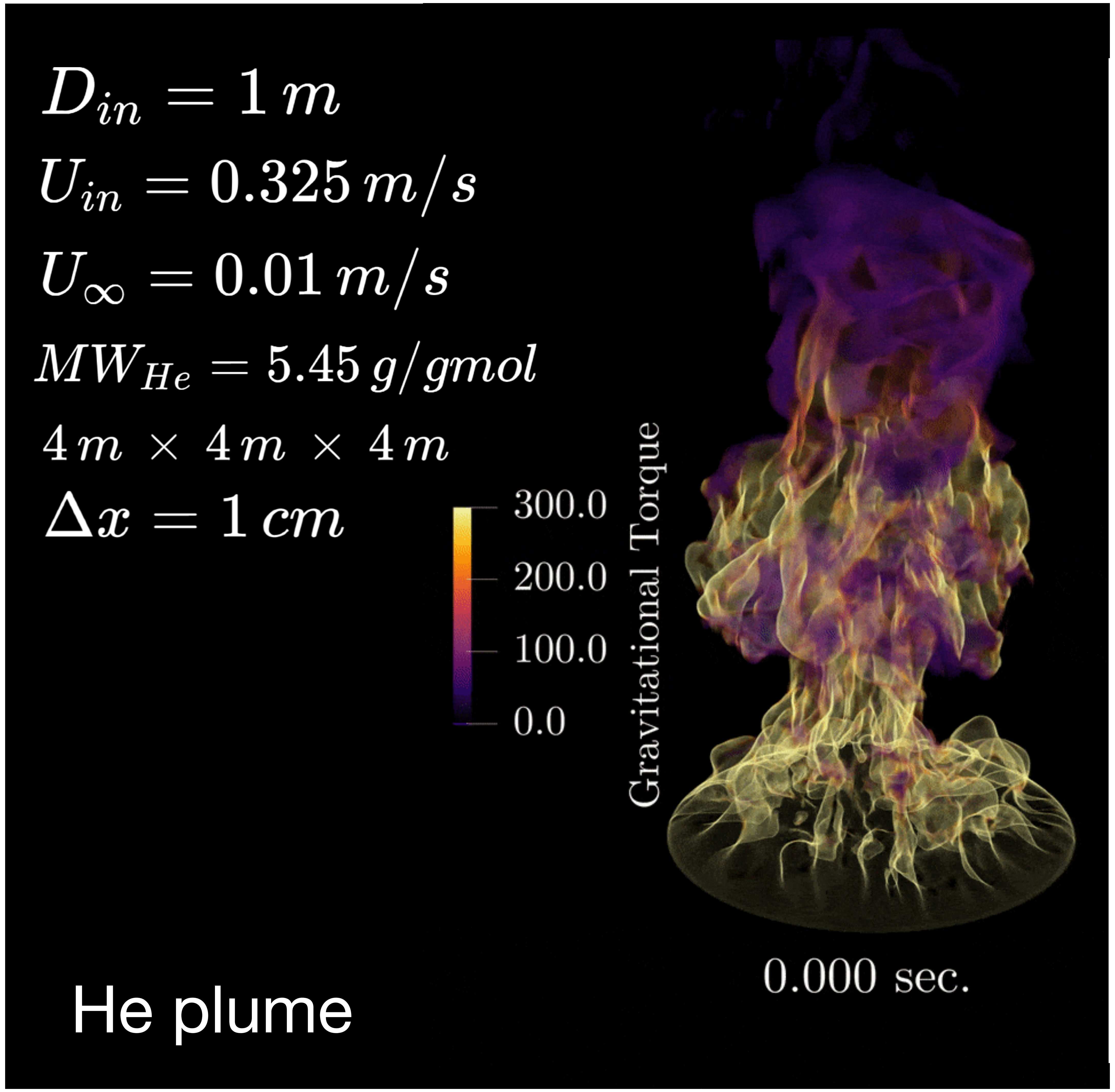
- The key is to understand what is the flux as computed from LBM.
  - Along a link, the flux through $\boldsymbol{x} + \frac{1}{2}\boldsymbol{c_i}\Delta t$ is $\Delta m_i \equiv f_i^{\mathrm{col}}(\boldsymbol{x} + \boldsymbol{c_i}\Delta t) - f_i^{\mathrm{col}}(\boldsymbol{x})$

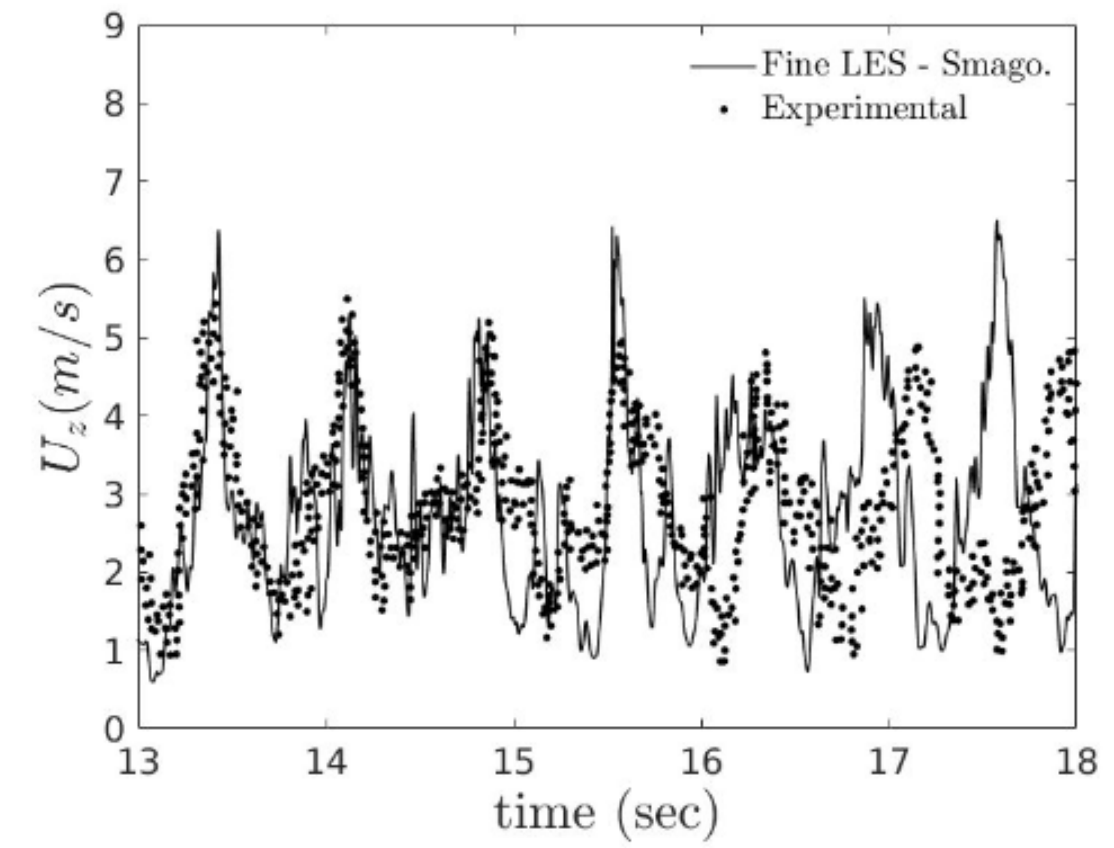
Osmanlic’s proposal $$(\boldsymbol{u} \cdot \nabla\phi)^{OS} \equiv \sum_i \frac{-\Delta m_i}{\rho(\boldsymbol{x}, t + \Delta t)} \begin{cases} \phi(\boldsymbol{x}, t) & \text{if } \Delta m_i \leq 0 \\ \phi(\boldsymbol{x} + \boldsymbol{c_i}\Delta t, t) & \text{otherwise.} \end{cases}$$

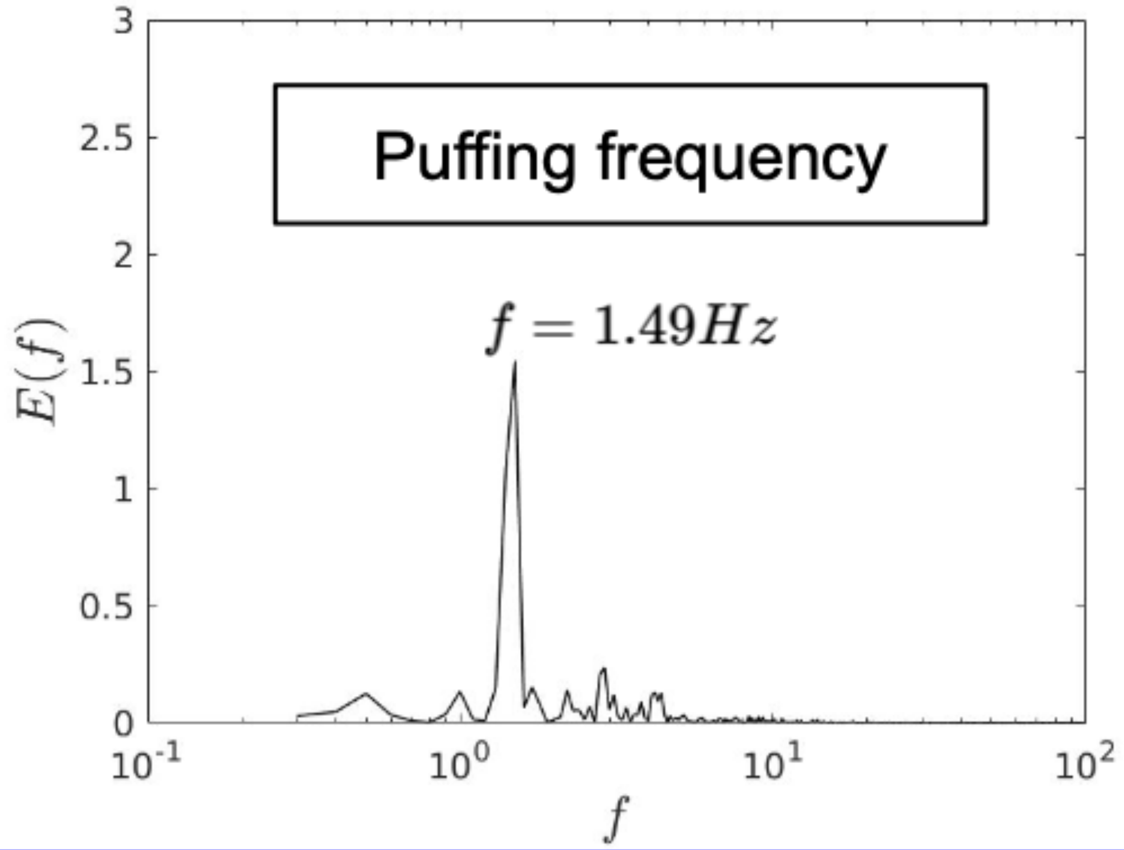
Colors for Directors CFD

Weakly compressible flow (multi-species)

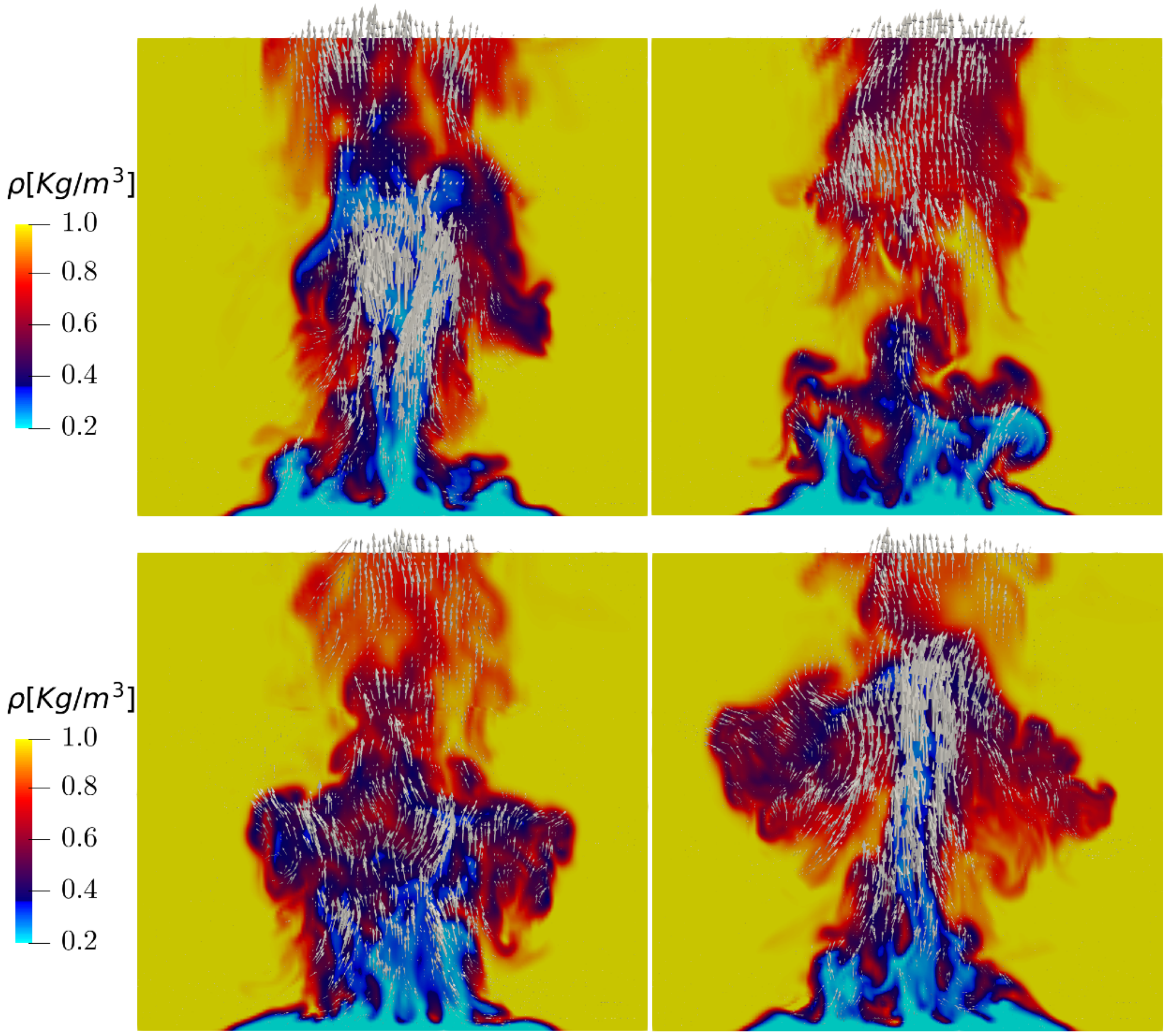
G. Wang, S. Zhao, P. Boivin, E. Serre, and P. Sagaut, “A new hybrid lattice-boltzmann method for thermal flow simulations in low-mach number approximation,” Physics of Fluids, vol. 34, no. 4, p. 046114, 2022.







Correct puffing frequency

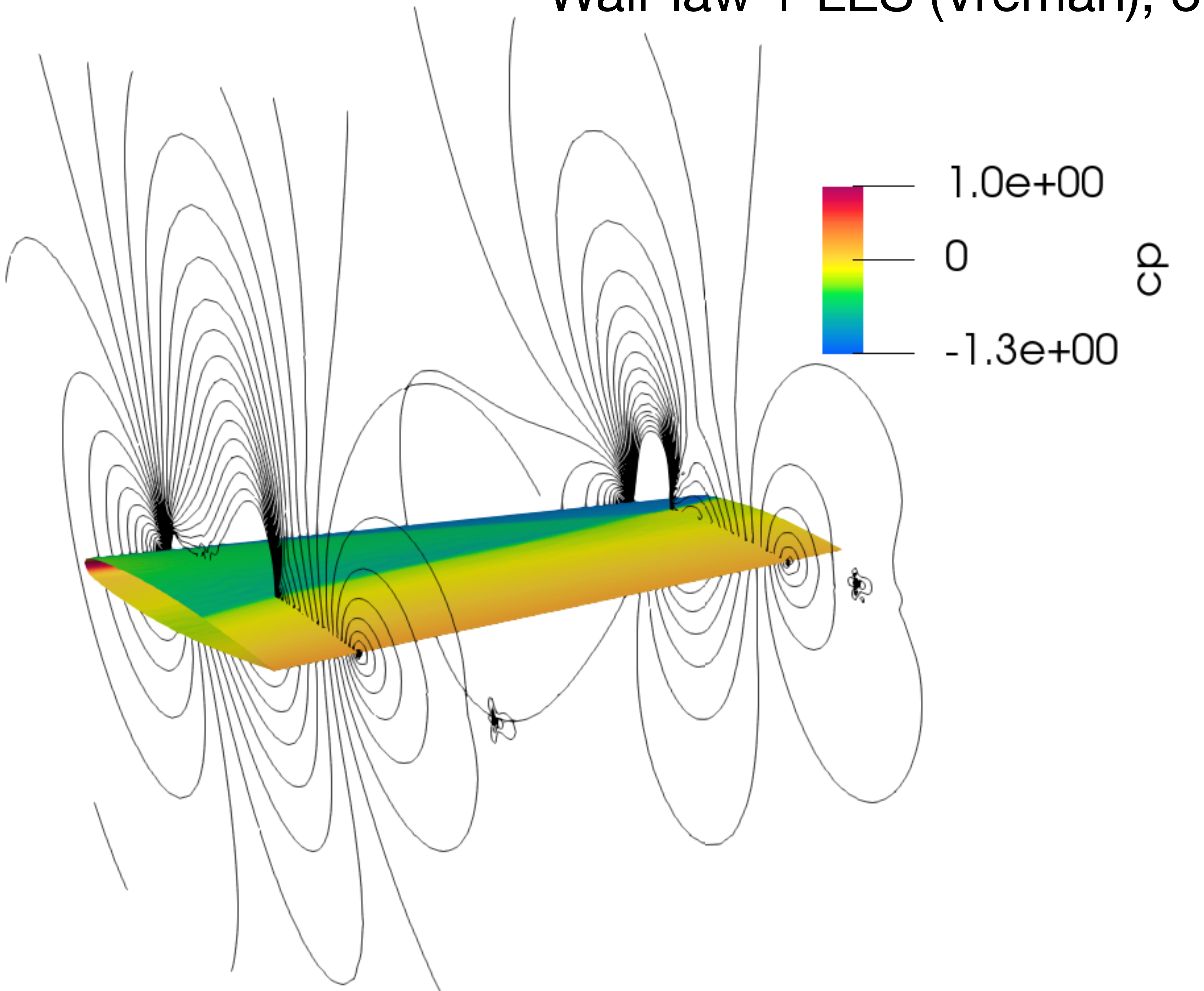


[1] M. Taha, S. Zhao, A. Lamorlette, J.-L. Consalvi, and P. Boivin, “Lattice-boltzmann modeling of buoyancy-driven turbulent flows,” Physics of Fluids, vol. 34, no. 5, p. 055131, 2022.
[2] M. Taha, S. Zhao, A. Lamorlette, J.-L. Consalvi, and P. Boivin, “Large eddy simulation of the Near-Field Region of a Turbulent Buoyant Helium Plume using Lattice-Boltzmann method”, 2024

3D aerodynamics

M6 wing

Wall-law + LES (Vreman), on turbulent M6 wing, Ma=0.84



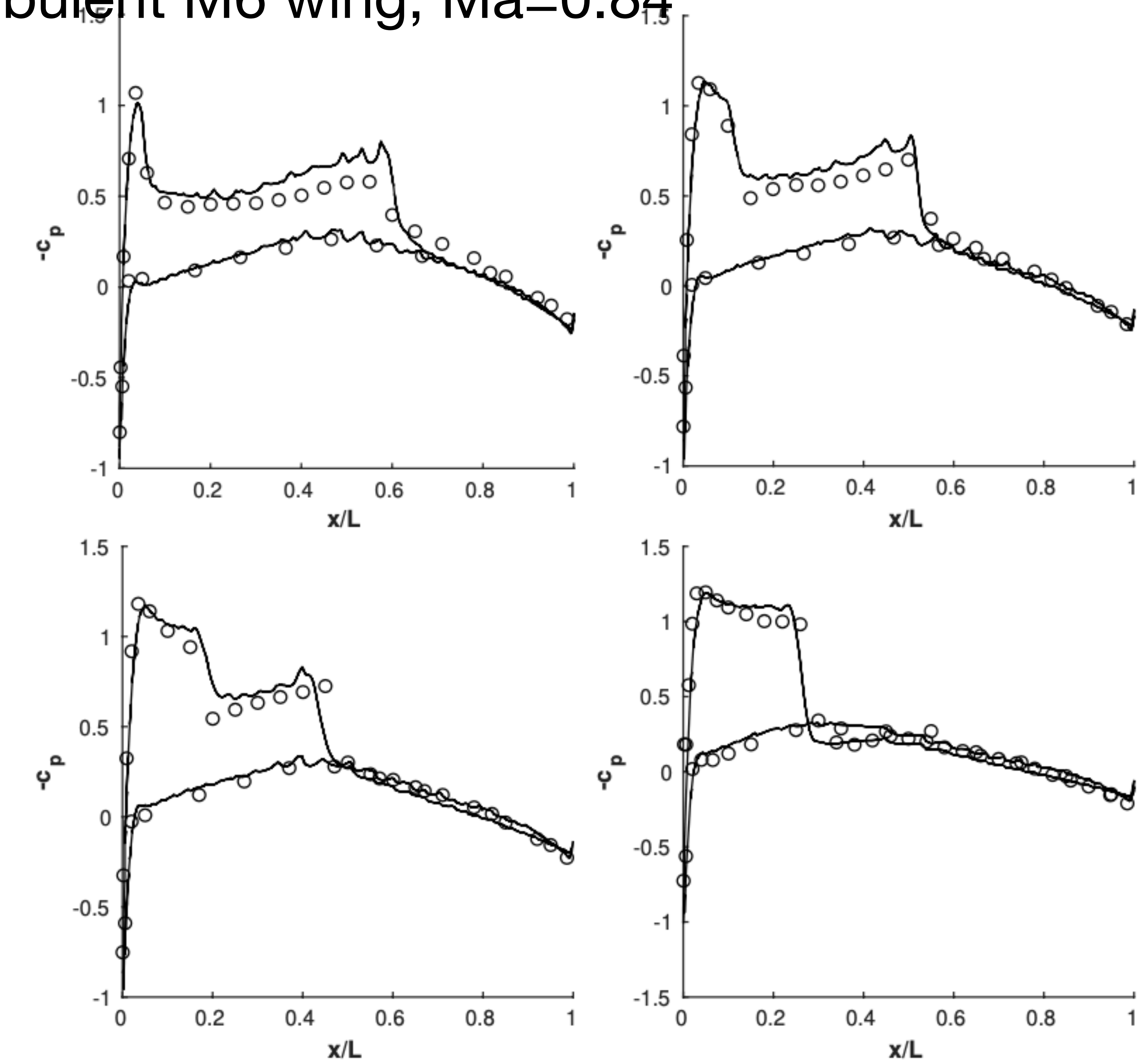
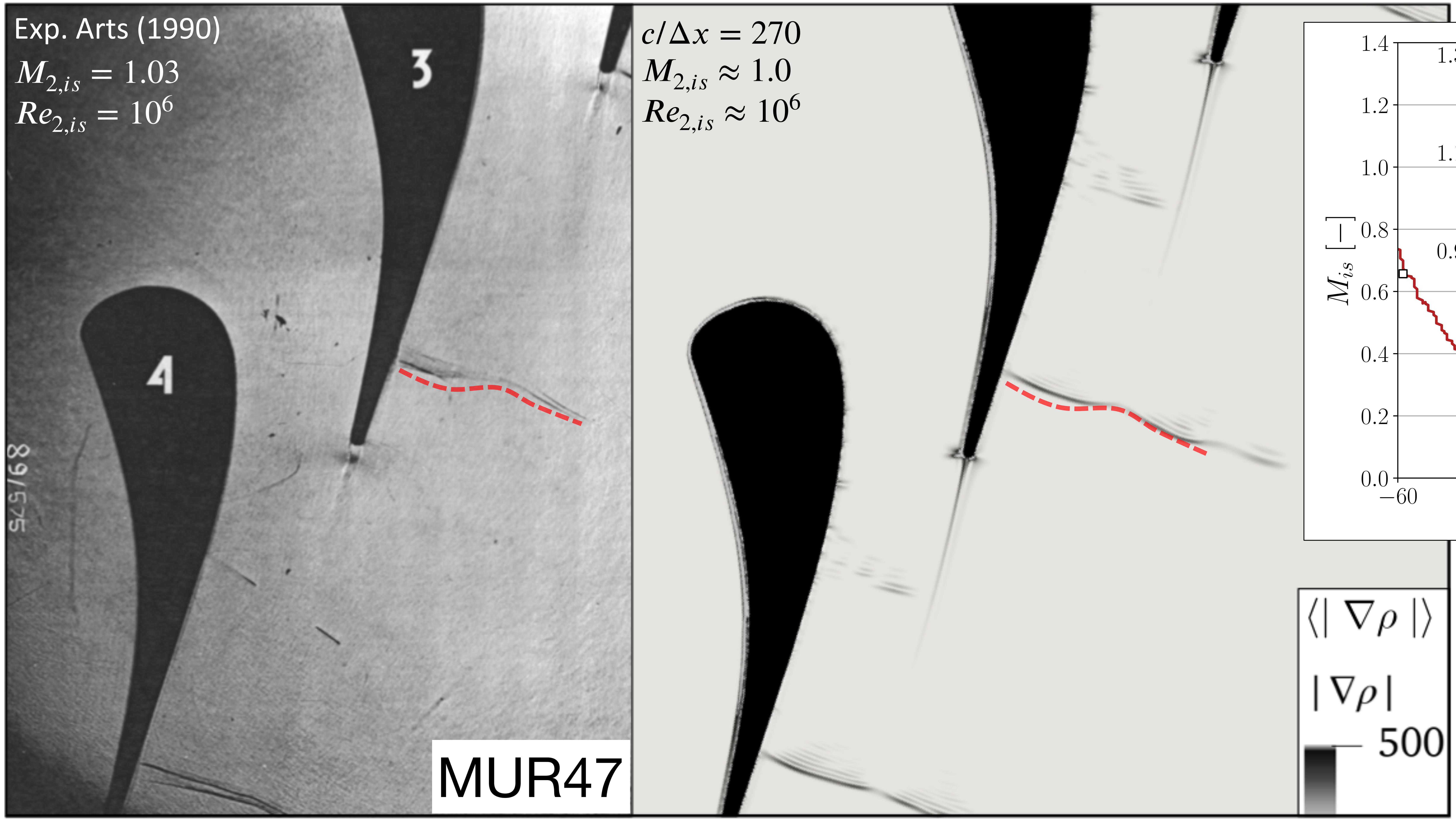


Figure 10: Pressure coefficient at (from top-left to bottom-right) $y = 20\%$, $y = 44\%$, $y = 65\%$ and $y = 90\%$; — LBM results; ∘ Expt.

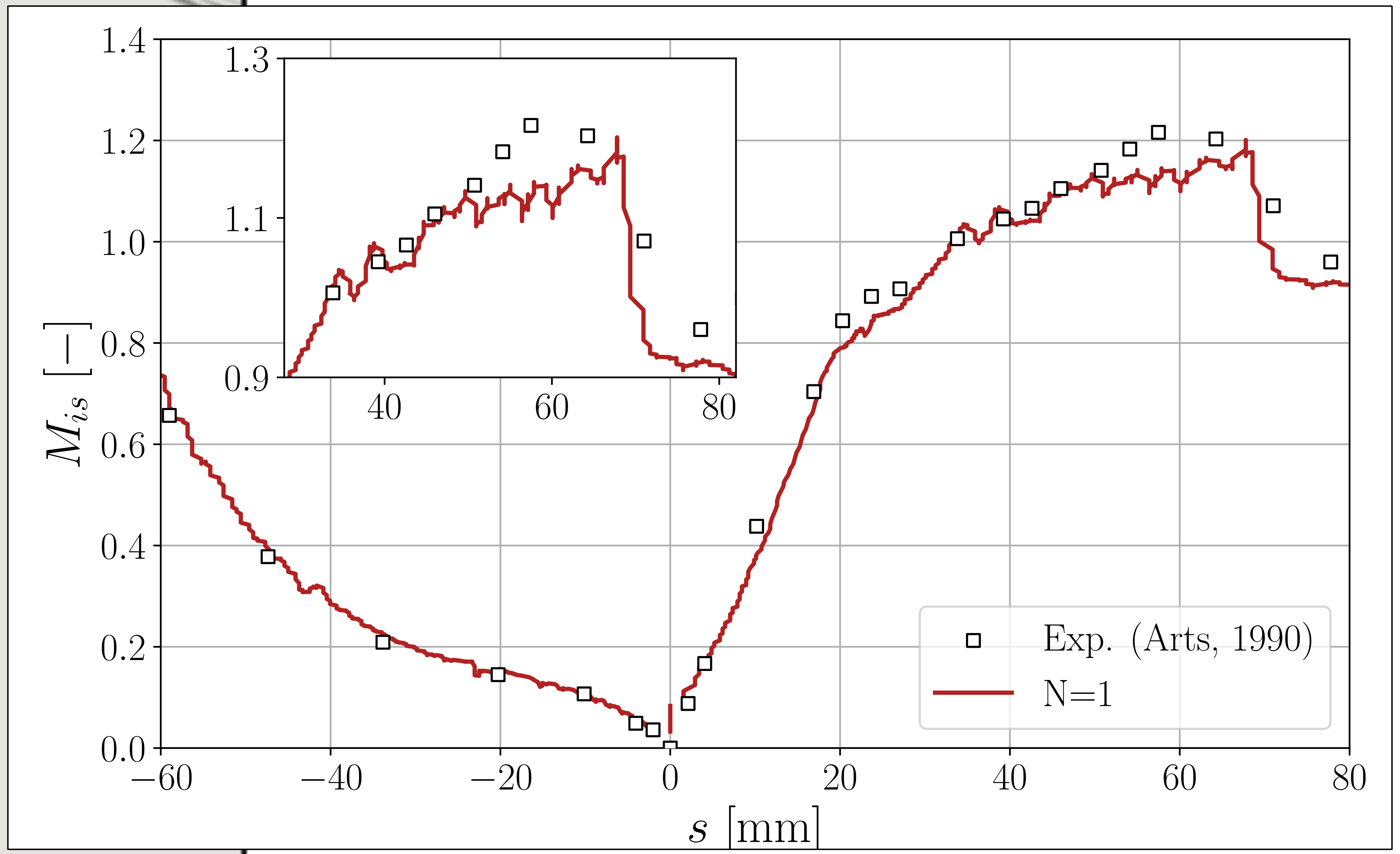
T. Coratger, G. Farag, S. Zhao, P. Boivin, and P. Sagaut, "Large-eddy lattice-boltzmann modelling of transonic flows," Physics of Fluids, 2021.

3D aerodynamics

LS89 blade cascade



Experimental (left) and numerical (right) Schlieren



Isentropic Mach number along the blade

Tsetsoglou et al. TurboExpo 2024

Non-conservative s/h equations ~ weak coupling

They are characteristics of the system

Outline

- Part I : Problem statement
- Part II : Additional scalar equations (weak coupling, non conservative)
- **Part III : Conservativity of scalar equations**
- Part IV : Application to hydrogen combustion & safety
- Part V: Discussion, perspectives

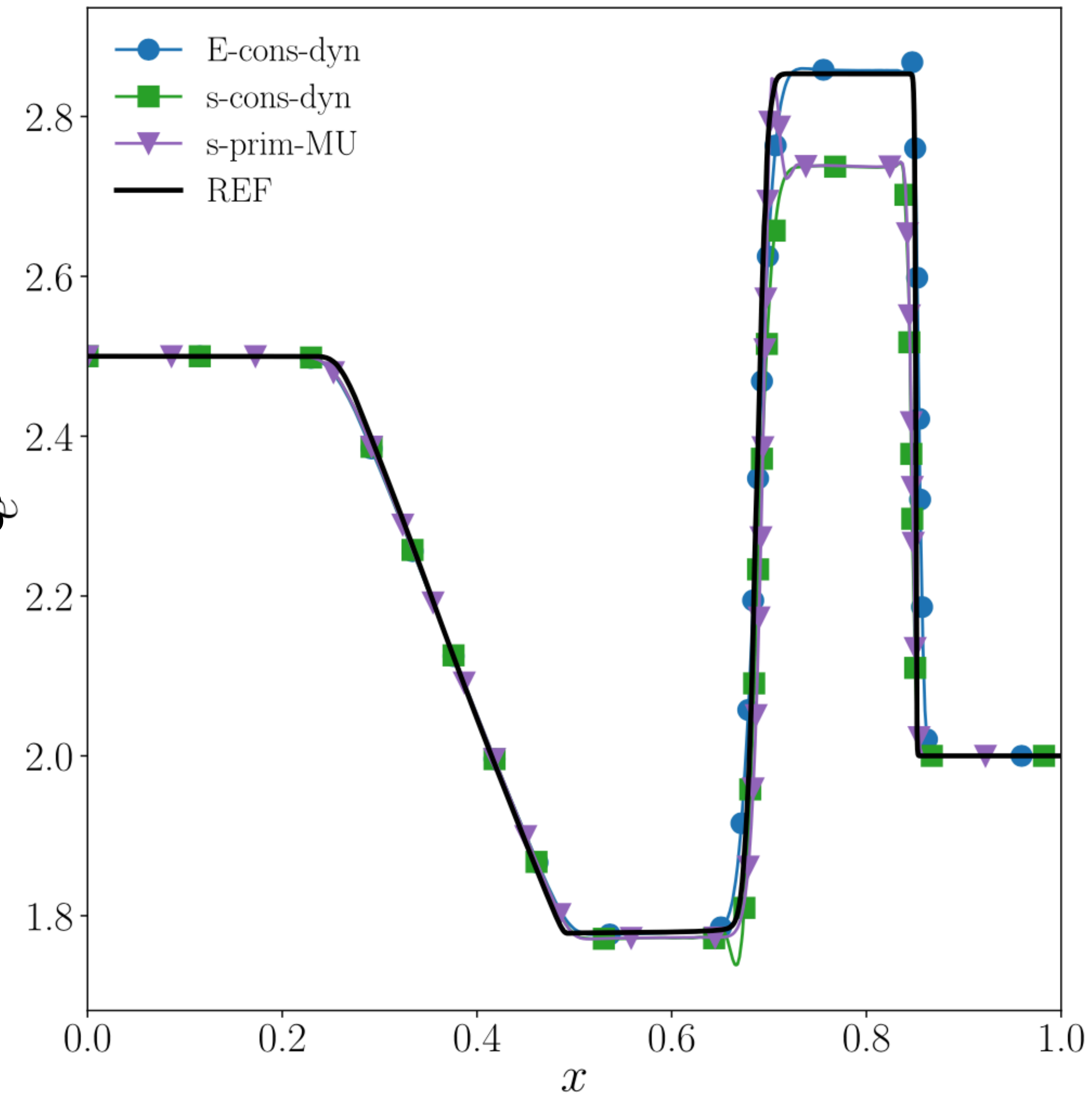
Conserving Scalars

Why ?

- Some scalar need to be conserved absolutely
  e.g. fuel/oxidizer for combustion

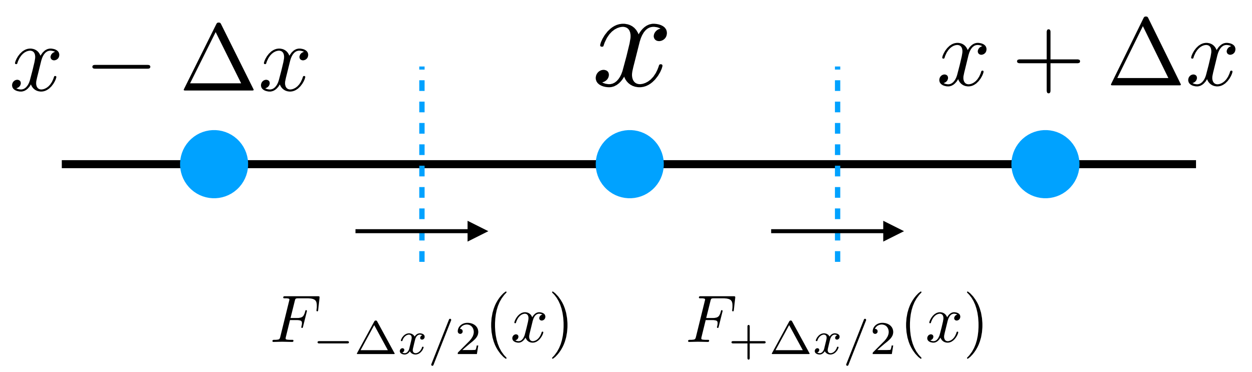
- Conservative form yield correct Hugoniot conditions

- …



How to make a system conservative ?

- General form of a conservative system in finite volume



$$\frac{U(x,t+\Delta t) - U(x,t)}{\Delta t} = \frac{F_{-\Delta x/2}(x,t) - F_{+\Delta x/2}(x,t)}{\Delta x}$$

- The system is conservative if the flux entering a cell is computed exactly in the same way as the corresponding existing flux (from the next cell)

$$\boxed{F_{-\Delta x/2}(x) = F_{+\Delta x/2}(x - \Delta x)}$$

- The conservative system may be written as (NB: this is exactly Godunov scheme, 1959):

$$\frac{U(x,t+\Delta t) - U(x,t)}{\Delta t} = \frac{F_{+\Delta x/2}(x - \Delta x,t) - F_{+\Delta x/2}(x,t)}{\Delta x}$$

Objective : Find the intercell flux

What about LBM ?

- Generic LBM scheme:

$$f_i(x, t+\Delta t) = f_i^{coll}(x - c_i \Delta t, t)$$

- Mass and momentum then follow [3] :

$$\frac{\rho(x, t+\Delta t) - \rho(x, t)}{\Delta t} = \frac{1}{\Delta t} \sum_i \left(f_i^{coll}(\boldsymbol{x} - \boldsymbol{c_i} \Delta t, t) - f_i^{coll}(\boldsymbol{x}, t) \right)$$

$$\frac{\rho u_\alpha(\boldsymbol{x}, t+\Delta t) - \rho u_\alpha(\boldsymbol{x}, t)}{\Delta t} = \frac{1}{\Delta t} \sum_i c_{i,\alpha} \left(f_i^{coll}(\boldsymbol{x} - \boldsymbol{c_i} \Delta t, t) - f_i^{coll}(\boldsymbol{x}, t) \right)$$

- Whcih can directly be recast as a flux (already mentioned previously) :

$$\boxed{\frac{\Phi(x, t+\Delta t) - \Phi(x, t)}{\Delta t} + \frac{F^{\Phi}_{+\Delta x/2}(x, t) - F^{\Phi}_{+\Delta x/2}(x - \Delta x, t)}{\Delta x} = 0 \qquad \Phi \in \{\rho, \rho u_\alpha\}}$$

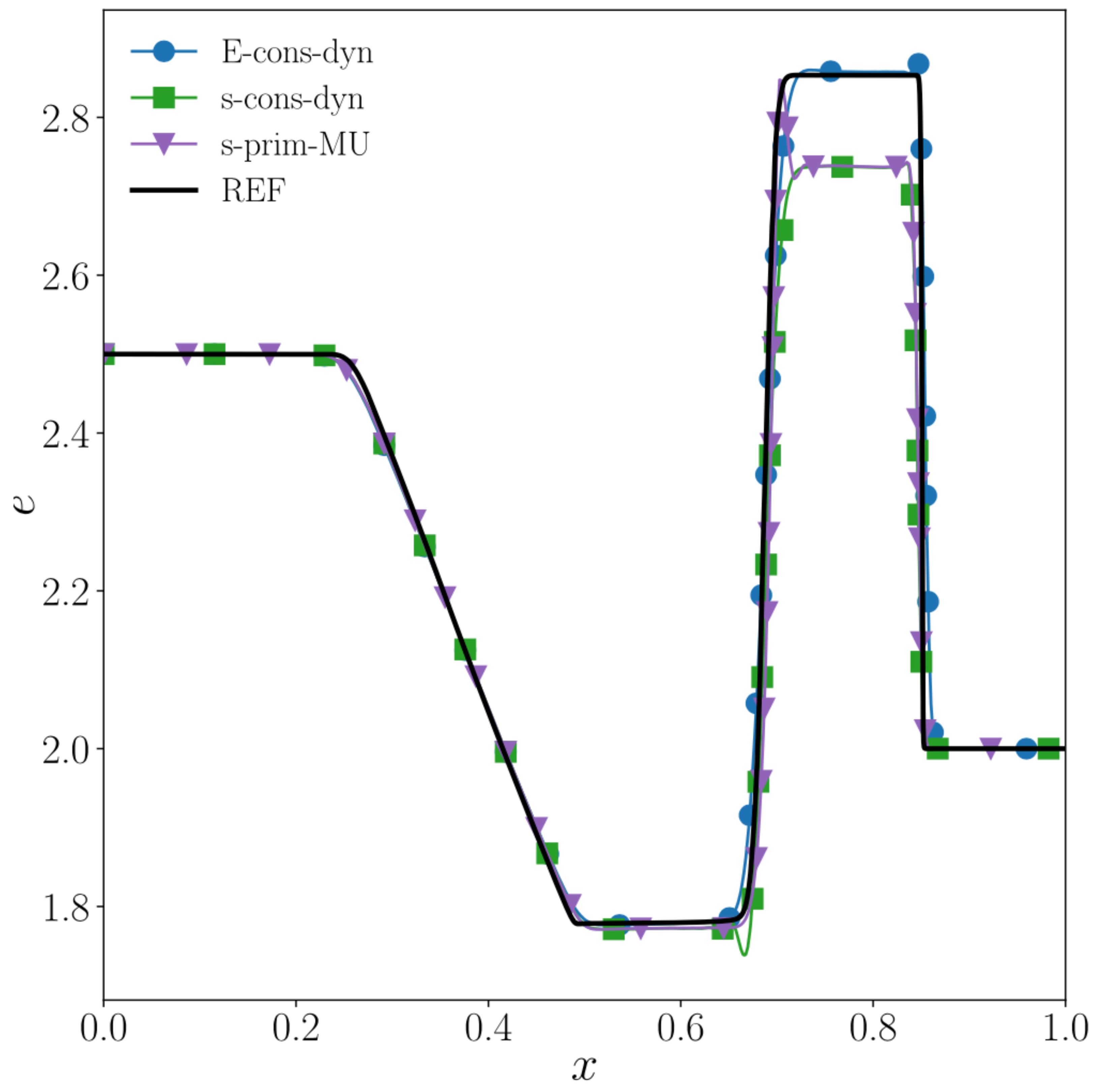
Any LBM scheme may be written as a conservative finite volume scheme [4]

[3] S. Zhao, G. Farag, P. Boivin, P. Sagaut, Toward fully conservative hybrid lattice Boltzmann methods for compressible flows. Physics of Fluids, 32(12) (2020).
[4] G. Wissocq, T. Coratger, G. Farag, S. Zhao, P. Boivin, Restoring the conservativity of characteristic-based segregated models: Application to the hybrid lattice Boltzmann method, Physics of Fluids.

Conserving Scalars

Basic idea

- For any advection equation $\dfrac{\partial \rho\phi}{\partial t} + \nabla \rho u \phi = 0,$
  - (= mass conservation + non-conservative scalar eq)
  - $\nabla^C \cdot (\rho \boldsymbol{u} \phi) \equiv \dfrac{1}{\Delta t} \sum_i \left[f_i^{\mathrm{col}} \dfrac{\phi^+ + \phi}{2} - f_i^{\mathrm{col}-} \dfrac{\phi + \phi^-}{2} \right]$
  - ~ Match the LBM mass flux computation to compute scalar eqs.
  - => numerically conserve $\rho\phi$ and $\rho\phi^2$
  - And respect the Hugoniot jump conditions



- Using the LBM fluxes is ~ to mimicking the 0th order of a second distribution (at no extra cost…)
  - *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.*

What if I want to use my own FV scheme (e.g. TVD or with limiter) ?

Conserving Scalars

A more advanced solution

- **Non-conservative scheme:**

LBM

FD / FV

$$\begin{cases} \delta_t \rho = -\delta_x F_\rho^{\mathrm{LBM}}, \\ \delta_t(\rho u) = -\delta_x F_{\rho u}^{\mathrm{LBM}}, \\ \delta_t s = -u\delta_x \mathcal{F}^{\mathrm{FD}}(s), \\ \delta_t Y = -u\delta_x \mathcal{F}^{\mathrm{FD}}(Y). \end{cases}$$

✦ Linearly stable
✦ **Characteristics are (linearly) decoupled**
✦ Total mass and momentum are conserved, **but total energy and mass of each species are not**

$$\Updownarrow$$

Linear equivalence

- **A new conservative FV scheme can be derived**

Finite Volumes

$$\begin{cases} \delta_t(\rho E) = -\delta_x F_{\rho E}, \\ \delta_t(\rho Y) = -\delta_x F_{\rho Y}. \end{cases}$$

✦ Linearly stable
✦ **Characteristics are (linearly) decoupled**

✦ Total mass, momentum, **total energy and mass of each species conserved**

G. Wissocq, T. Coratger, G. Farag, S. Zhao, P. Boivin, and P. Sagaut, "Restoring the conservativity of characteristic-based segregated models: application to the hybrid lattice boltzmann method," Physics of Fluids, 2022.

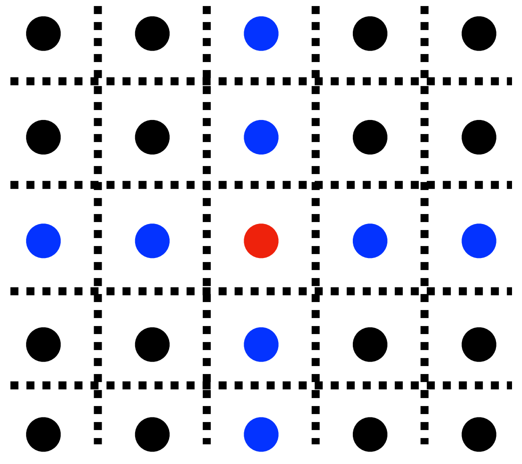
Conserving Scalars

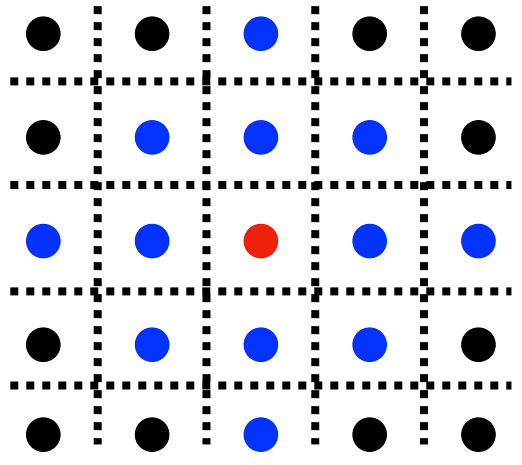
A more advanced solution

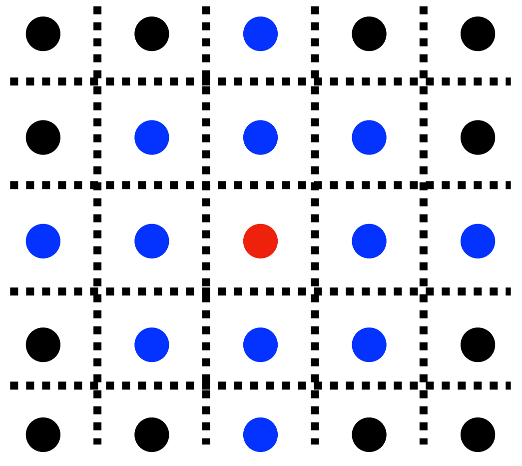
- **Expression of fluxes:**

$$
\begin{aligned}
F_{\rho E} &= \mathcal{F}^{\mathrm{FD}}(\rho H u) + (h - u^2/2)\left(F_{\rho}^{\mathrm{LBM}} - \mathcal{F}^{\mathrm{FD}}(\rho u)\right) + u\left(F_{\rho u}^{\mathrm{LBM}} - \mathcal{F}^{\mathrm{FD}}(\rho u^2 + p)\right), \\
F_{\rho Y} &= \underbrace{\mathcal{F}^{\mathrm{FD}}(\rho u Y)}_{\textit{Expected flux}} + \underbrace{Y\left(F_{\rho}^{\mathrm{LBM}} - \mathcal{F}^{\mathrm{FD}}(\rho u)\right)}_{\textit{Numerical corrections}}
\end{aligned}
$$

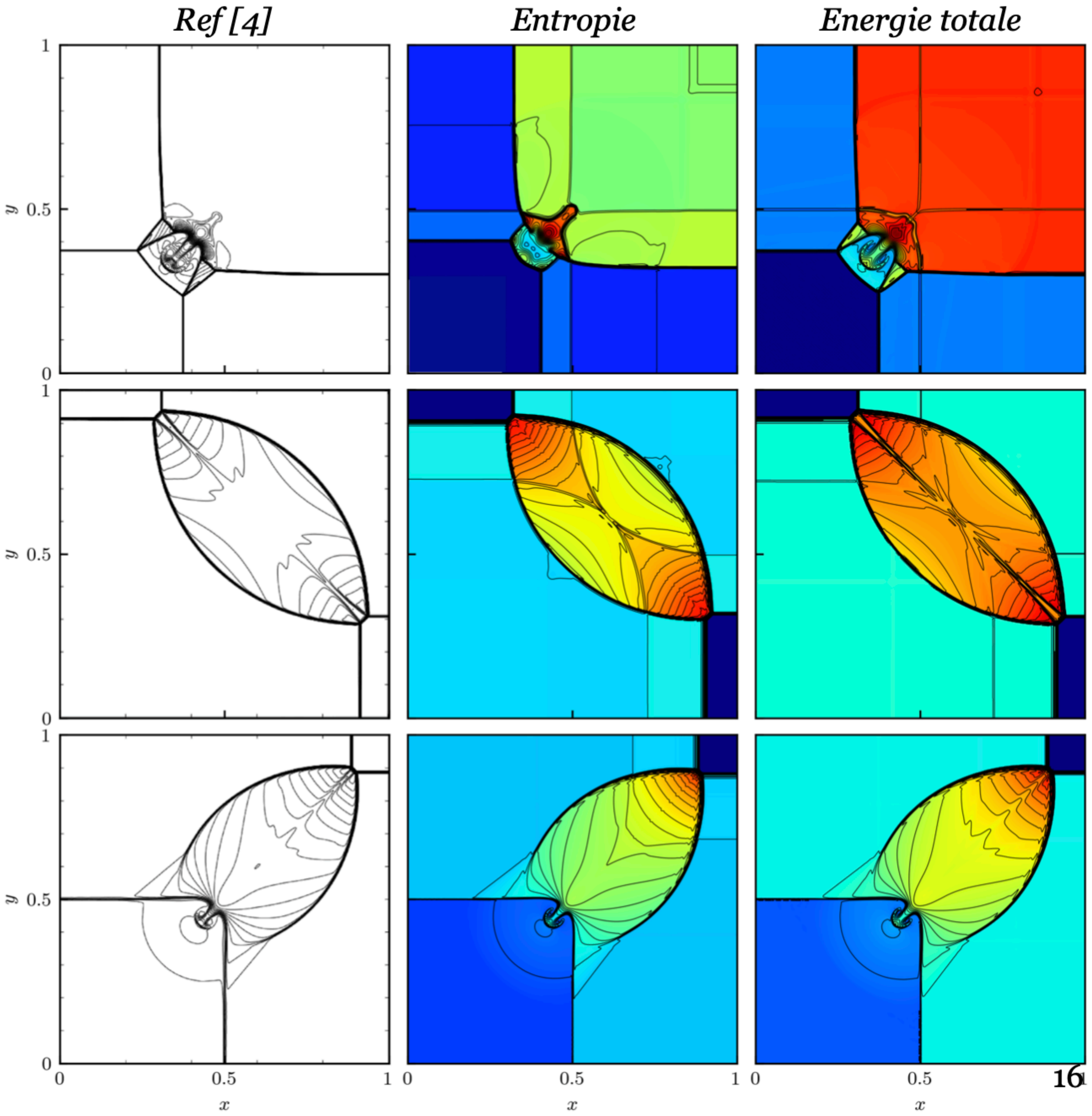
- **Choices for the discretization operator $\mathcal{F}^{\mathrm{FD}}$:**

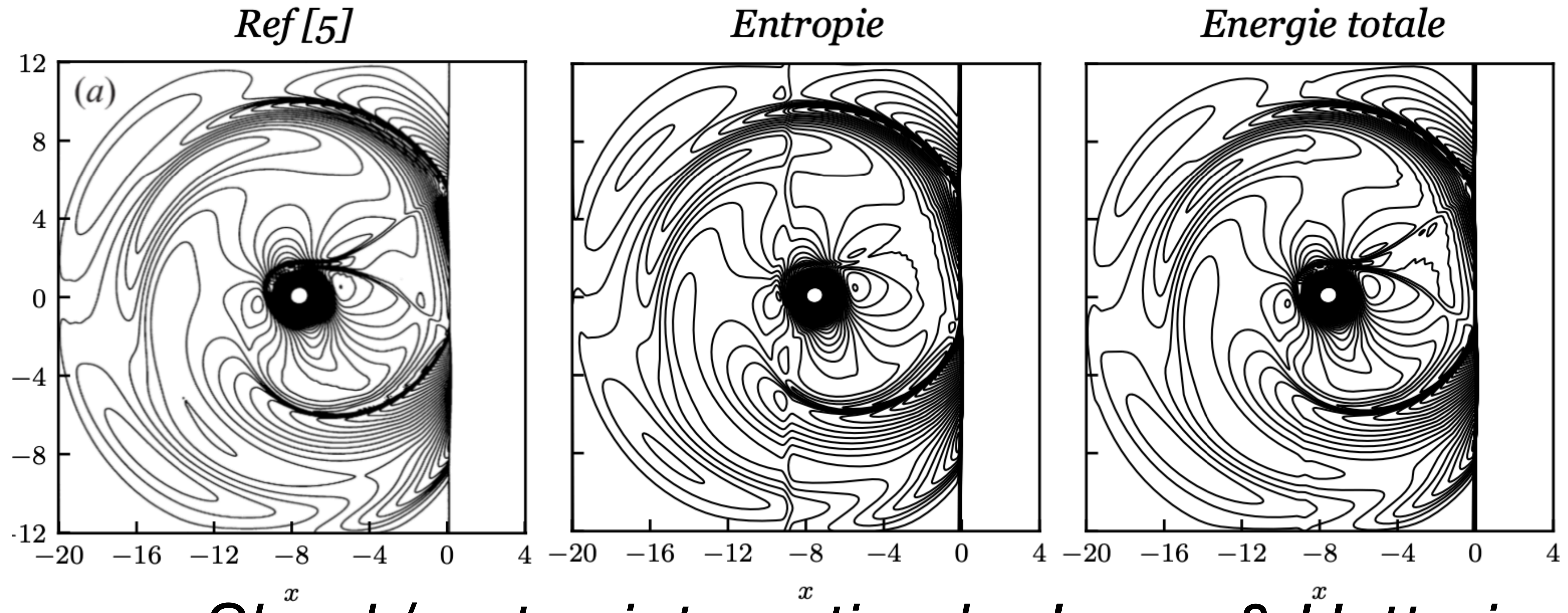
1) MHM 1D [2] 

2) MHM 2D [3] 

3) Heun (TVD) 

Compressible core - total energy





Shock/vortex interaction by Inoue & Hattori
Ma_s = 1.29, Ma_v=0.39, Re = 800

Shock sensors:

[1] 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.
[2] G. Wissocq, T. Coratger, G. Farag, S. Zhao, P. Boivin, and P. Sagaut, “Restoring the conservativity of characteristic-based segregated models: application to the hybrid lattice boltzmann method,” Physics of Fluids, 2022.

[3] upcoming LBMOOD - preprint available

Outline

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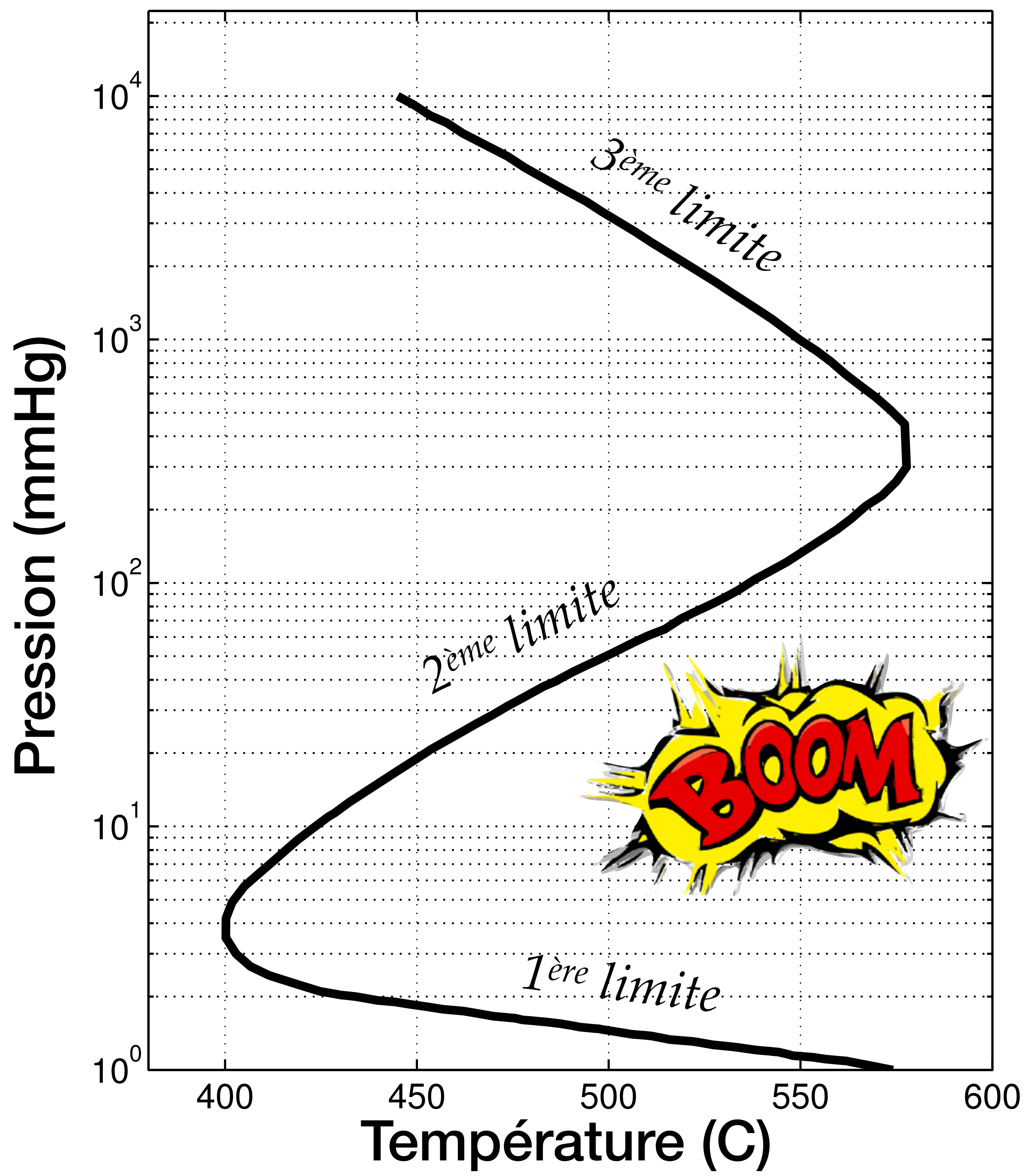
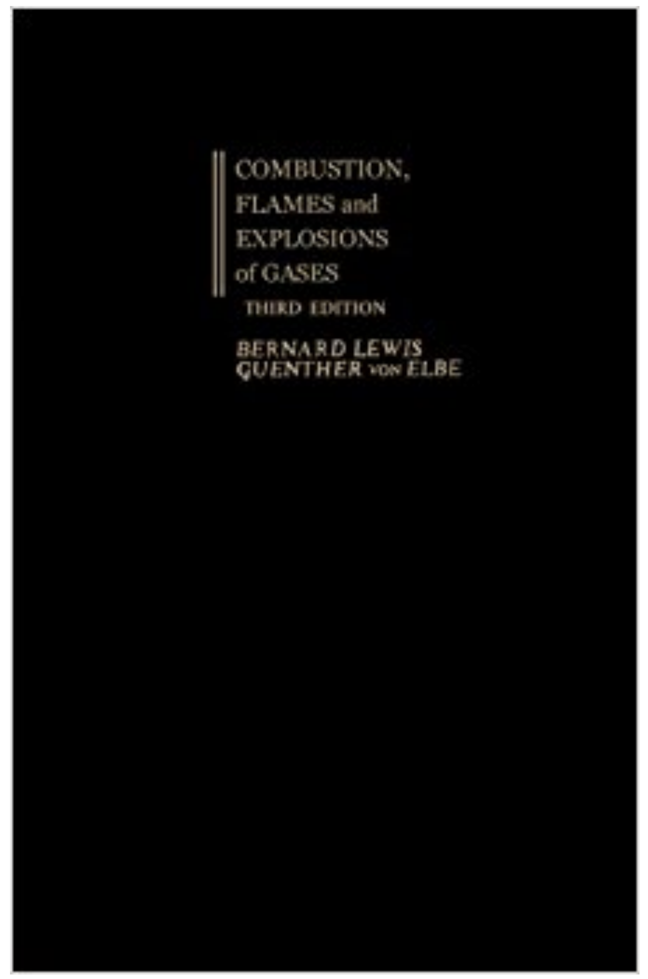
H_2 = problems

- NOx emissions
- Combustion instabilities
- Impact on radiative fluxes
- Blends H_2 et natural gas.
- Safety (H_2 leaks)
- Transition to detonation



Experimental explosion limits of a stoichiometric hydrogen-oxygen mixture in a 3.7 cm radius spherical vessel, from the classical Lewis & von Elbe textbook

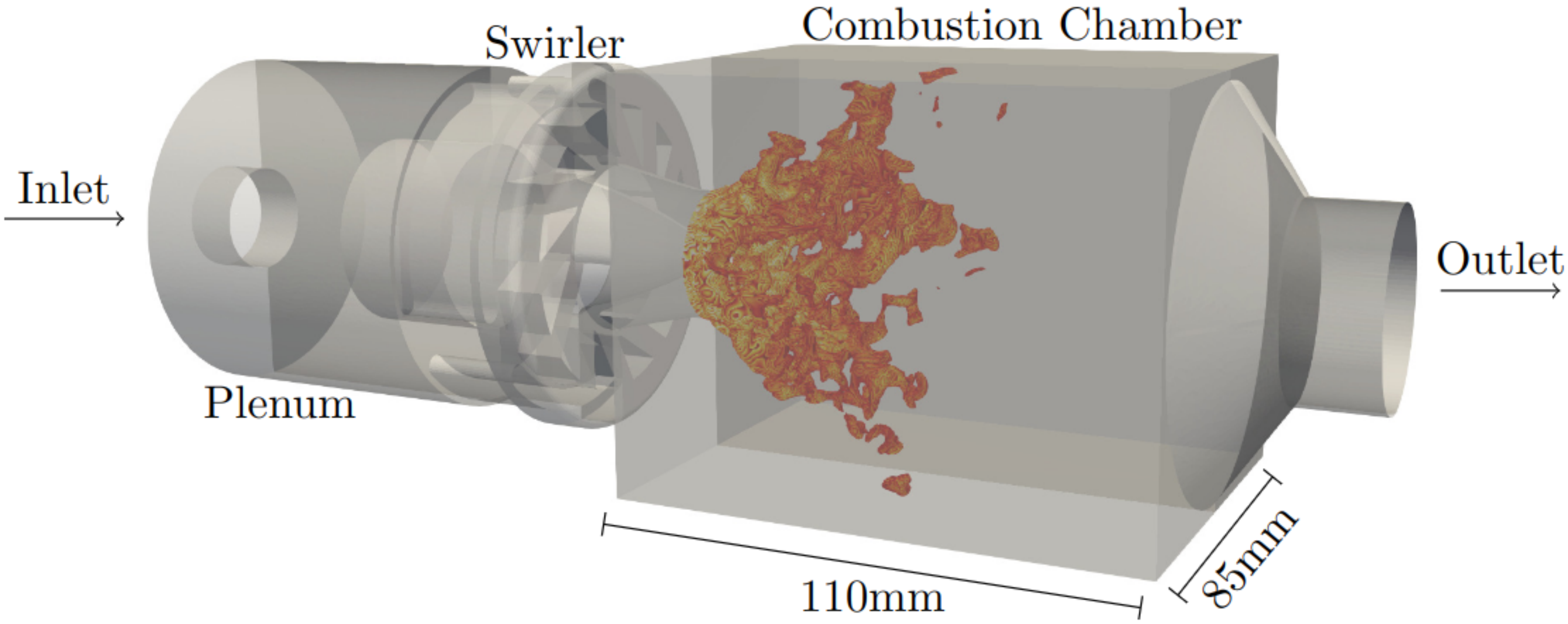
Hinshelwood & Semonov
~1920-1940
Nobel 1956



Turbulent premixed combustion

Aeronautical engine

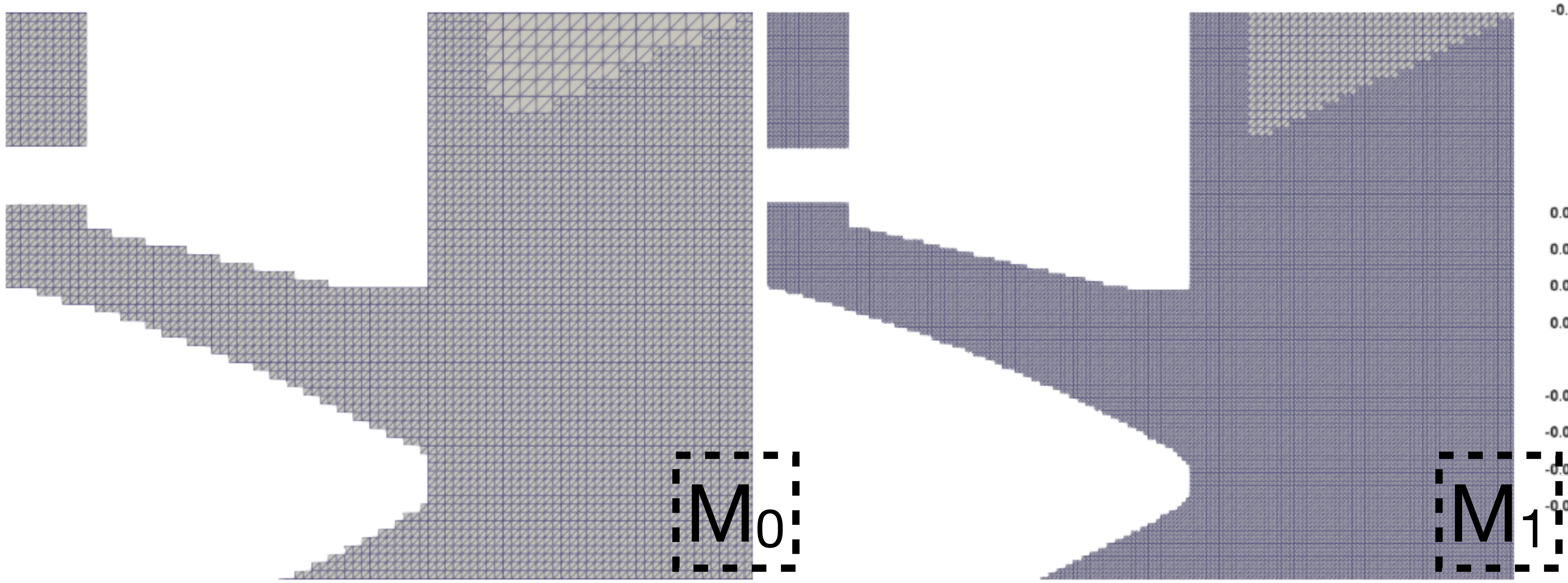
Preccinsta

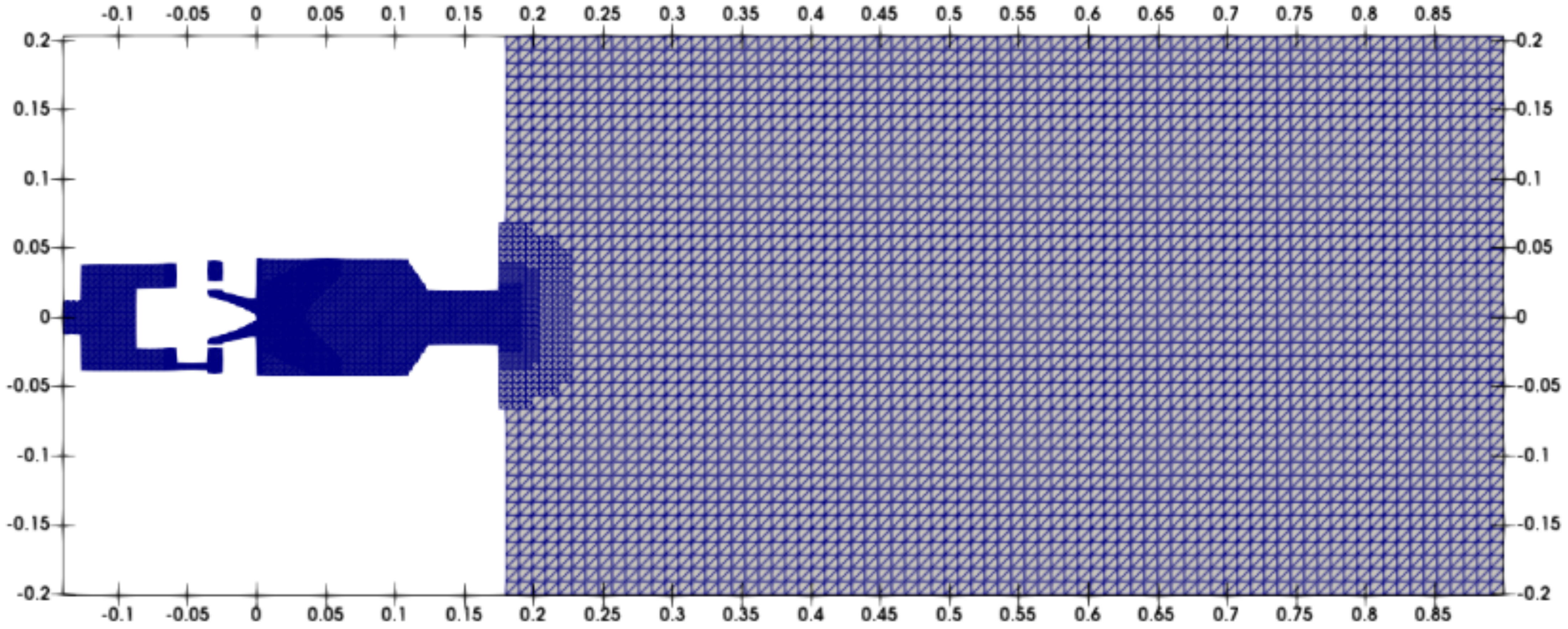


Aeronautical engine

Set-up — Mesh

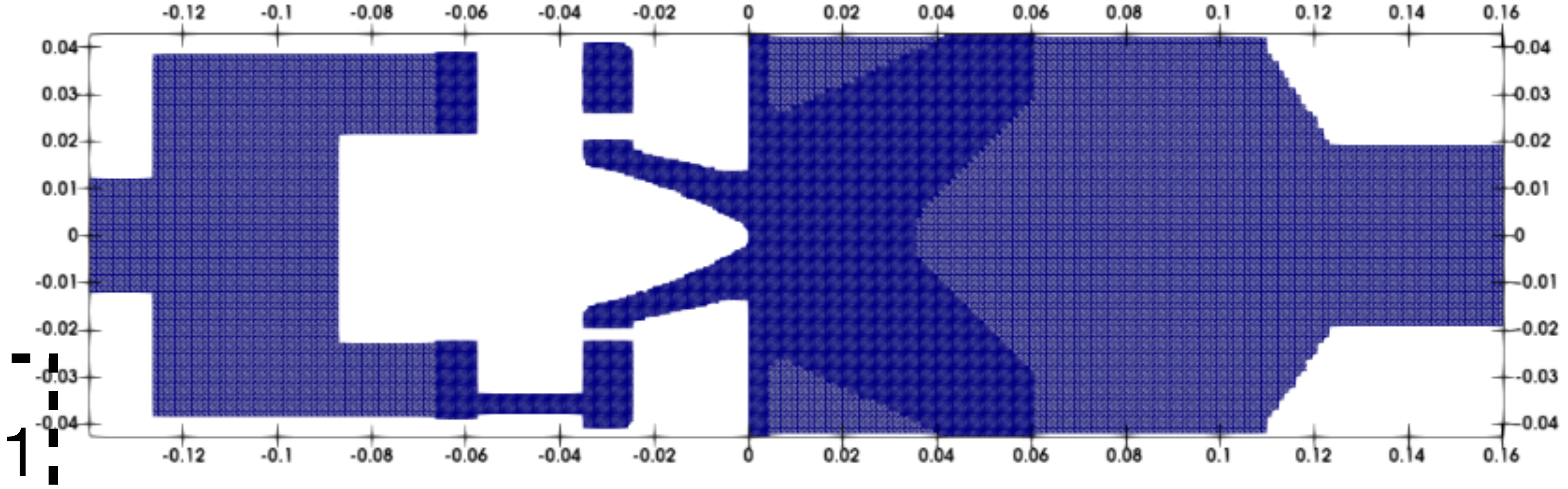
	M0	M1	M2	M1-Lu17	M1-LMNA
No. of pts.	2.4M	19.9M	81.2M	19.9M	19.9M
Minimum Δx	0.6 mm	0.3 mm	0.15 mm	0.3 mm	0.3 mm
LBM strategy	comp.	comp.	comp	comp.	LMNA
Chemistry	BFER	BFER	BFER	Lu17	BFER
Pts. in thickened δ_T^L	10	6	6	13	6





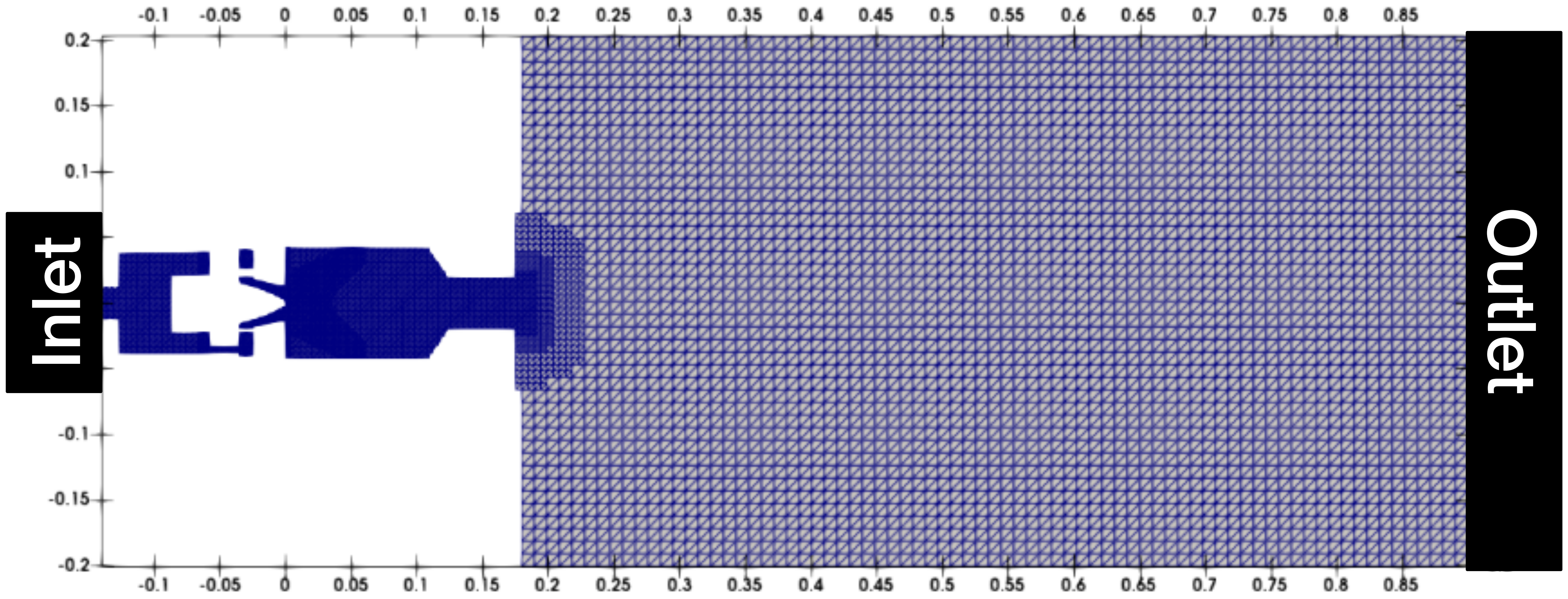
(a) M1

Mesh M_1



Aeronautical engine

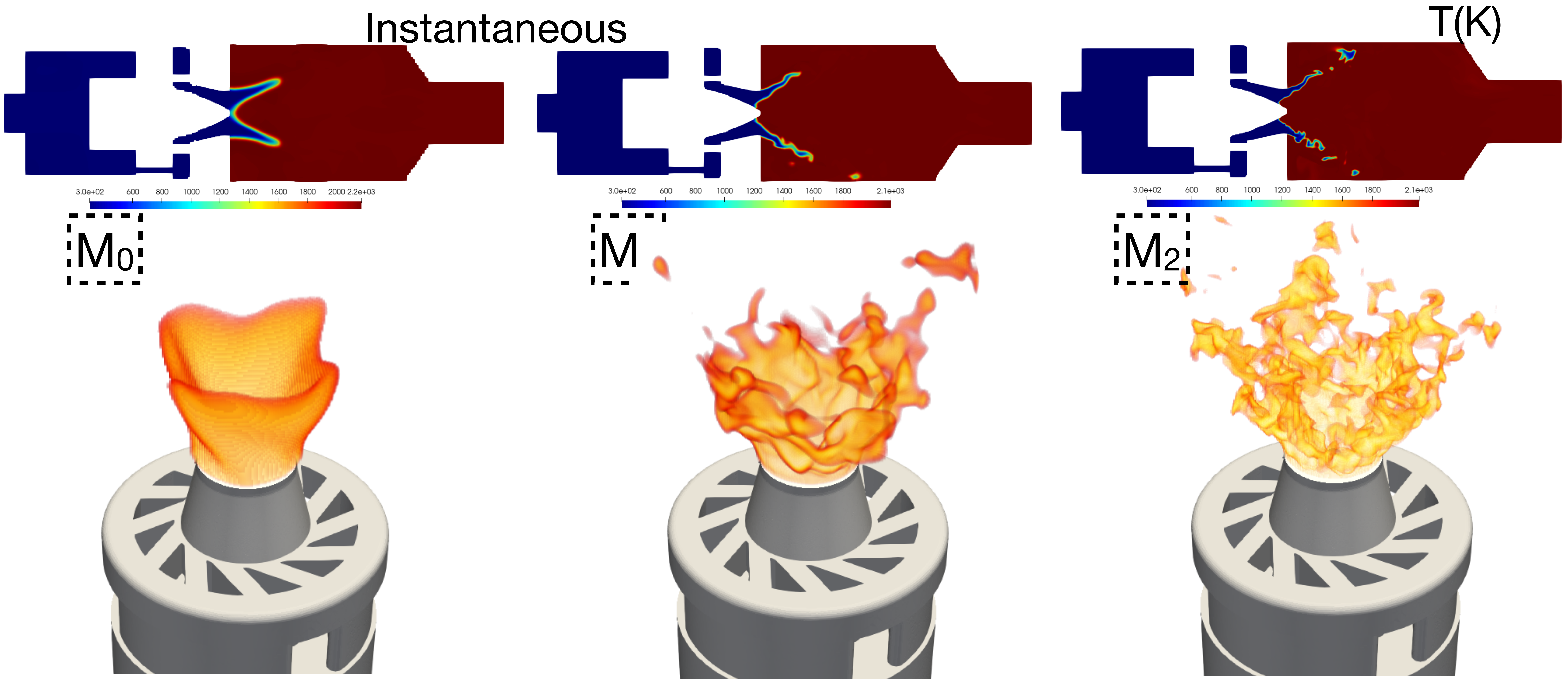
Set-up & models



- Inlet > characteristic non-reflecting BC, target mass flow rate
- Outlet > Non-reflecting BC, target atmospheric pressure.
- Everything else > Adiabatic, non-slip walls.

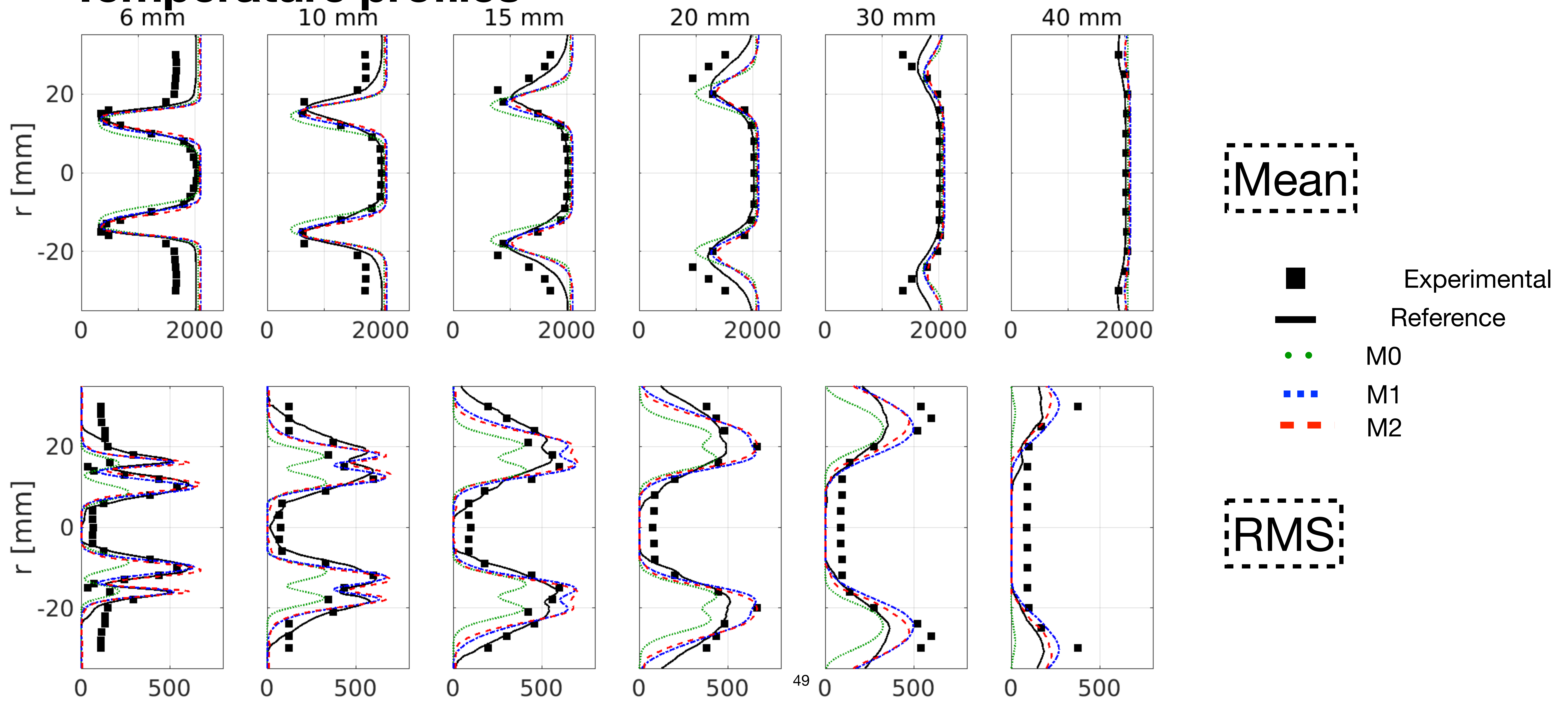
- Turbulence:
  - Vreman (ν_t)
  - $Sc_t = Pr_t = 0.7$
  - TFLES [1], $\beta = 0.5$
- Chemistry
  - 2s_BFER, *1s_CnHm, Lu17.*
- Transport
  - (Pr, Sc_k); or mixture-averaged.

Results — qualitative



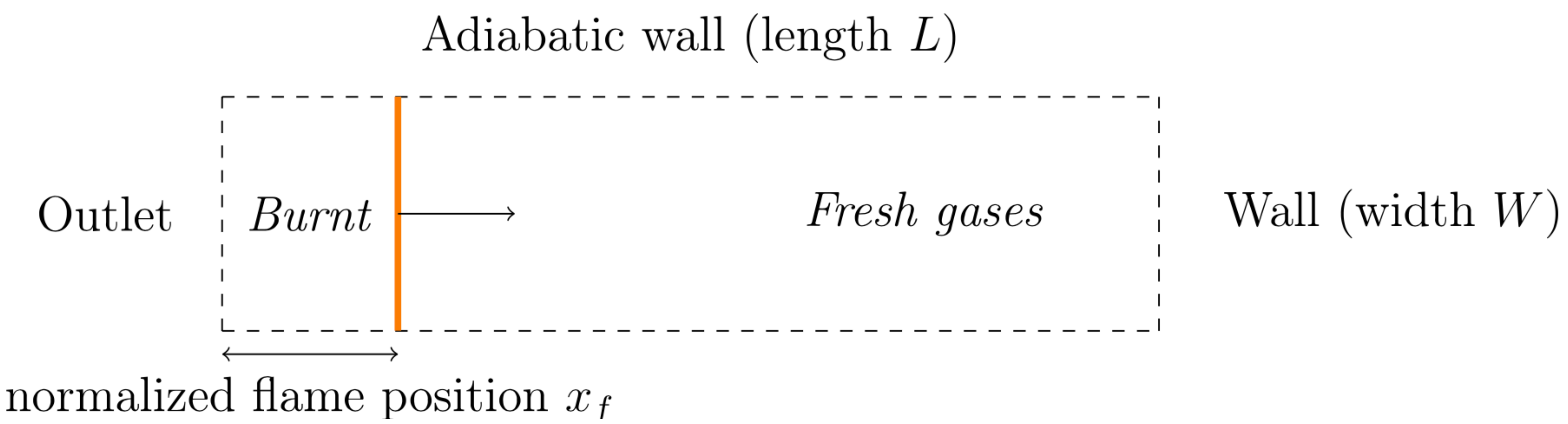
Results — quantitative

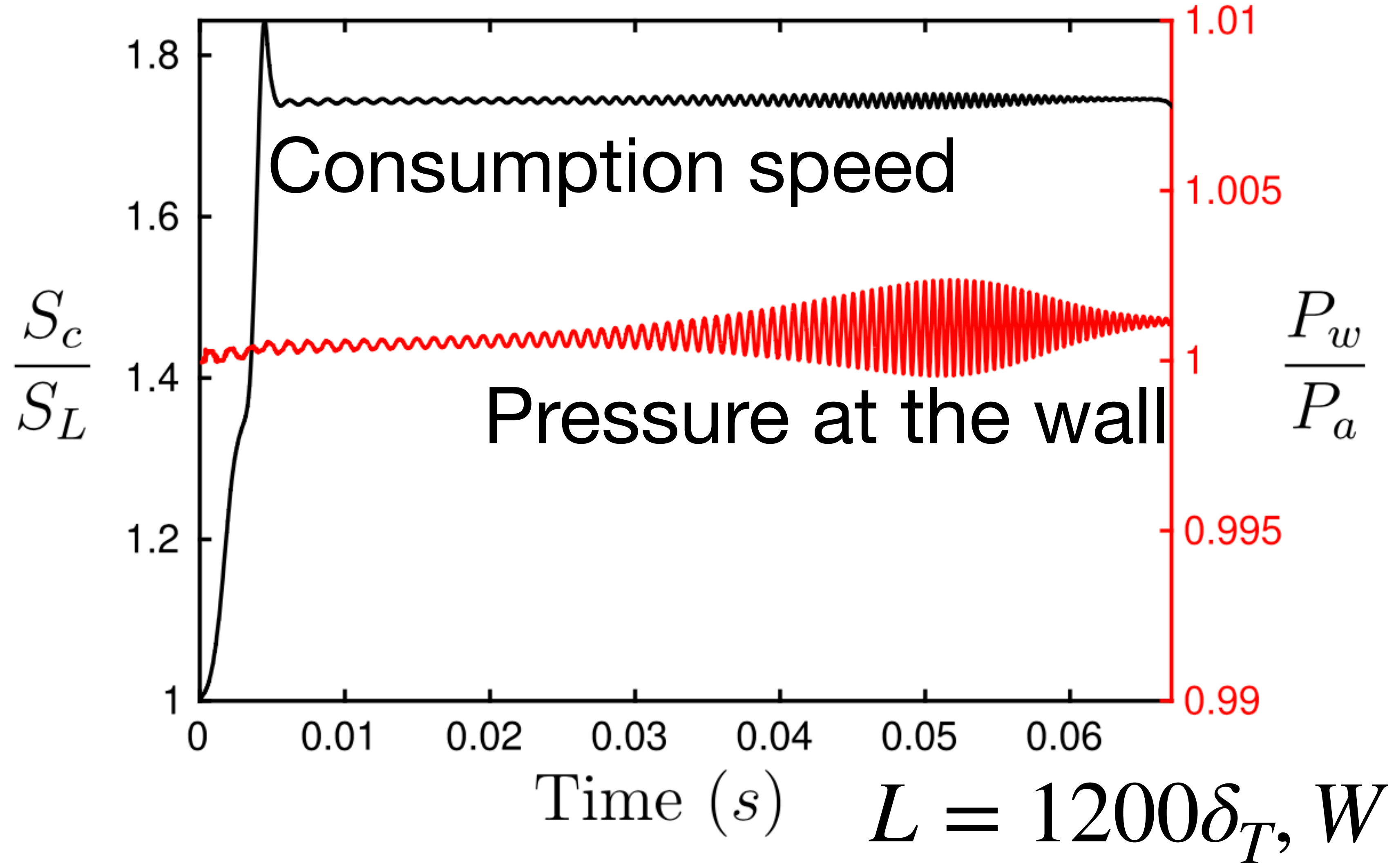
Temperature profiles



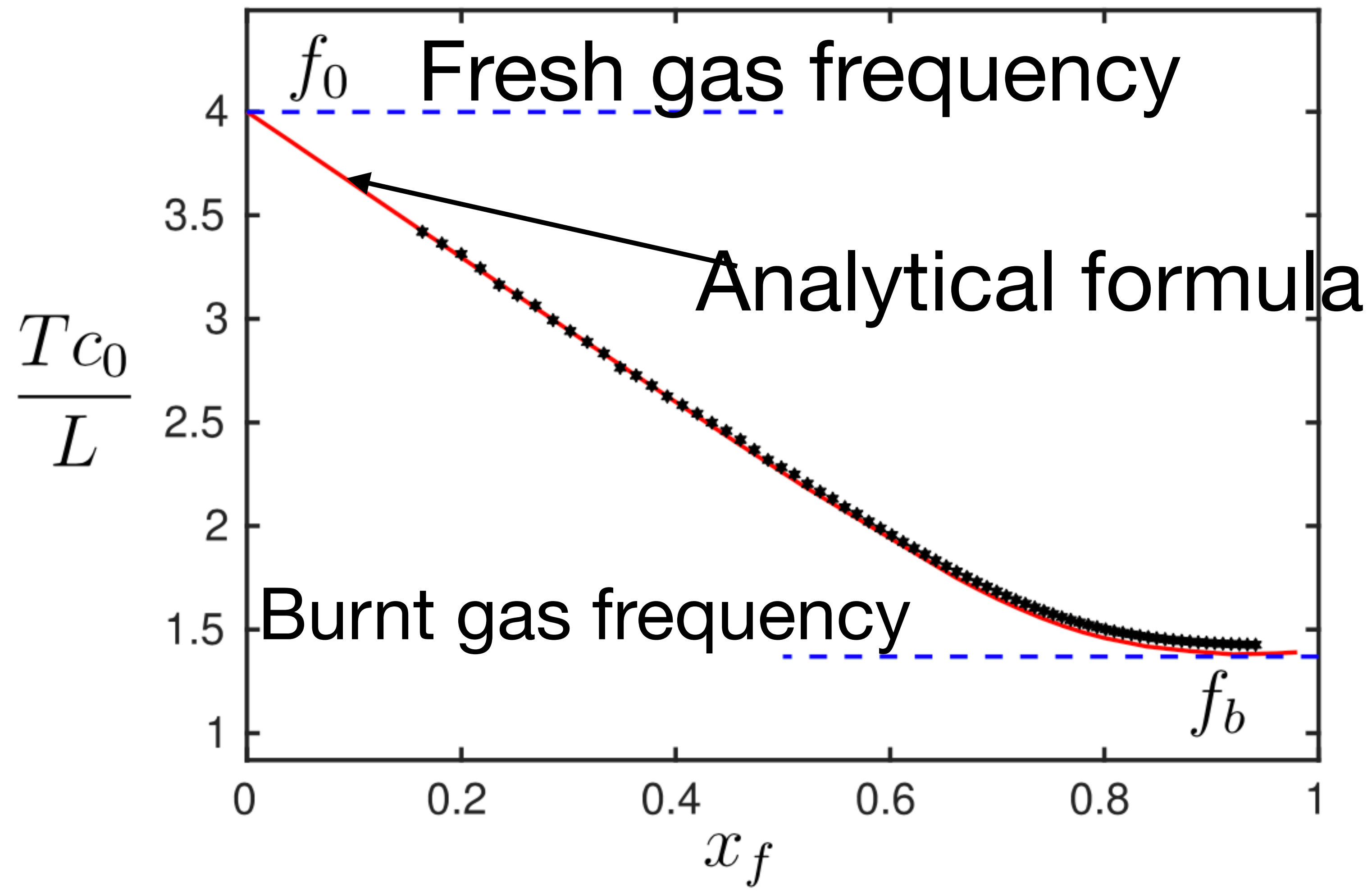
Thermoacoustic instabilities

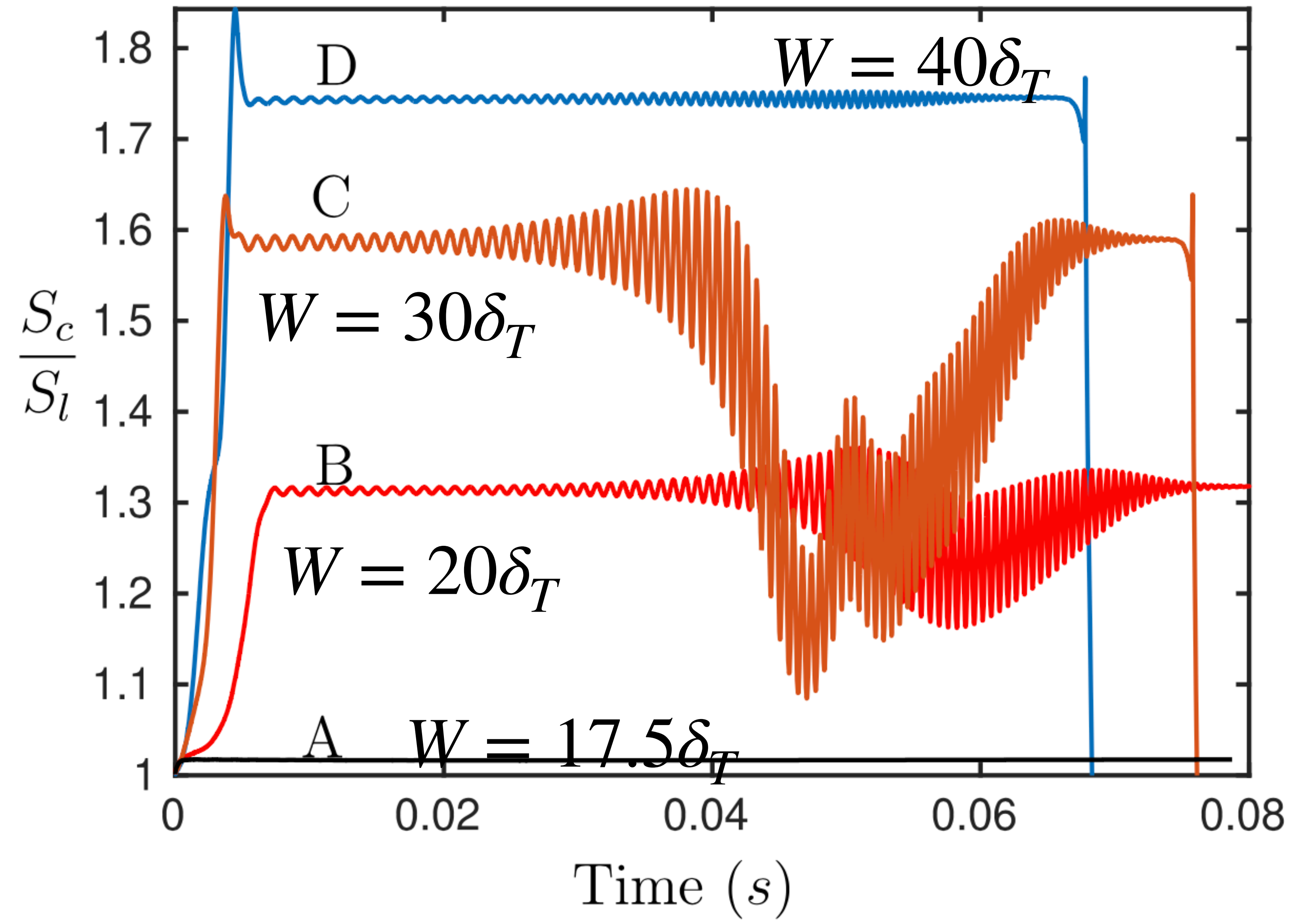
Thermo-acoustic instabilities





$L = 1200\delta_T, W = 40\delta_T$

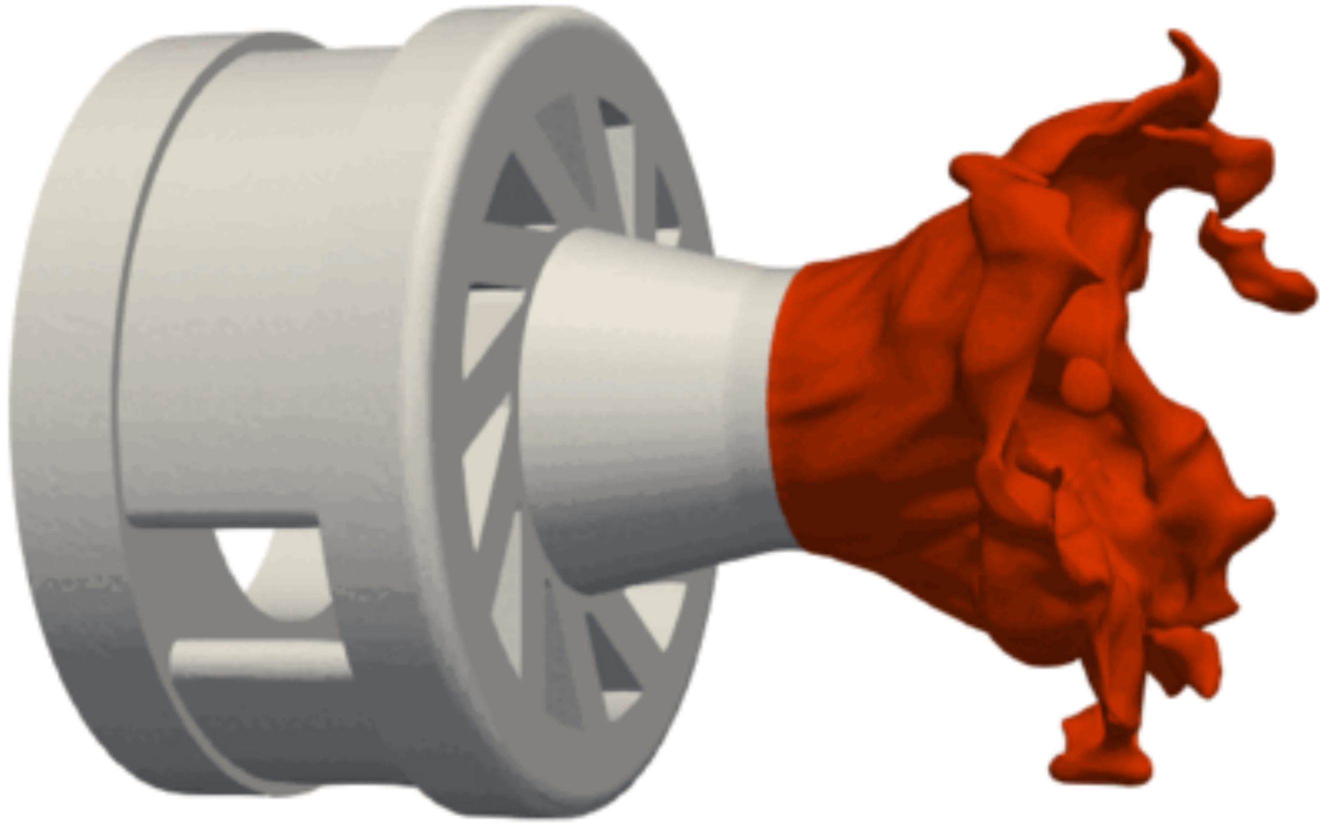


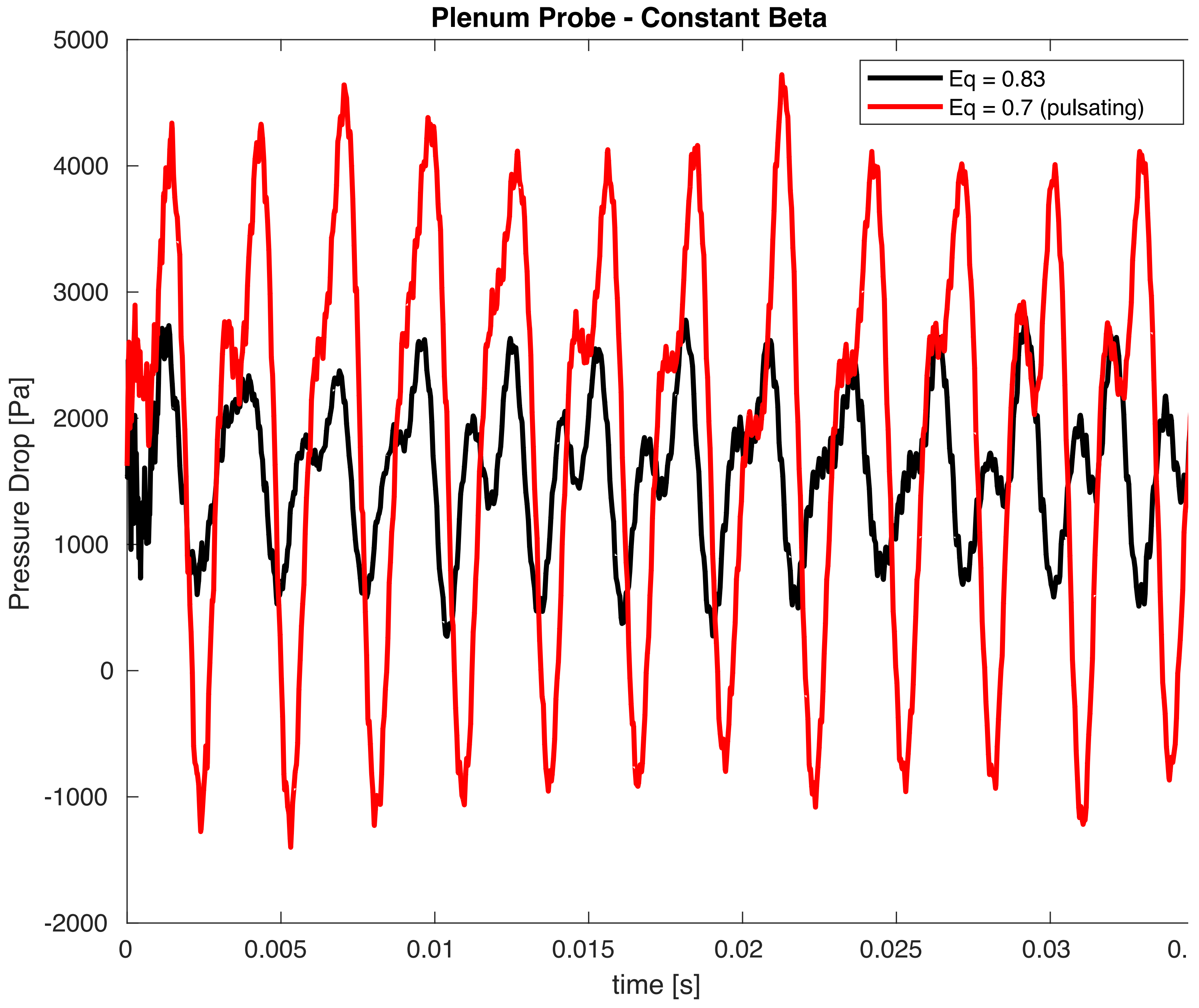


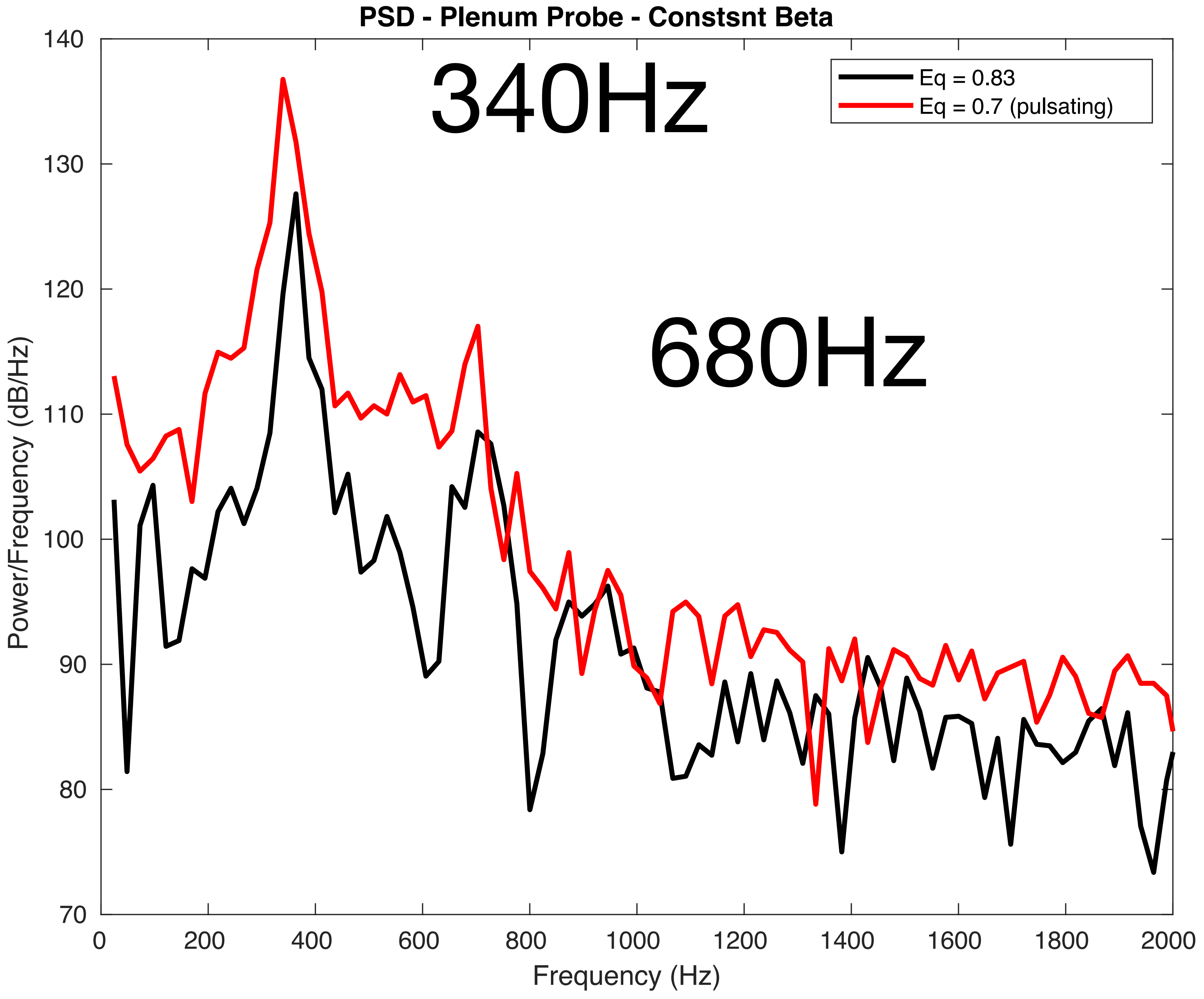
Back on Preccinsta

Unstable case $\varphi = 0.7$

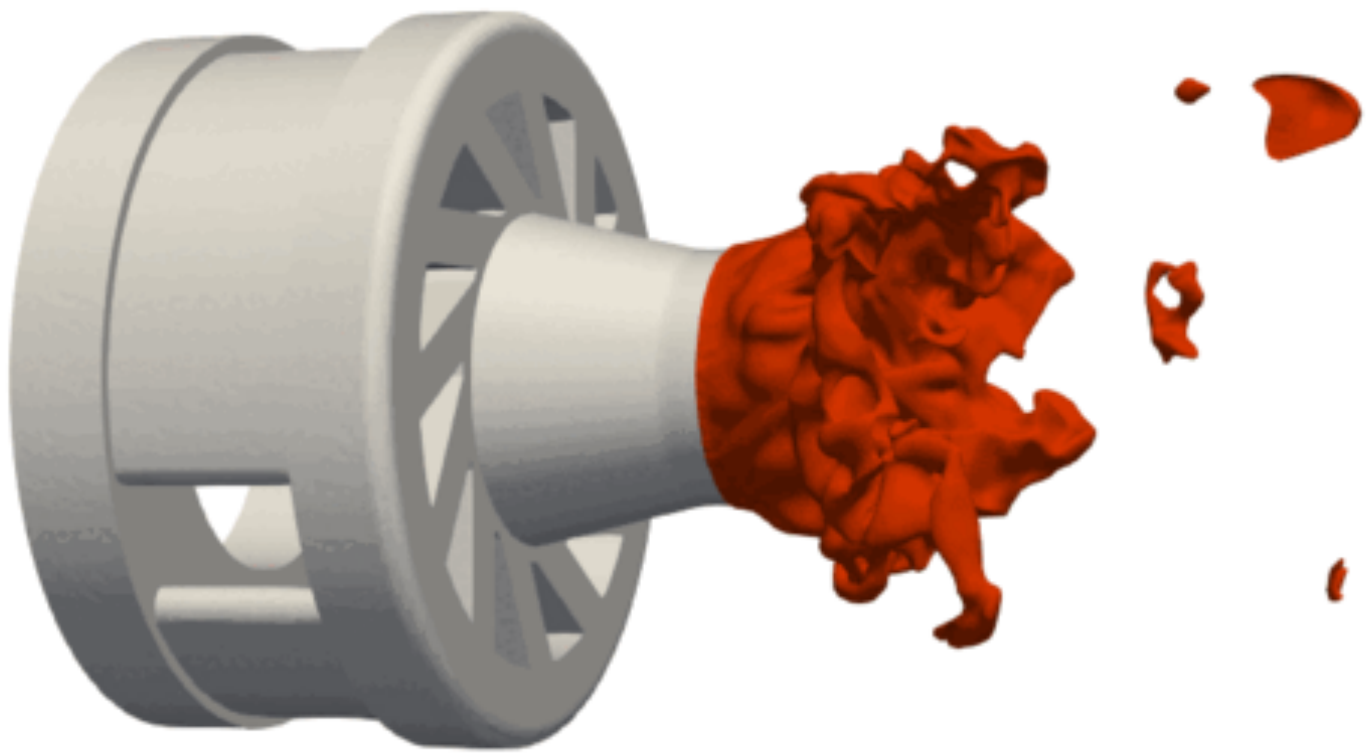
M1, $\varphi = 0.83$



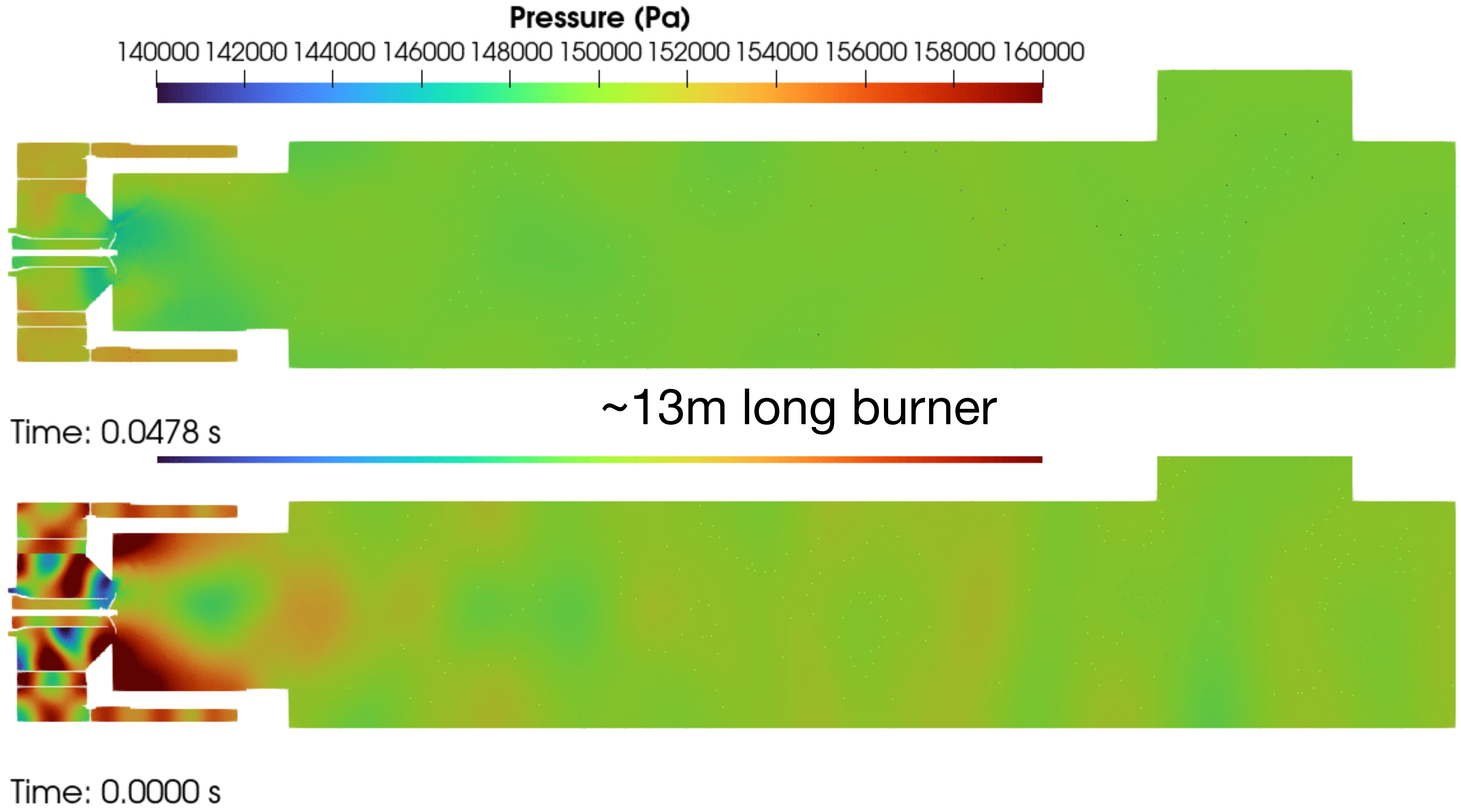




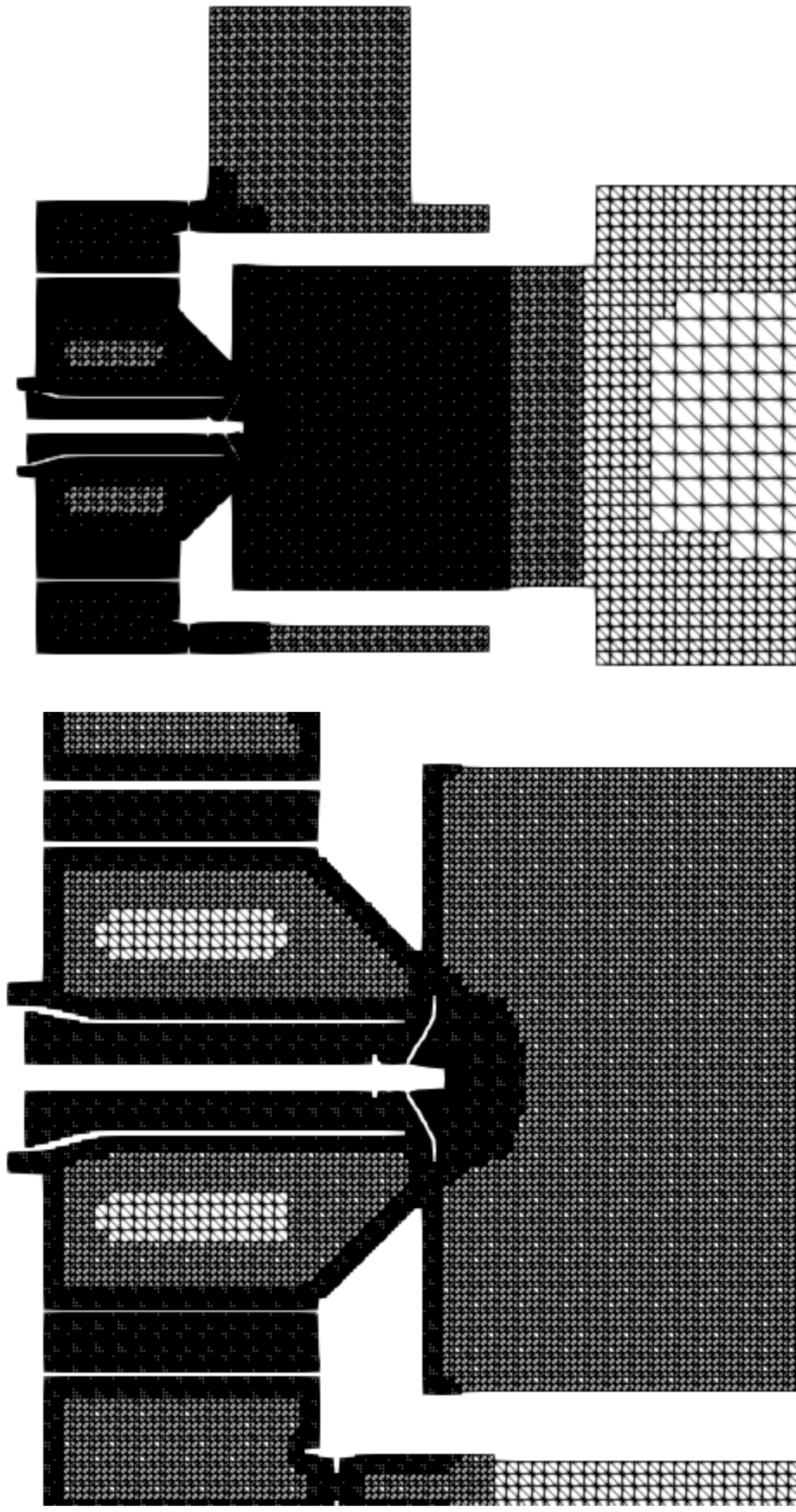
M1, $\varphi = 0.7$



Industrial burner



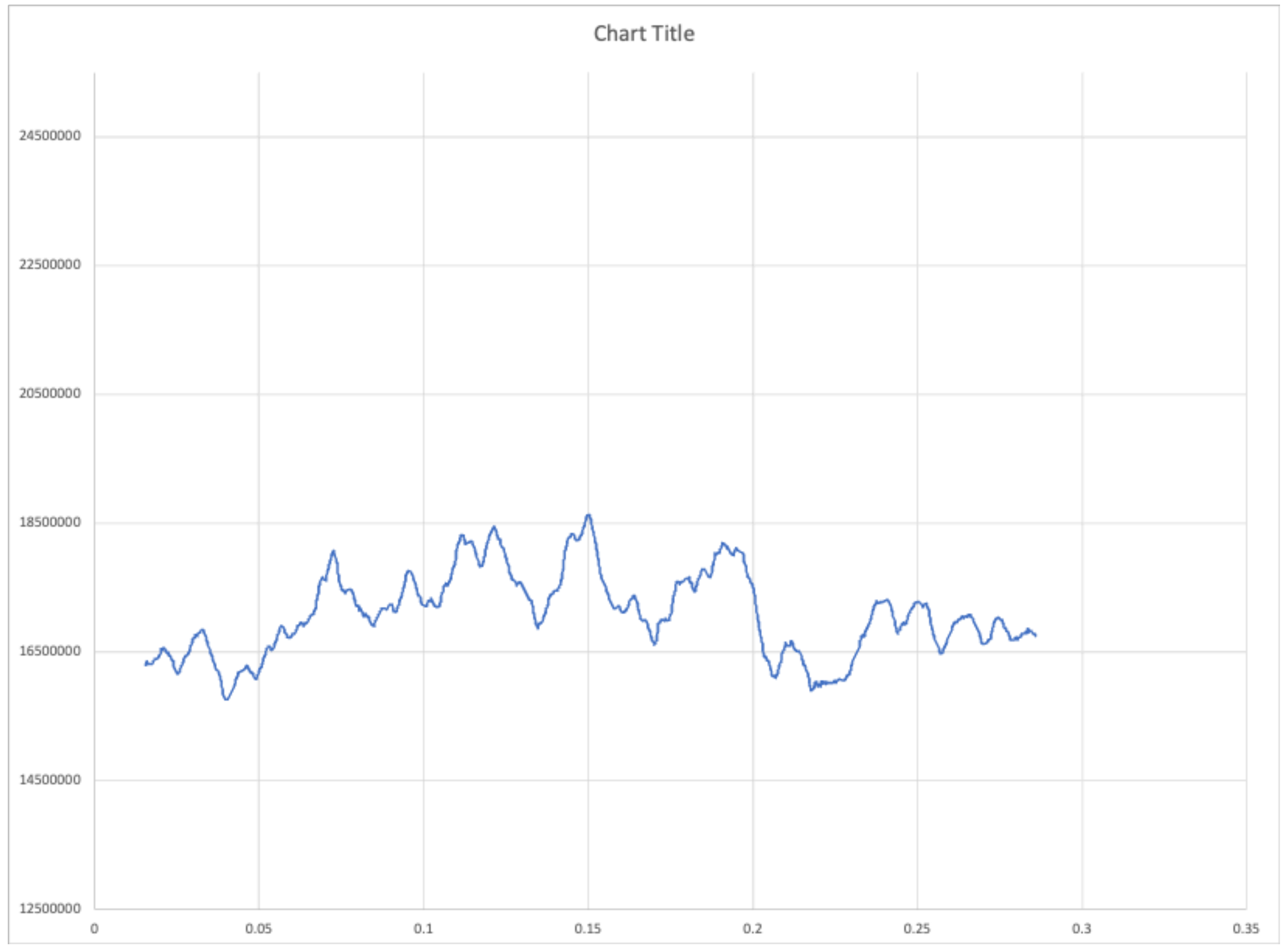
~13m long burner

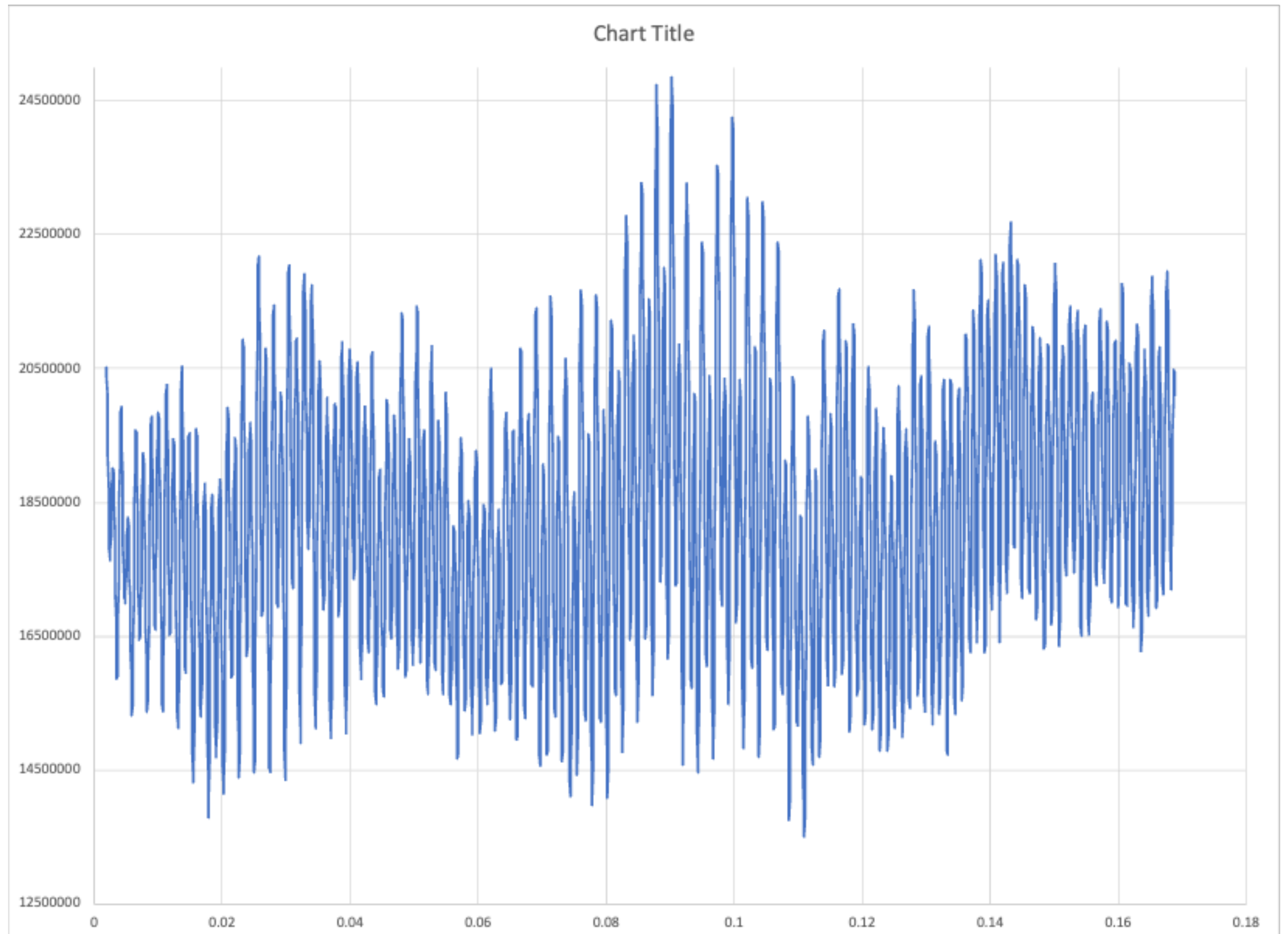


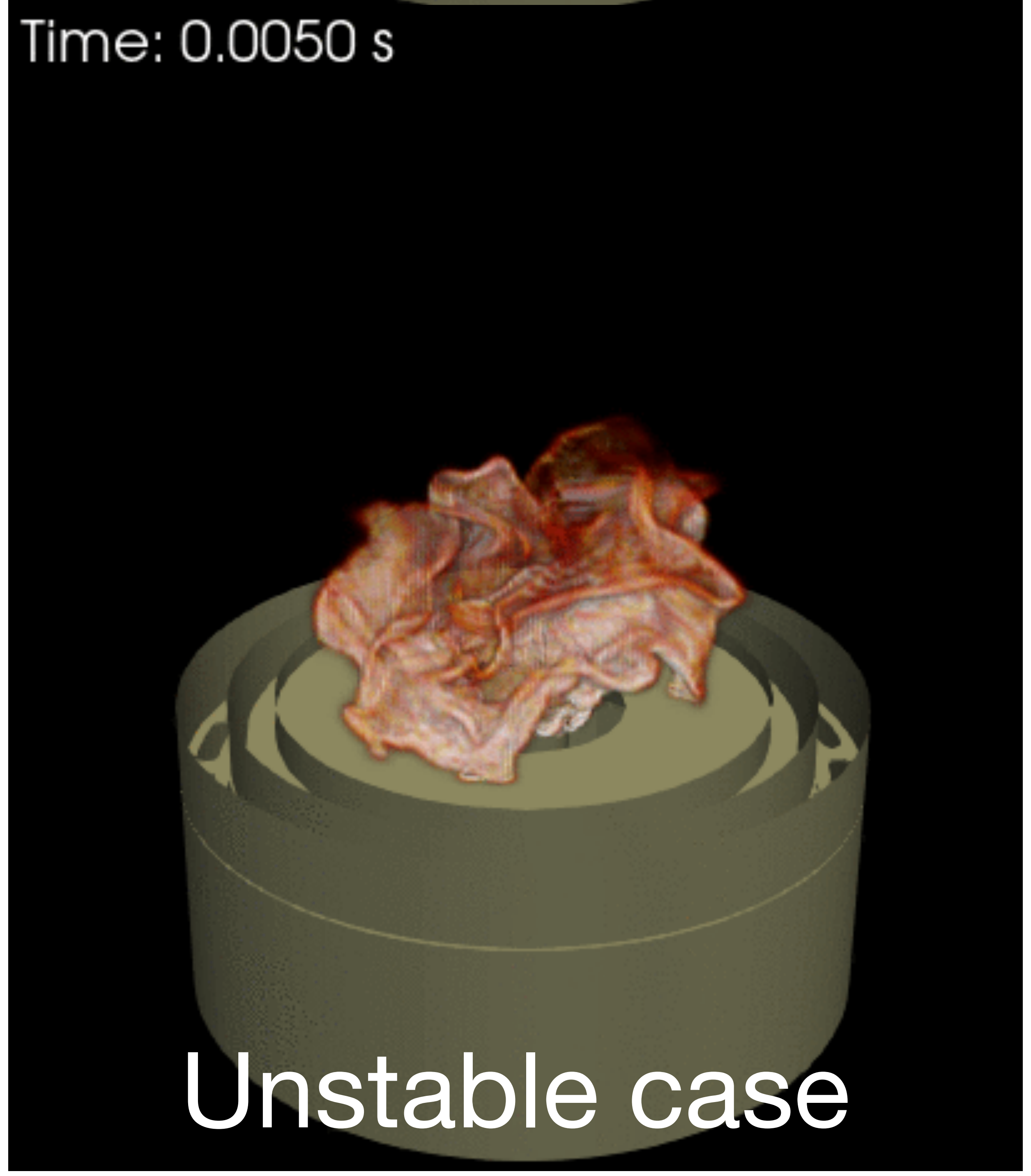
Industrial burner

Pressure probes

- Natural gas burner
- Same power
- Different injection







Radiation

Radiation modelling

$$\nabla \cdot \left(\frac{1}{k_i} \nabla G_i \right) - 3 \cdot k_i \cdot G_i = -12\pi a_i k_i I_{bi}$$

G is the incident radiation for band i

We solve the equation for 4 bands

$$k_{i,c} = p_c \cdot k_{p_i,c}$$

Kic is the sum of the absorption coef. for participating species

$$a_i(T) = \sum_{j=0} b_{i,j} \cdot T^j$$

a(T) is a temperature dependent coefficient

$$I_{bi}(T) = \frac{\sigma T_i^4}{\pi}$$

Ib is the black body intensity

$$\nabla \cdot \mathbf{q} = \sum_{1}^{4} \kappa_i (4\pi a_i I_{bi} - G_i)$$

The radiation flux « div q » is subtracted to energy the equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}(\rho Y_k u_i) = -\frac{\partial}{\partial x_i}(J_{k,i}) + \dot{\omega}_k \quad (k = 1, 2, ..., N_S)$$

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + \rho g_j$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i}(\rho E u_i) = -\frac{\partial}{\partial x_i}(u_i p) + \frac{\partial}{\partial x_i}(\tau_{ij} u_j) - \frac{\partial}{\partial x_i} q_i + \dot{\omega}_T + \boxed{P^R}$$

Radiation modelling

Case	Participating gas	Temperature (K)	Concentration
5	$CO_2 + H_2O$	Non- isothermal: Eq. (27)	Homogeneous: 10% CO_2 + 20% H_2O

T wall = 0 K

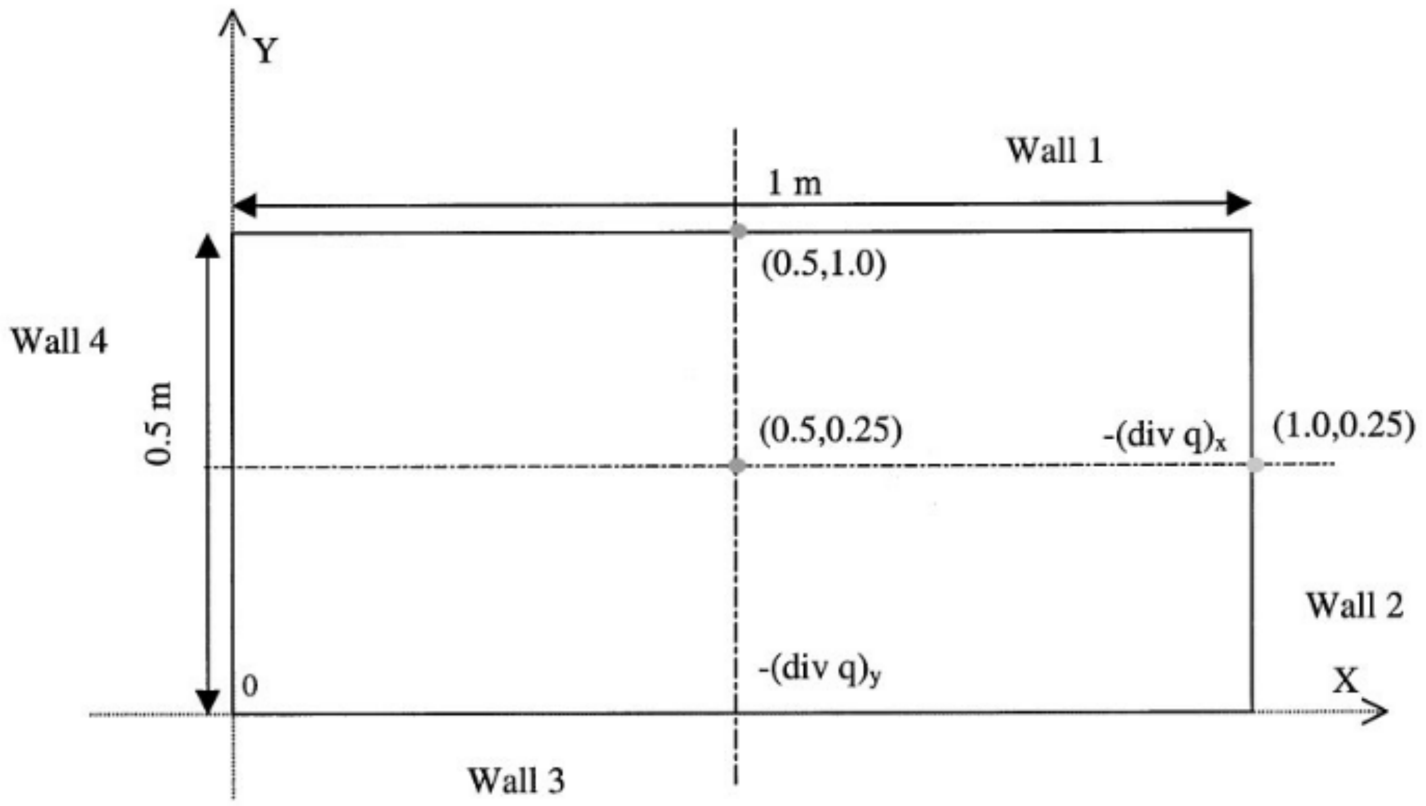
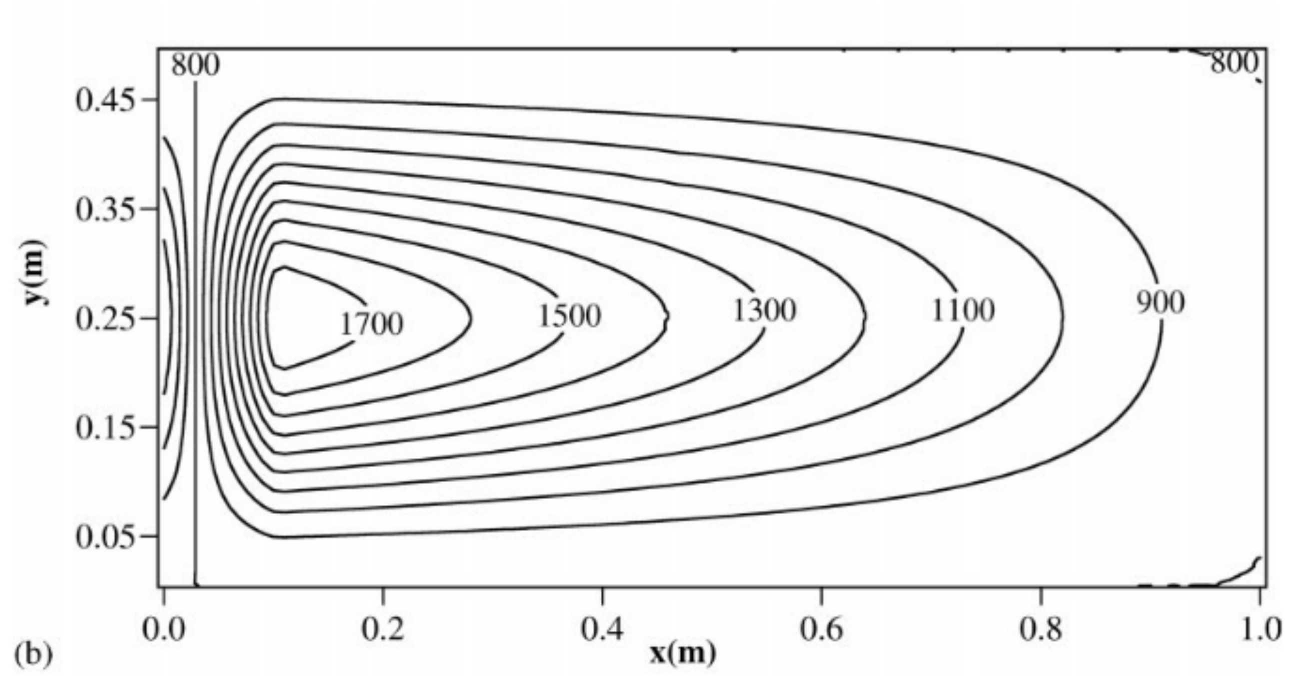
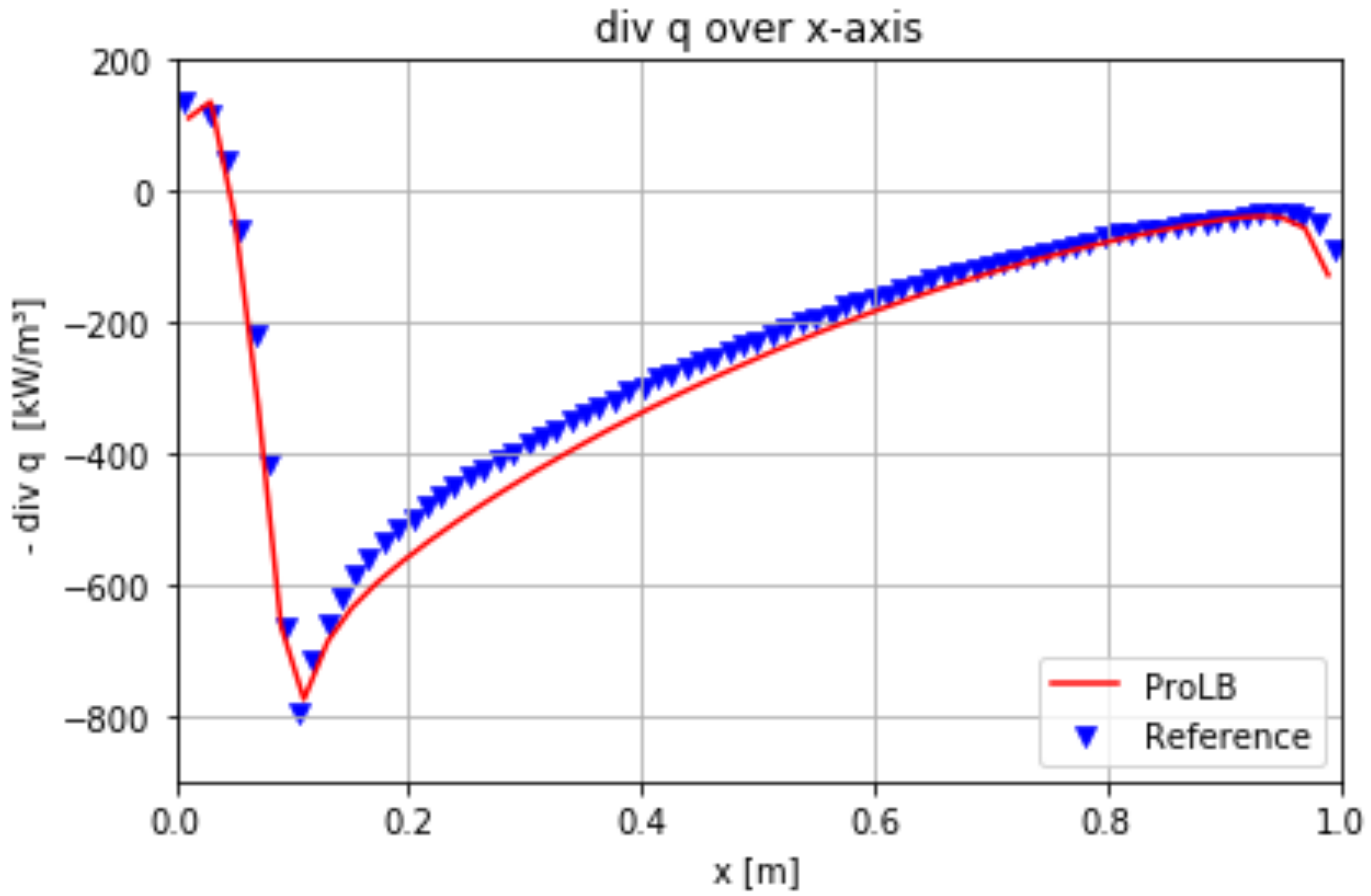
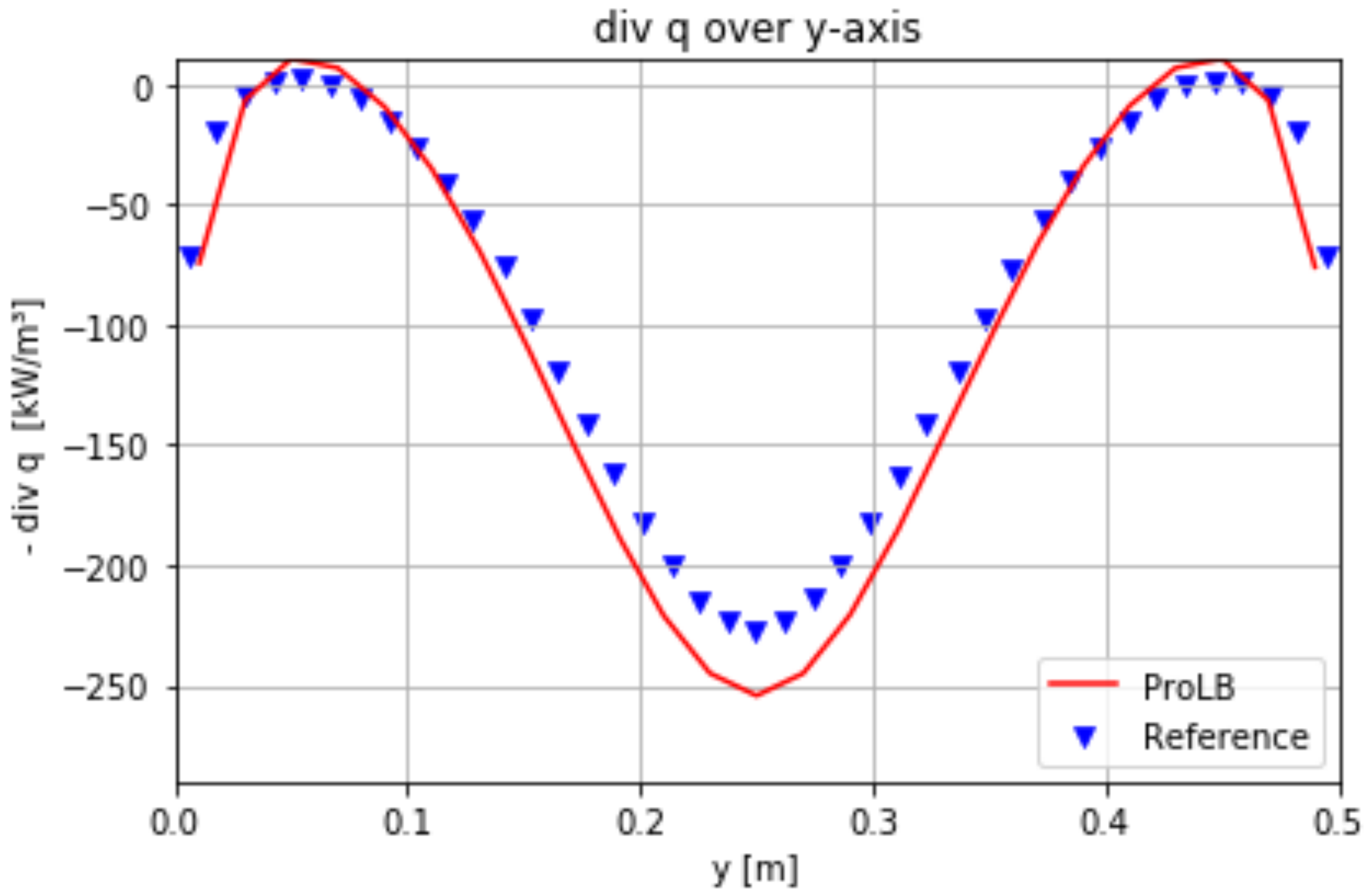


Fig. 1. The enclosure.

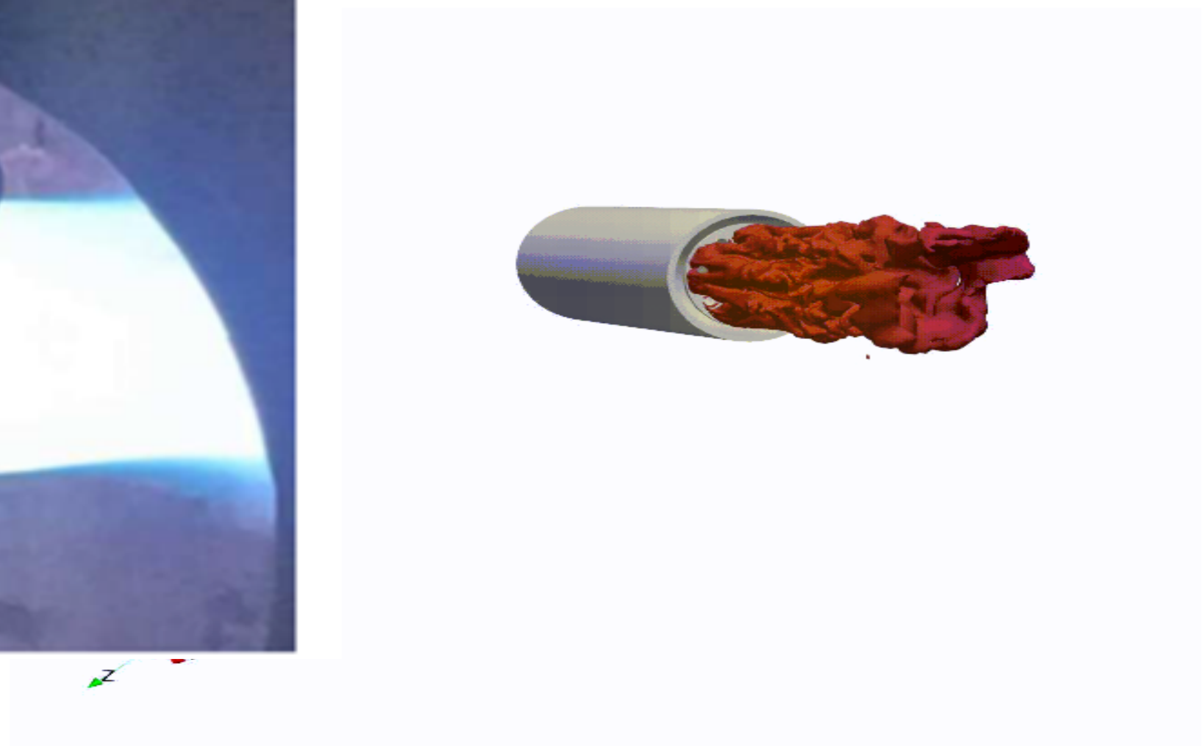


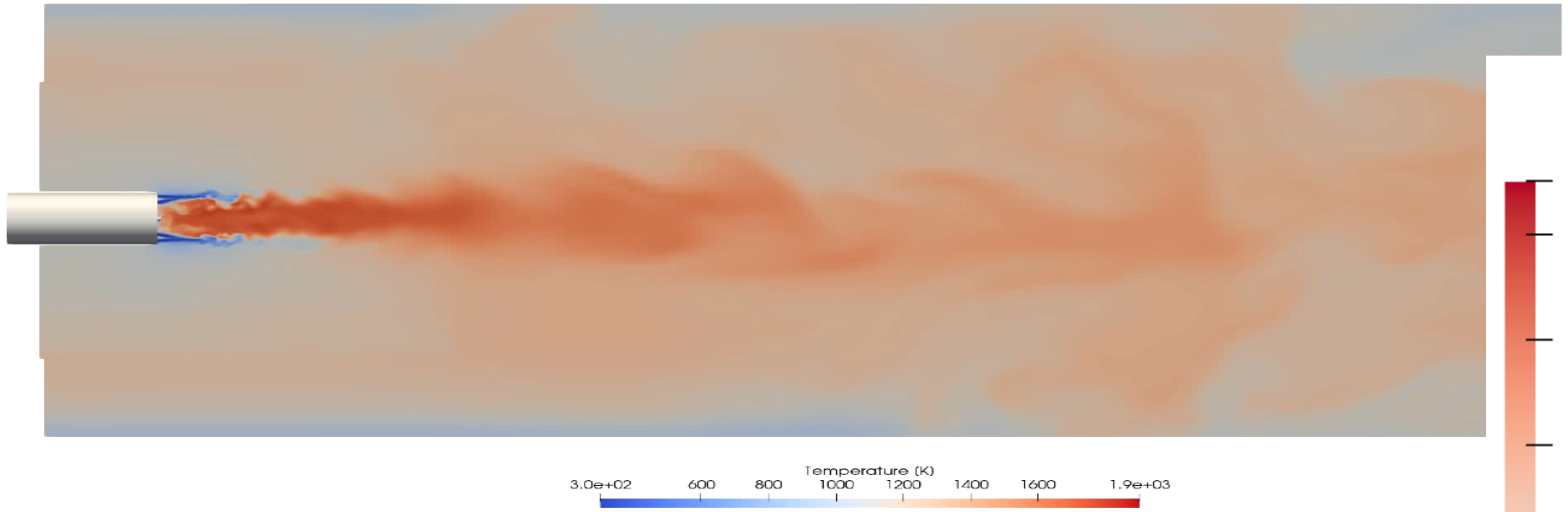




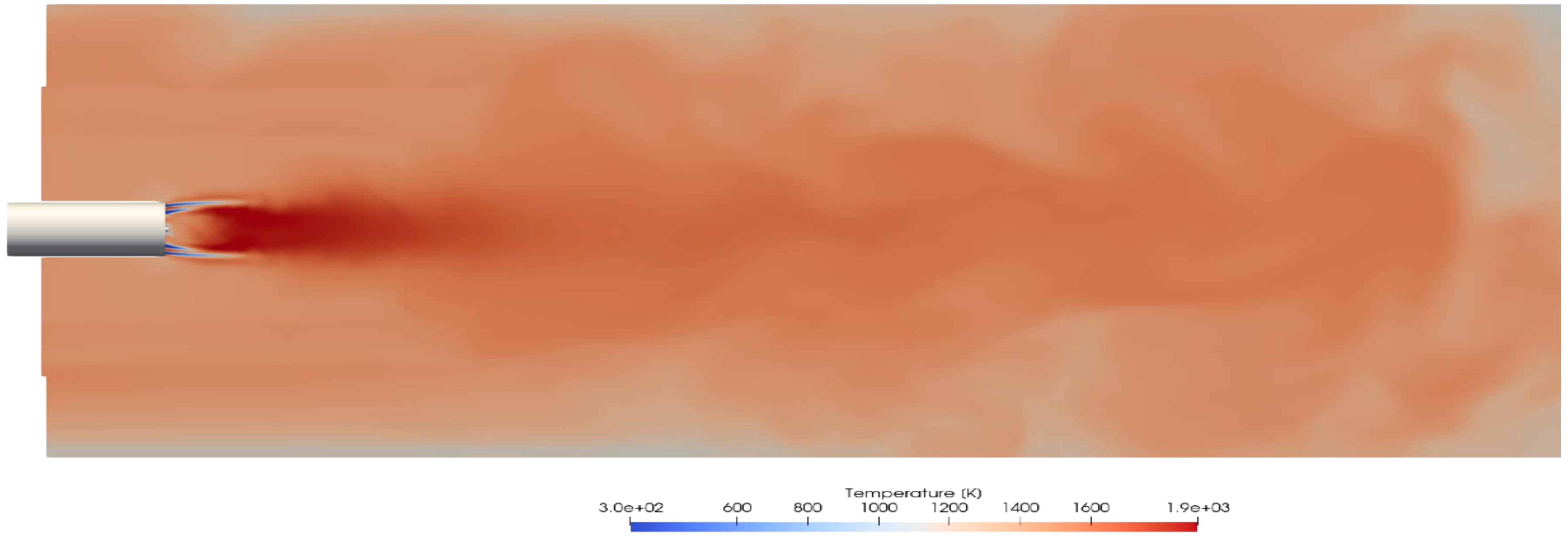
Radiation effect and H_2 dilution

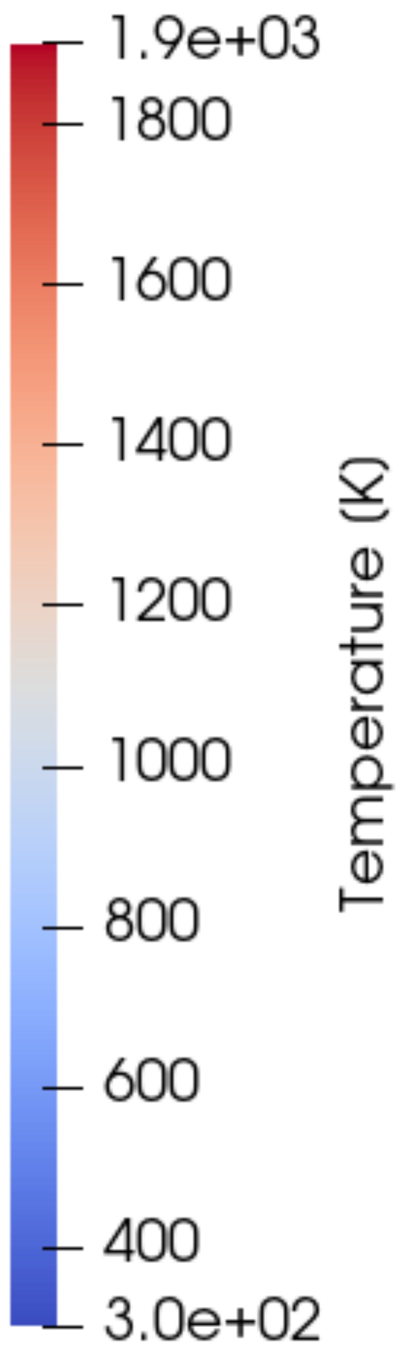
100% CH4





70% H2
30% CH4



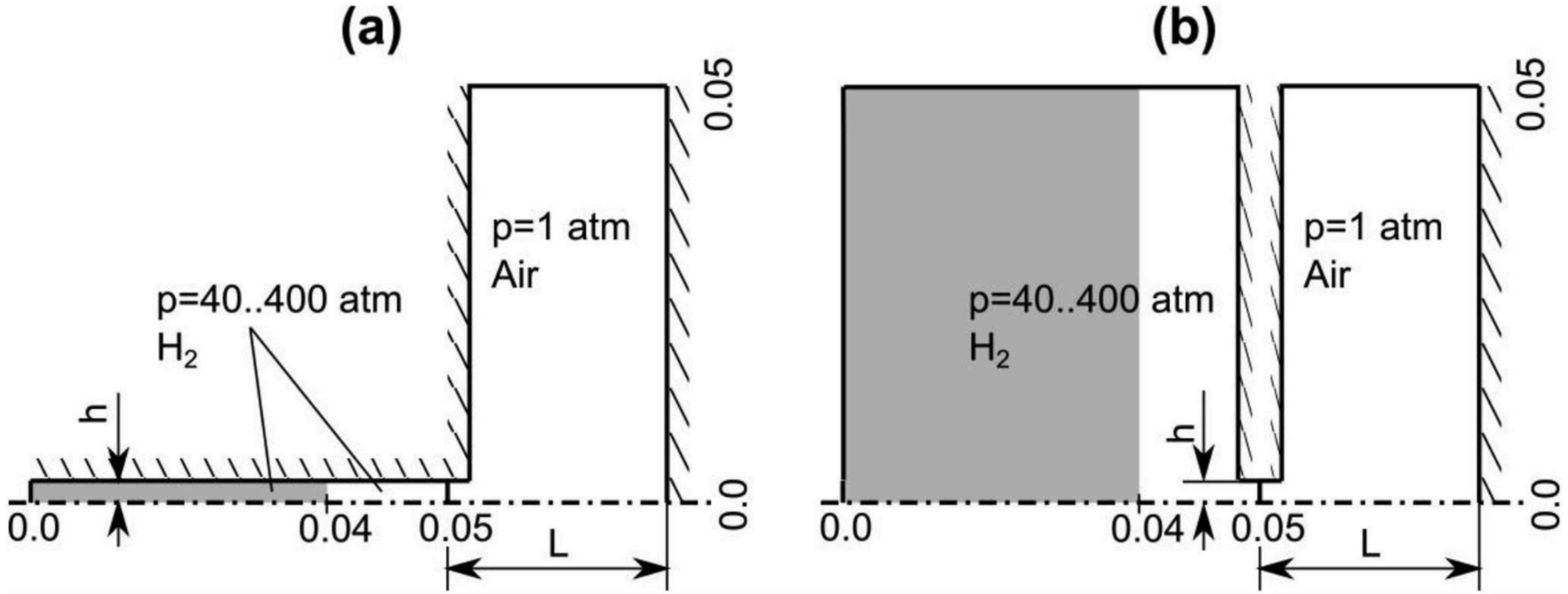


H_2 leaks

H_2 leakage problem

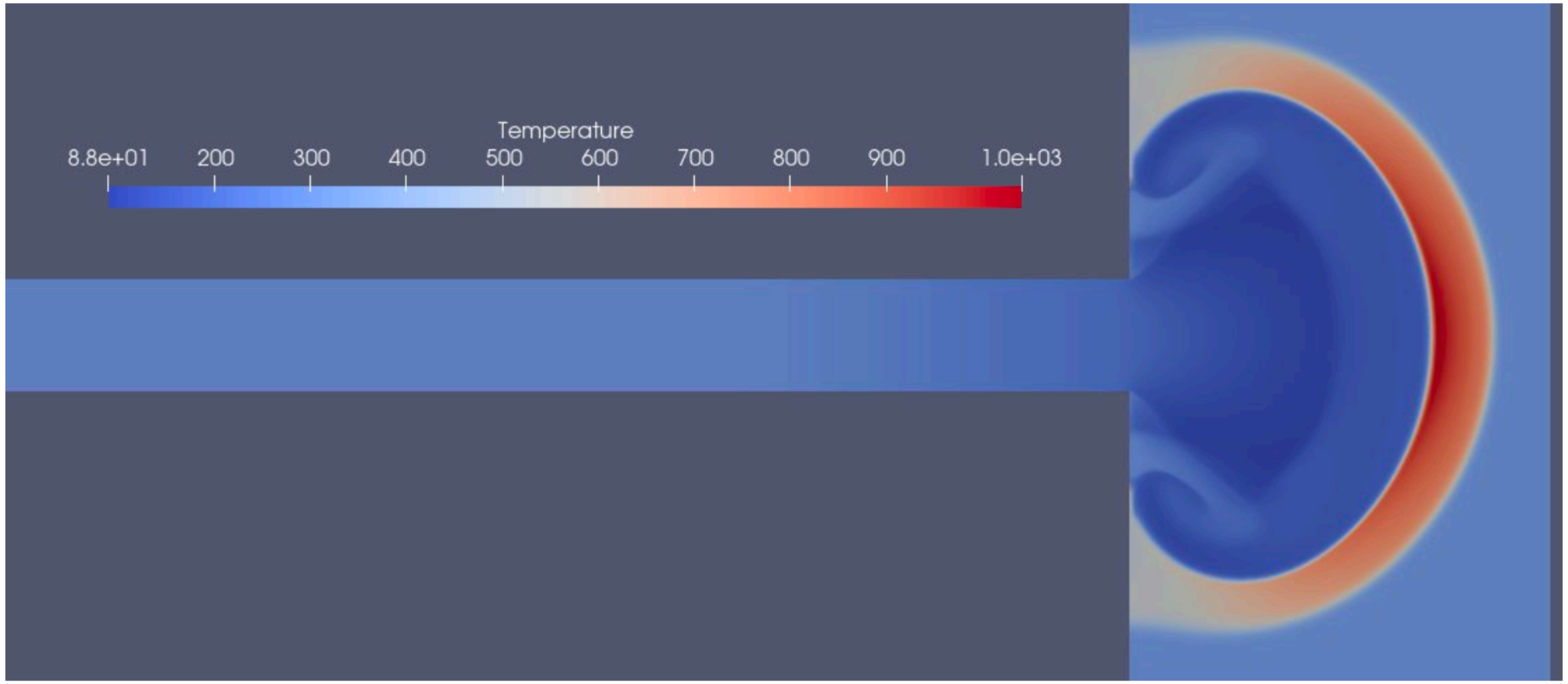
- Planar 2D configuration

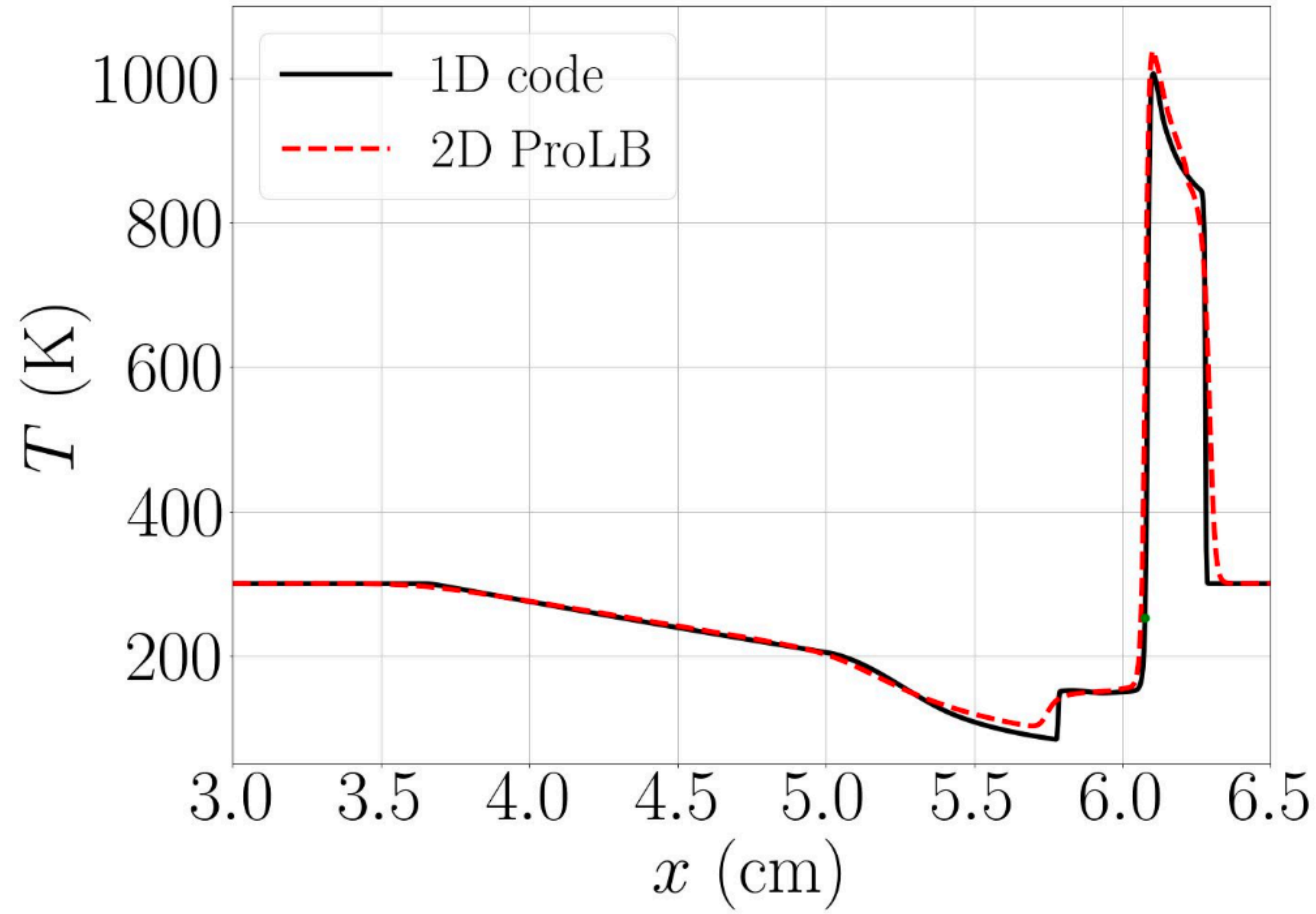
A.E. Smygalina and A.D. Kiverin, **Self-ignition of hydrogen jet due to interaction with obstacle in the obstructed space**. International journal of hydrogen energy, 2022.



H_2 safety

Case : h=4mm, p=100atm (variable Cp, H2 and air)





Detonations

ZND profiles

- **Initialization of a ZND profile with the following parameters:**

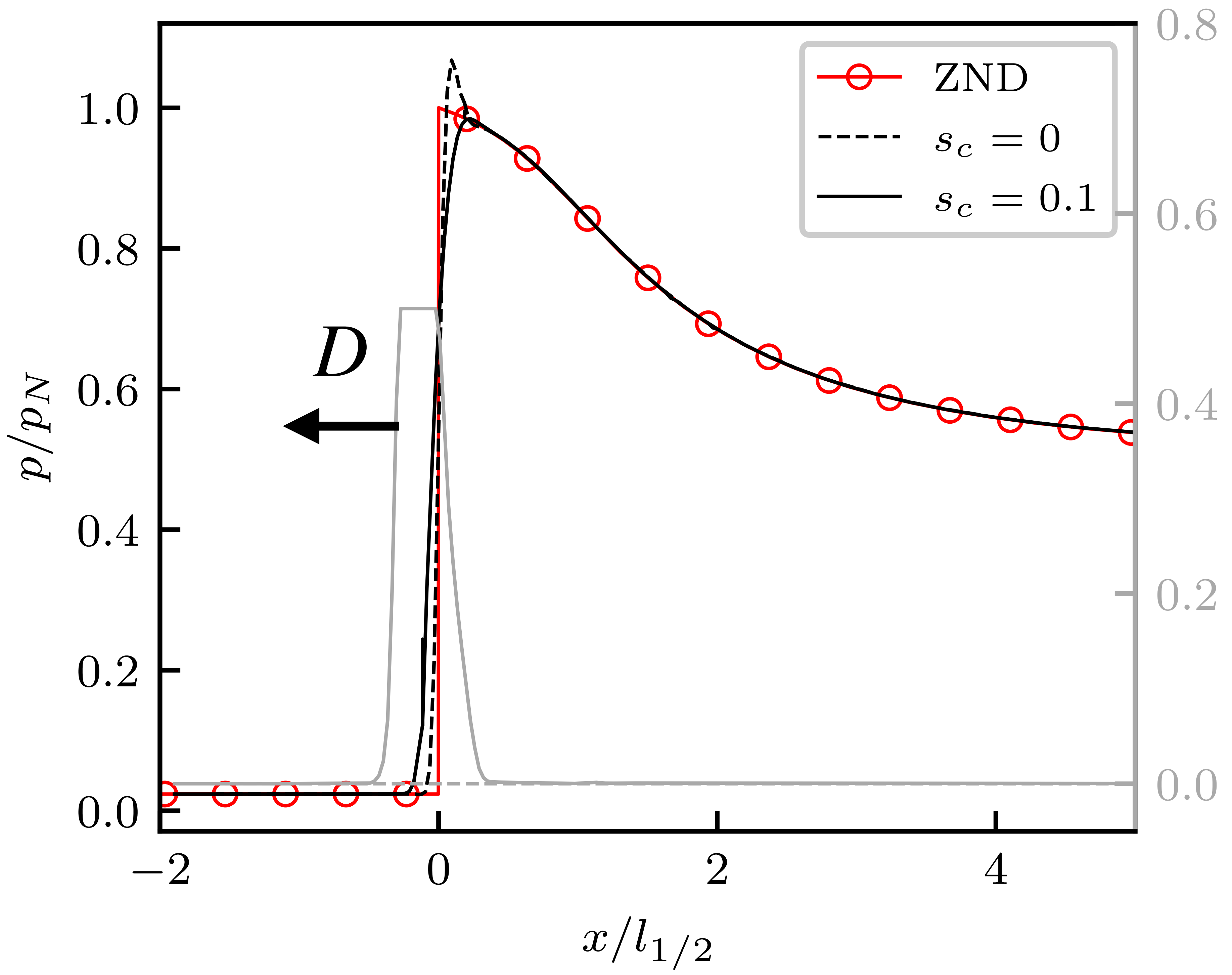
Points per half reaction length: $N_{1/2} = 32$

$\gamma = 1.2,$

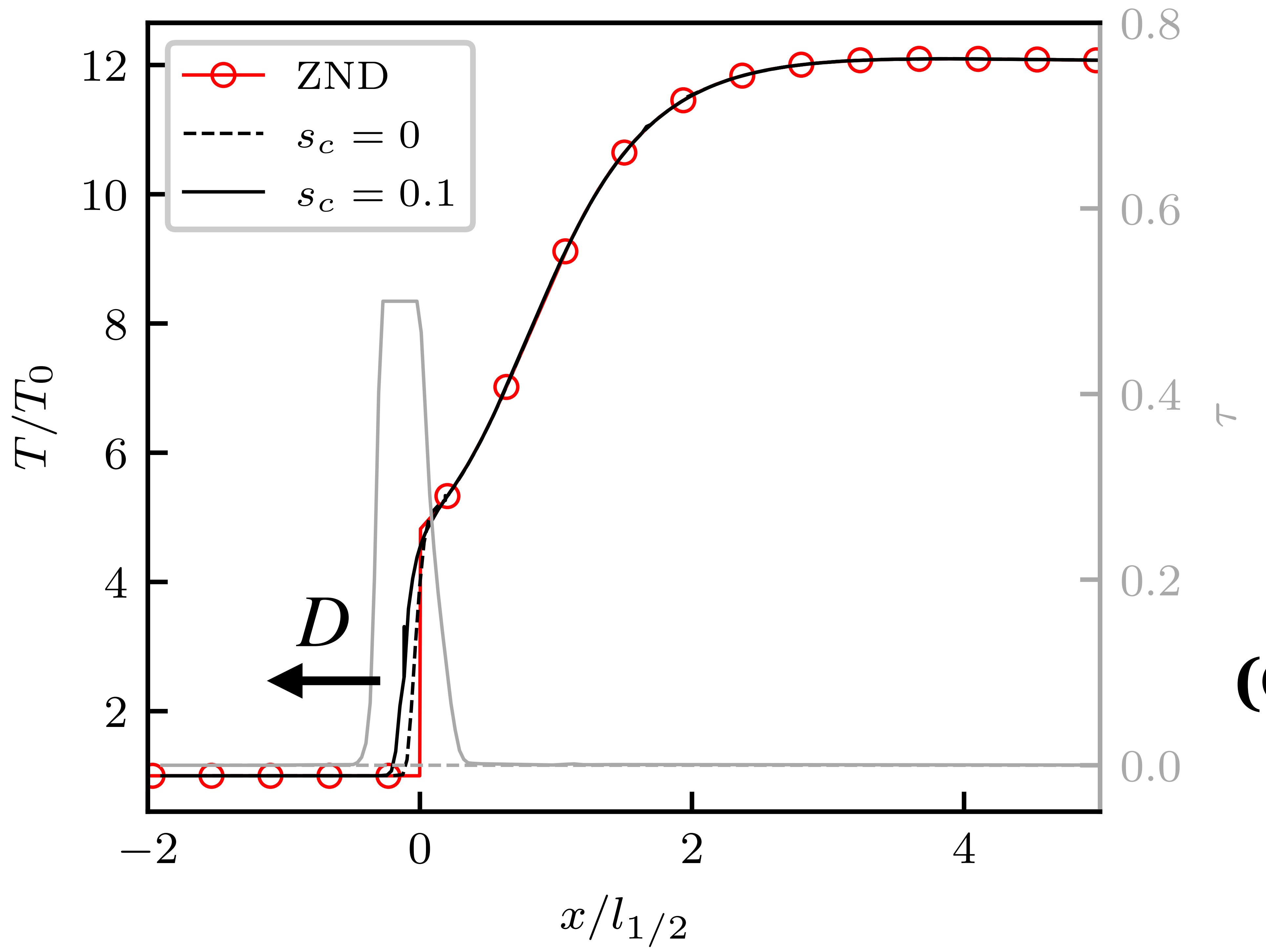
$E_a = 24\,RT_0,$

$Q = 50\,RT_0,$

$L_{1/2} = 6.92e-4\ m$



$p_N \approx 4.26 \times 10^6$ Pa



Detonation velocity:

$D \approx 3078.64$ m/s

$D_{CJ} \approx 3078.66$ m/s

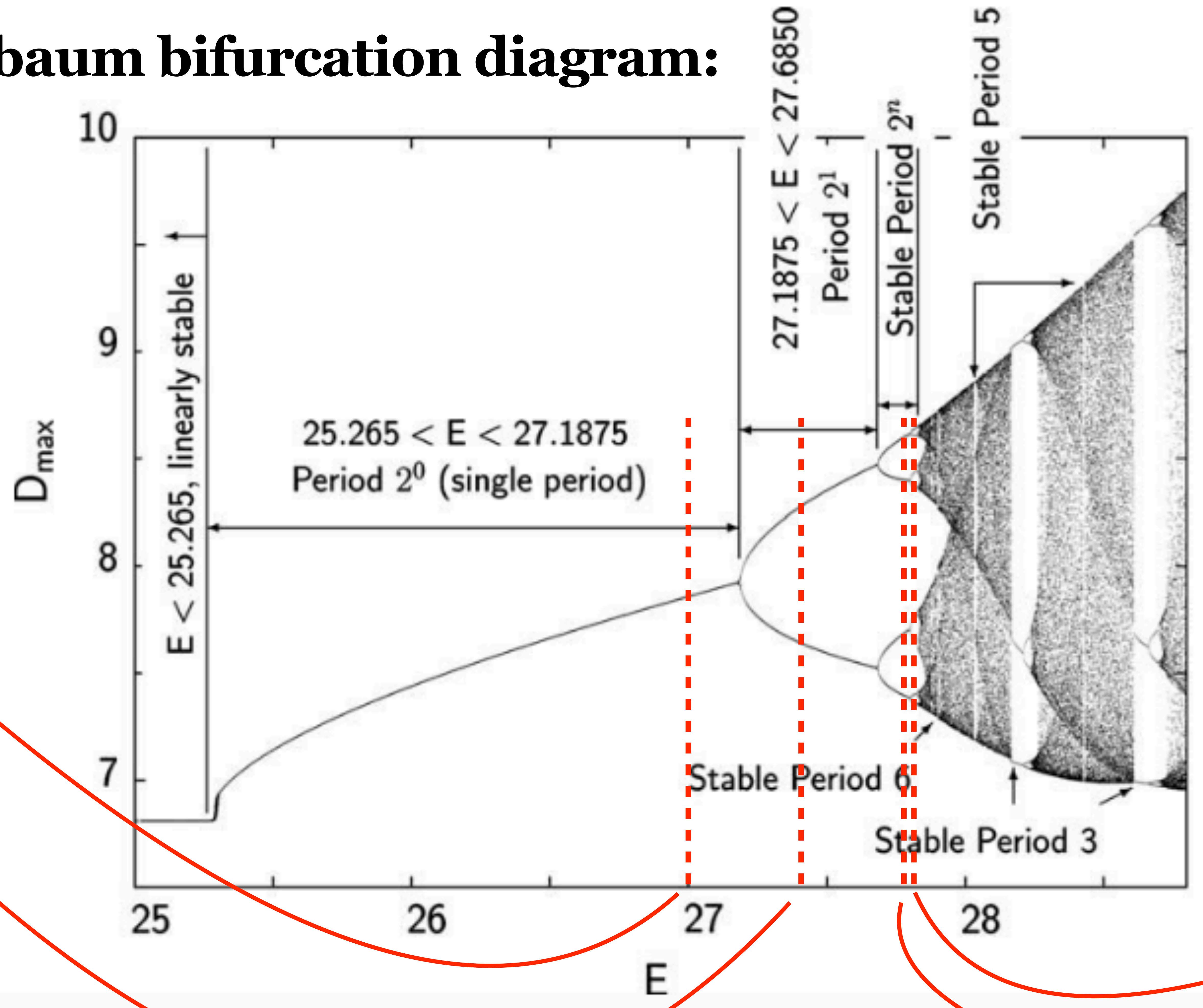
(Chapman-Jouguet theory)

G. Wissocq, S. Taileb, S. Zhao, and P. Boivin, "A hybrid lattice boltzmann method for gaseous detonations," Journal of Computational Physics, vol. 494, p. 112525, 2023.

Detonation instabilities

Effect of activation energy

- **Feigenbaum bifurcation diagram:**



Ea=27 RT0: 1 mode

Ea=27.4 RT0: 2 modes

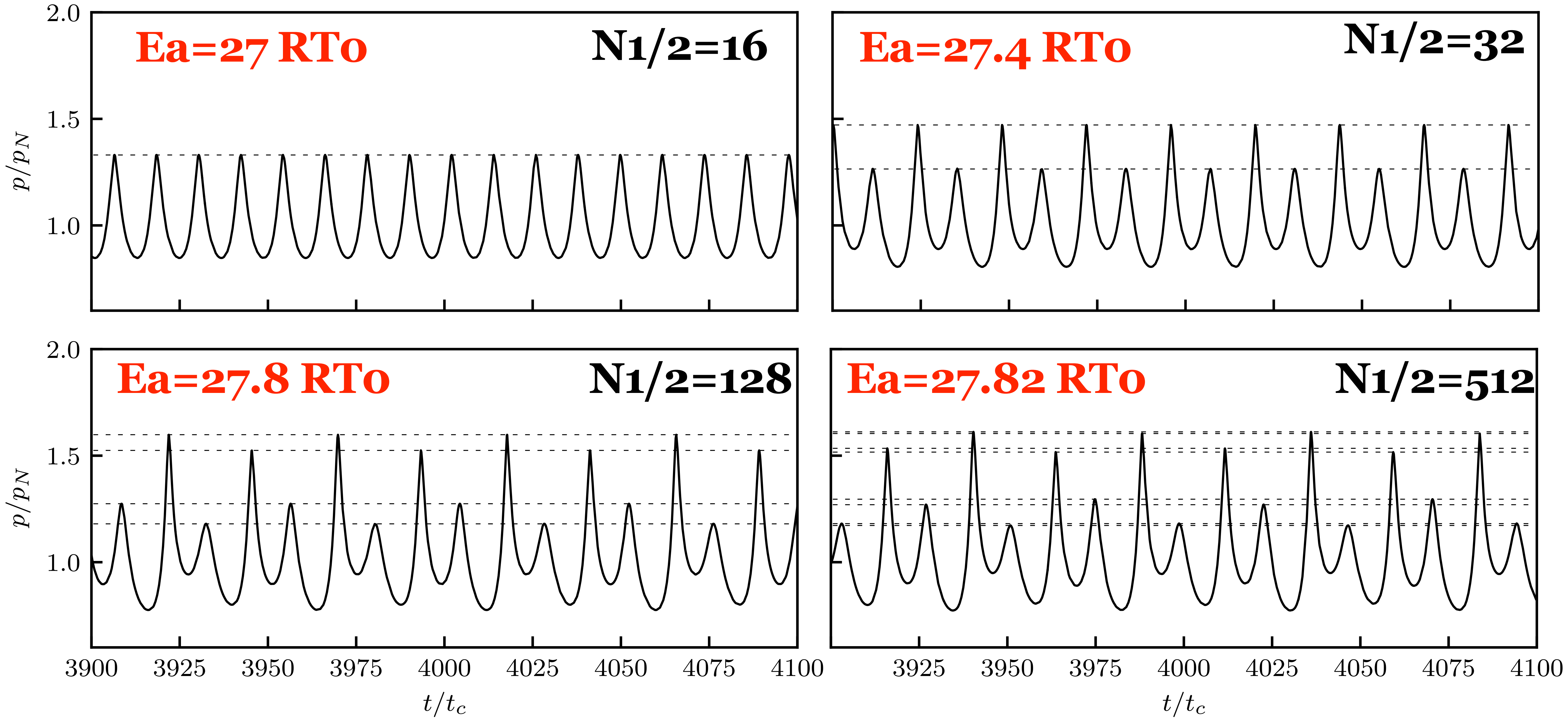
Ea=27.82 RT0: 8 modes

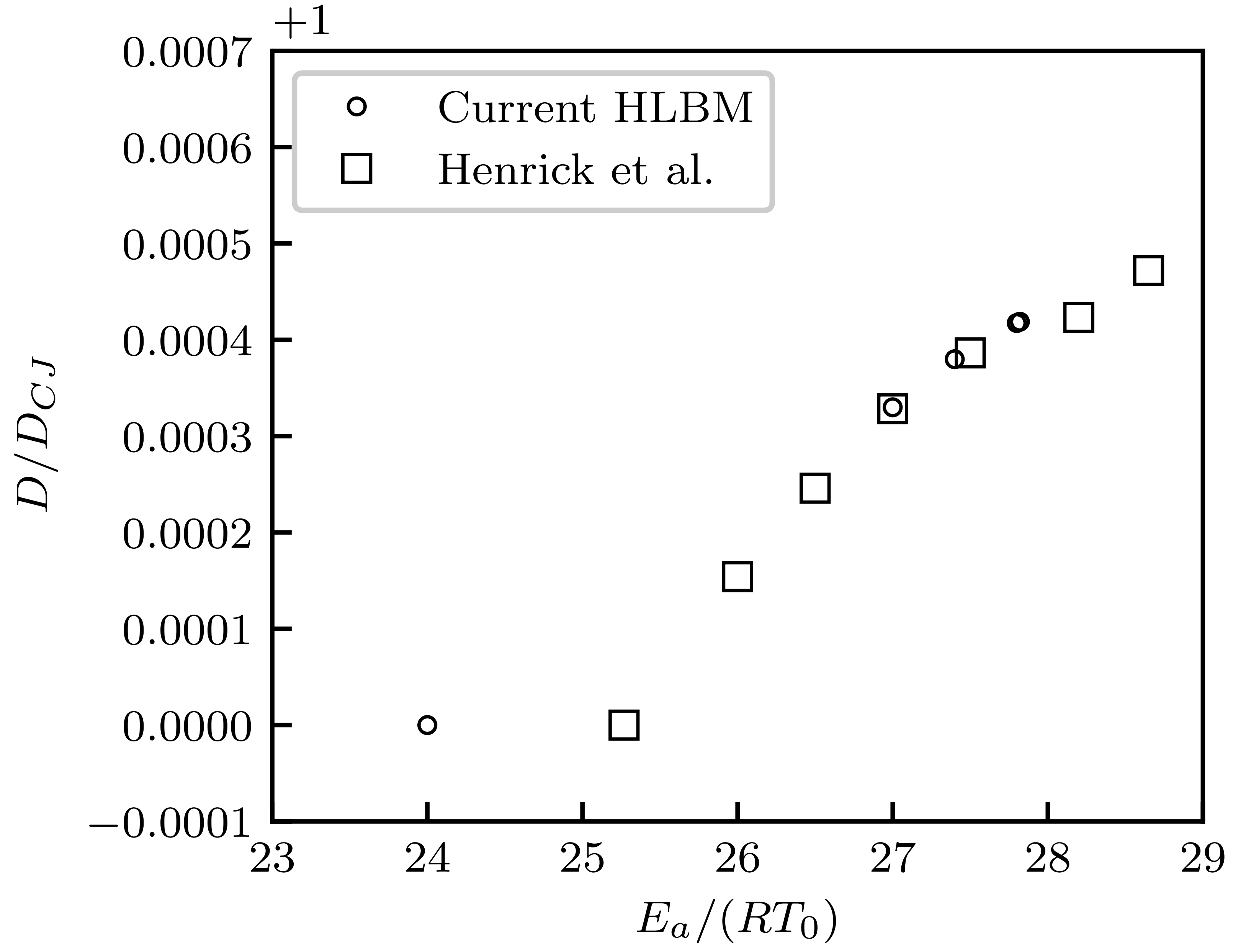
Ea=27.80 RT0: 4 modes

Detonation instabilities

Effect of activation energy

Time history of the shock pressure:





D : **Detonation velocity**

D_{CJ} : **Chapman-Jouguet theory**

Detonations

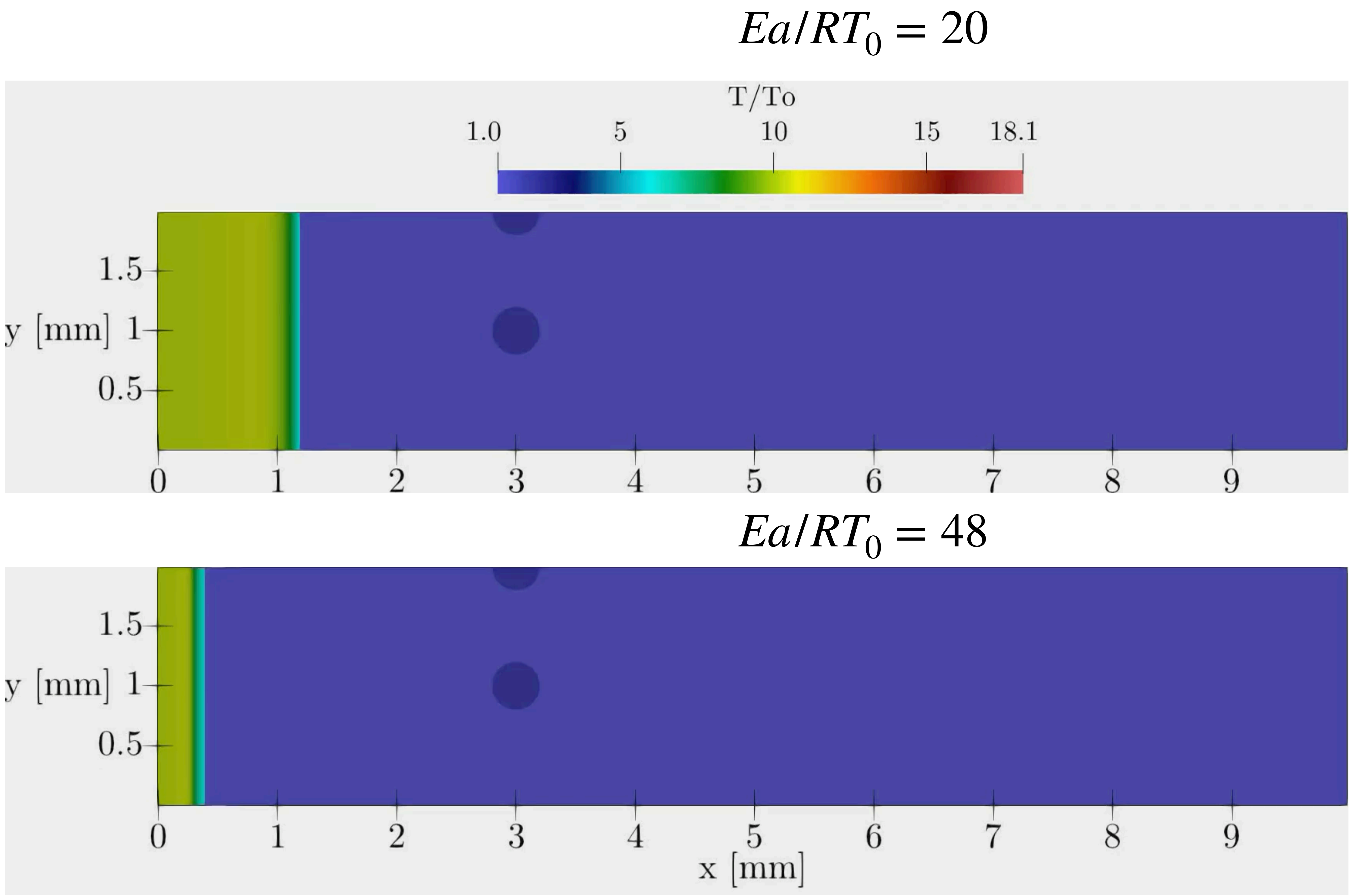
2D propagation in channel

$Ea/RT_0 = 20$ **:**

- **Detonation front is regular**
- **Alternation of mach stems and incident shock**
- **Absence of unburned pockets**

$Ea/RT_0 = 48$ **:**

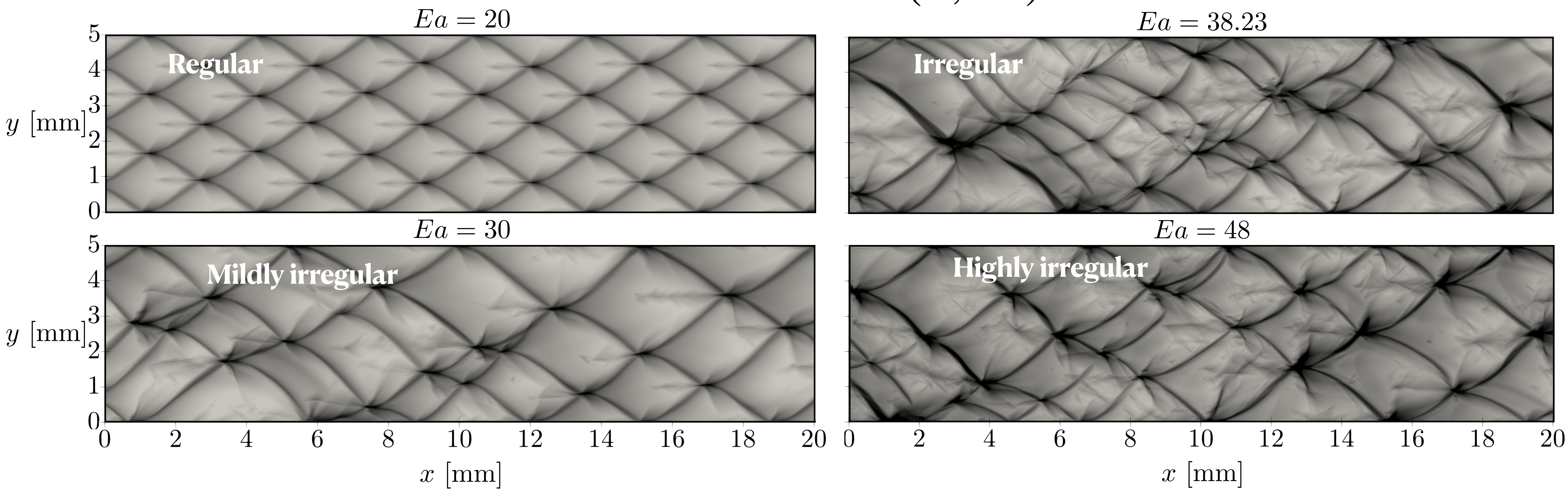
- **Detonation front is irregular**
- **Chaotic front behavior**
- **Presence of unburned pockets**



Detonations

Cellular patterns

- …recovered for all the mixtures : $TP = max(P, TP)$



Cell regularity classification based on Strehlow and Crooker (1974) and Libouton et al. (1981)

G. Wissocq, S. Taileb, S. Zhao, and P. Boivin, “A hybrid lattice boltzmann method for gaseous detonations,” Journal of Computational Physics, vol. 494, p. 112525, 2023.

Outline

- Part I : LBM 101 (isothermal)
- Part II : Compressible & reactive LBM
- Part III : Application to hydrogen combustion & safety
- **Part IV: Discussion, perspectives**

Conclusions

Take-home message

- LBM is a numerical method suitable for reacting flows.
  - A fully conservative version
  - A LMNA version
- Does it go beyond NS solvers ?
  - Not that I’m aware of.
- Is it worth it ?
  - Yes, very. Cases shown all << 10000cpuh. Local time-step is life for real applications.
- What’s next ?
  - discontinuities, multiphase flows, radiation. Help needed.

Questions ?

Ad 1: *LBM Spring School (AMU/KIT) — May 19-23 2025, CIRM, Marseille*

Ad 2: *Several open positions (PhD & postdocs)*

Equivalent equations

LBM ++

$$\boxed{\frac{\partial \Pi^{f,(n)}_{\alpha_1 \cdots \alpha_n}}{\partial t} + \frac{\partial \Pi^{f,(n+1)}_{\alpha_1 \cdots \alpha_n \alpha_{n+1}}}{\partial x_{\alpha_{n+1}}} = -\frac{1}{\tau} \Pi^{f^{neq},(n)}_{\alpha_1 \cdots \alpha_n} + \mathcal{O}(\Delta t^2)}$$

n = 0

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\beta}{\partial x_\beta} = \mathcal{O}(\Delta t^2)$$

n = 1

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \left[\rho u_\alpha u_\beta + \rho c_s^2 \delta_{\alpha\beta} + \Pi^{f^{neq},(2)}_{\alpha\beta}\right]}{\partial x_\beta} = \mathcal{O}(\Delta t^2)$$

n = 2

$$\frac{\partial \left[\Pi^{f^{eq},(2)}_{\alpha\beta} + \Pi^{f^{neq},(2)}_{\alpha\beta}\right]}{\partial t} + \frac{\partial \left[\Pi^{f^{eq},(3)}_{\alpha\beta\gamma} + \Pi^{f^{neq},(3)}_{\alpha\beta\gamma}\right]}{\partial x_\gamma} = -\frac{1}{\tau} \Pi^{f^{neq},(2)}_{\alpha\beta} + \mathcal{O}(\Delta t^2)$$

n = ...

$$\cdots$$

HRR collision kernel

Hybrid-recursive-regularized

J. Jacob, O. Malaspinas, and P. Sagaut, "A new hybrid recursive regularised bhatnagar–gross–krook collision model for lattice boltzmann method-based large eddy simulation," Journal of Turbulence, 2018.

$\Pi_{\alpha\beta}^{\overline{f}^{\mathrm{neq}},(2)}$ is weighted with finite differences using $0 \leq \sigma \leq 1$,

$$\tilde{\Pi}_{\alpha\beta}^{neq,(2)} = \sigma \Pi_{\alpha\beta}^{\overline{f}^{\mathrm{neq}},(2)} - (1-\sigma)\rho c_s^2 \overline{\tau} \left[\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right]_{FD} \tag{40}$$

- $\sigma = 1$: Standard (recursive & regularized) model
- $0 < \sigma < 1$: Hybrid $\Pi_{\alpha\beta}^{\overline{f}^{\mathrm{neq}},(2)}$
- $\sigma = 0$: Completely FD/FV $\Pi_{\alpha\beta}^{\overline{f}^{\mathrm{neq}},(2)}$

➔ How to interpret $\sigma < 1$? ➔

HRR collision kernel

Hybrid-recursive-regularized

PhD Gabriel Farag, 2022.

Relaxation equation,

$$\frac{\partial \Pi_{\alpha\beta}^{f^{neq},(2)}}{\partial t} + \cdots = -\frac{1}{\tau}\left(\Pi_{\alpha\beta}^{f^{neq},(2)} + \mu\left[\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right]\right) \quad (41)$$

with its target value

$$\Pi_{\alpha\beta}^{f^{neq},(2)} \approx -\mu\left[\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right] \quad (42)$$

Replaced by a toy-model,

$$\frac{d\phi}{dt} = -\frac{1}{\tau}\left(\phi - \phi^{eq}(t)\right) \quad (43)$$

with its own target value

$$\phi \approx \phi^{eq}(t) \quad (44)$$

➔ Toy-model, easier to understand than Lattice-Boltzmann ➔

HRR collision kernel

Hybrid-recursive-regularized

PhD Gabriel Farag, 2022.

We consider, $$\frac{d\phi}{dt} = -\frac{1}{\tau}\left[\phi - \sin\left(\frac{2\pi t}{\lambda^{eq}}\right)\right], \quad \text{with } \tau \ll \lambda^{eq} \tag{45}$$

Analytical and Crank-Nicolson $\Delta t = 10^6 \tau$ *i.e.* under-resolved relaxation.

Same integration as HRR LBM: Crank-Nicholson + small target contribution

$$\phi(t+\Delta t) = \sigma \phi^{CN}(t+\Delta t) + (1-\sigma)\,\phi^{eq}(t+\Delta t).$$

HRR collision kernel

Hybrid-recursive-regularized

PhD Gabriel Farag, 2022.

We consider, $$\frac{d\phi}{dt} = -\frac{1}{\tau}\left[\phi - \sin\left(\frac{2\pi t}{\lambda^{eq}}\right)\right], \quad \text{with } \tau \ll \lambda^{eq} \tag{45}$$

Analytical and Crank-Nicolson $\Delta t = 10^6\tau$ *i.e.* under-resolved relaxation.

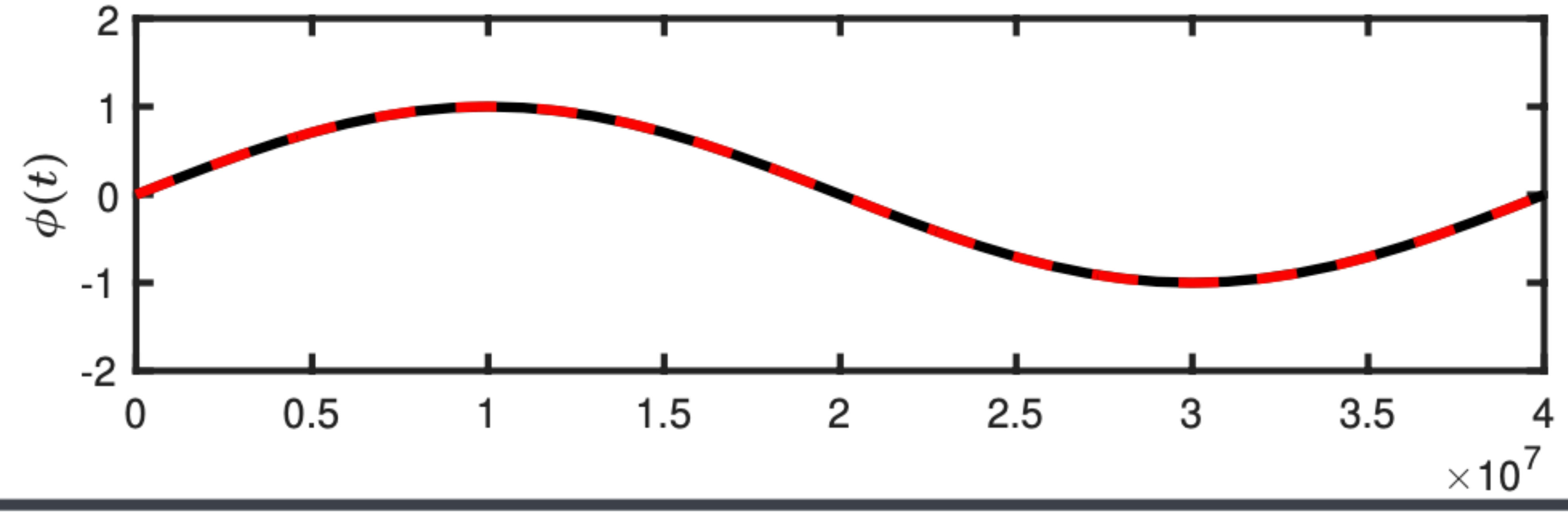


Figure 11: $\phi(t=0) = \phi^{eq}(t=0)$ and $0 \leq \sigma \leq 1$

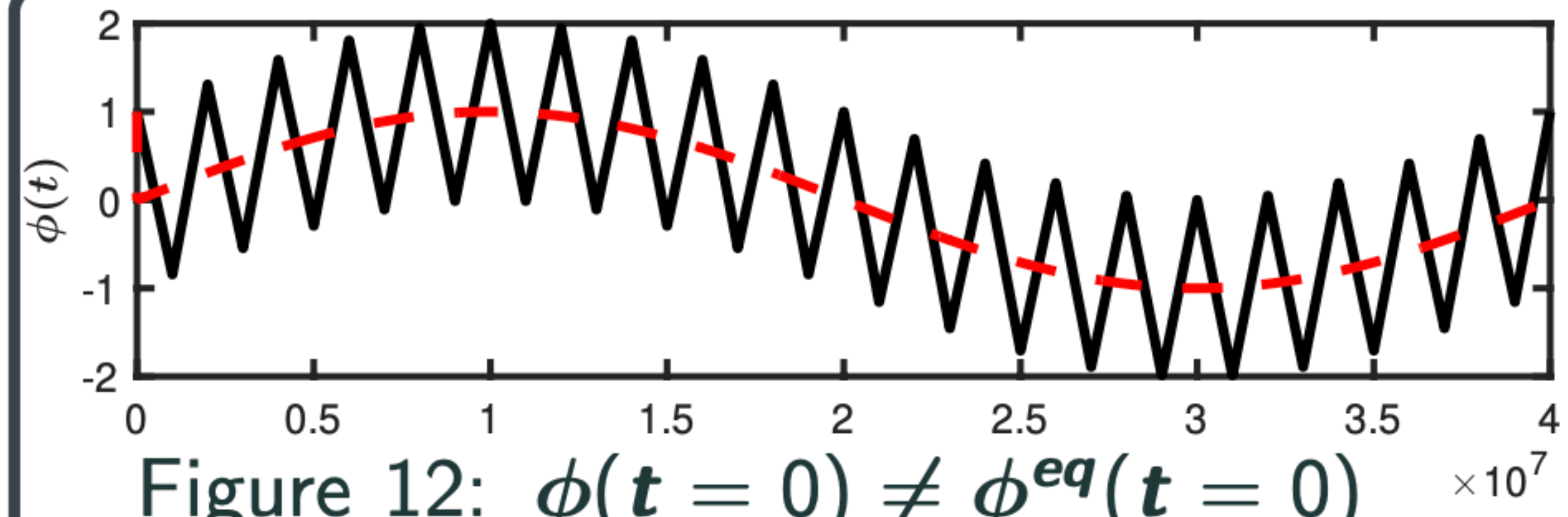


Figure 12: $\phi(t=0) \neq \phi^{eq}(t=0)$ and $\sigma = 1$

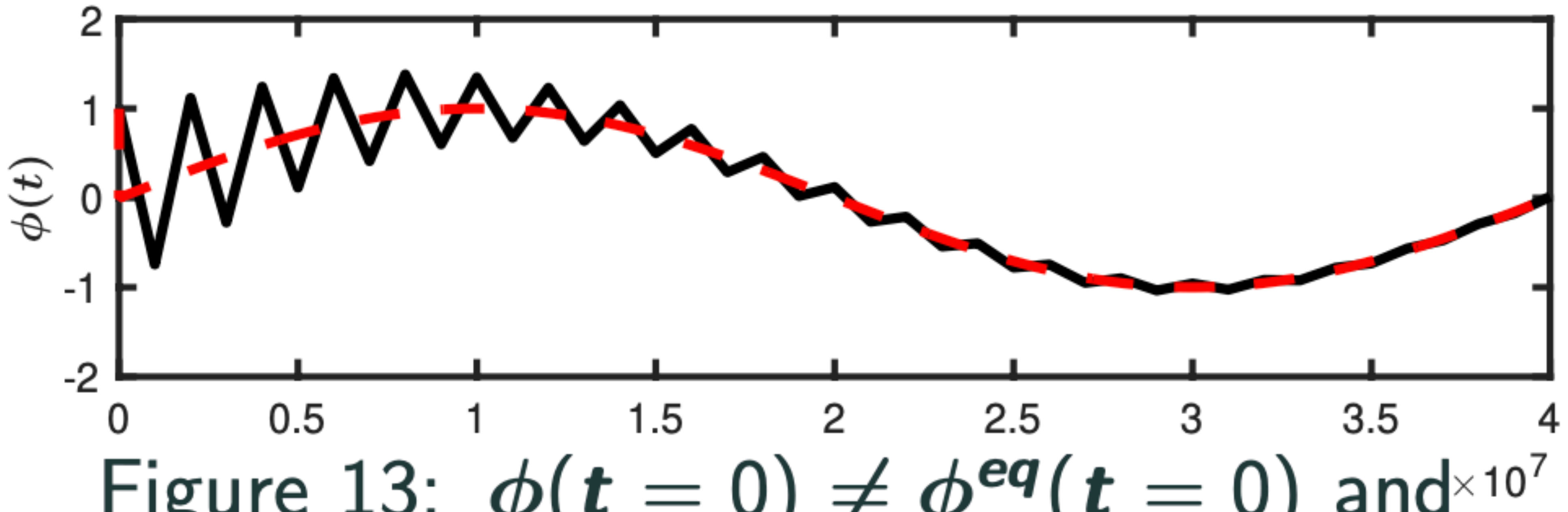
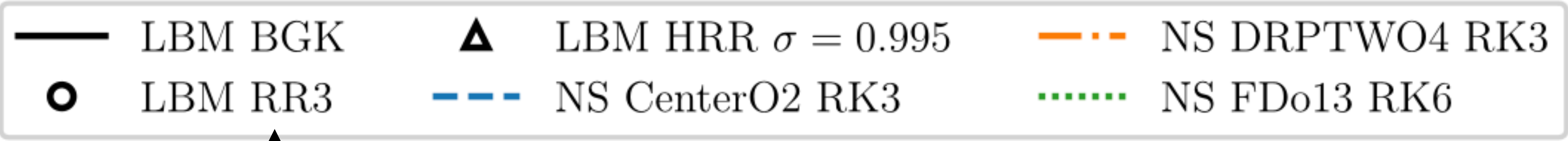


Figure 13: $\phi(t=0) \neq \phi^{eq}(t=0)$ and $\sigma = 0.9$

Numerical properties

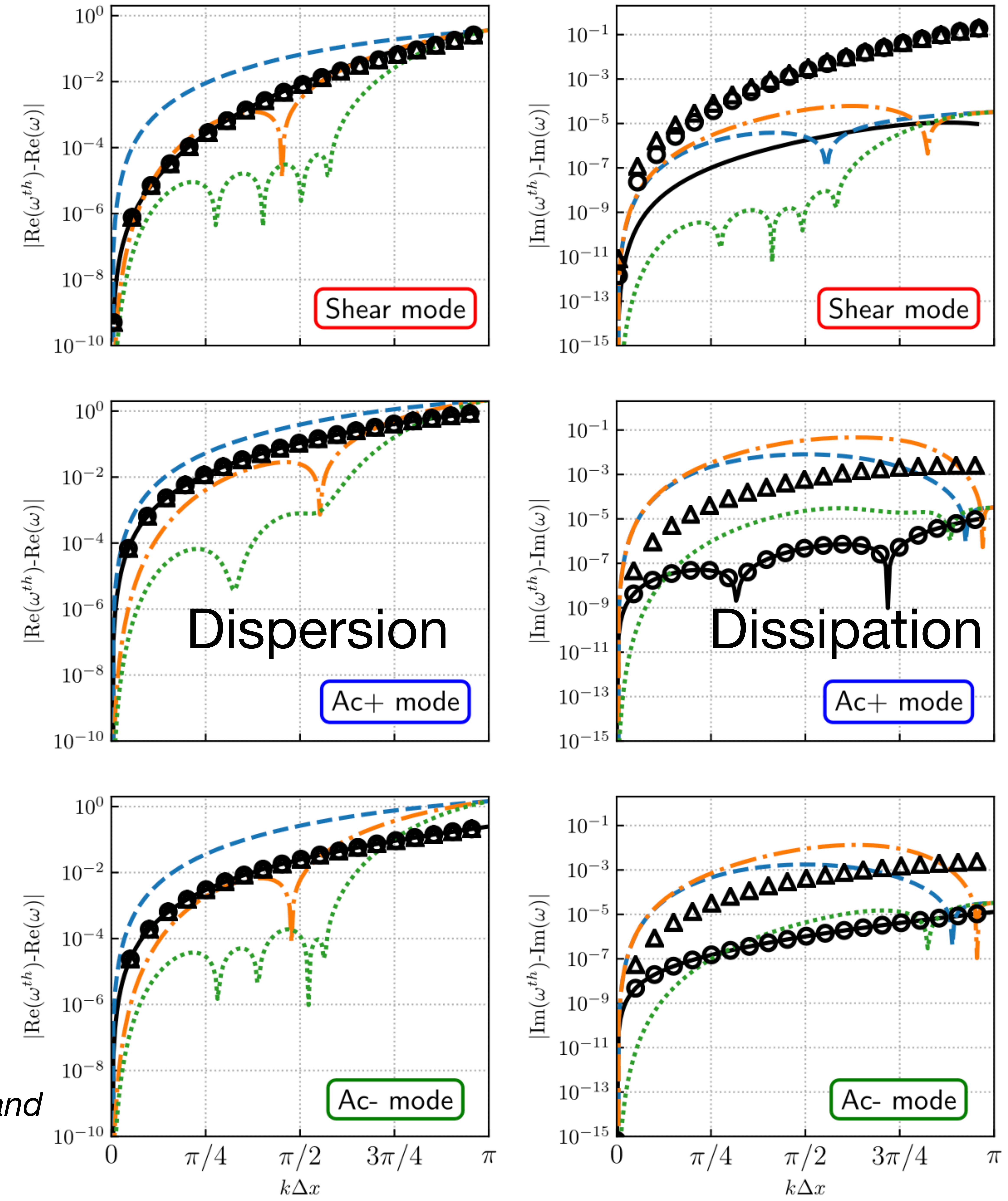
HRR dispersion/dissipation

Used for most industrial cases



Used for all academic cases

NS 6th order in space and time
JCP 2004: Bogey C, Bailly C. A family of low dispersive and low dissipative explicit schemes for flow and noise computations.



A. Suss, I. Mary, T. Le Garrec, and S. Marié, "Comprehensive comparison between the lattice boltzmann and navier–stokes methods for aerodynamic and aeroacoustic applications," Computers & Fluids, vol. 257, p. 105881, 2023.