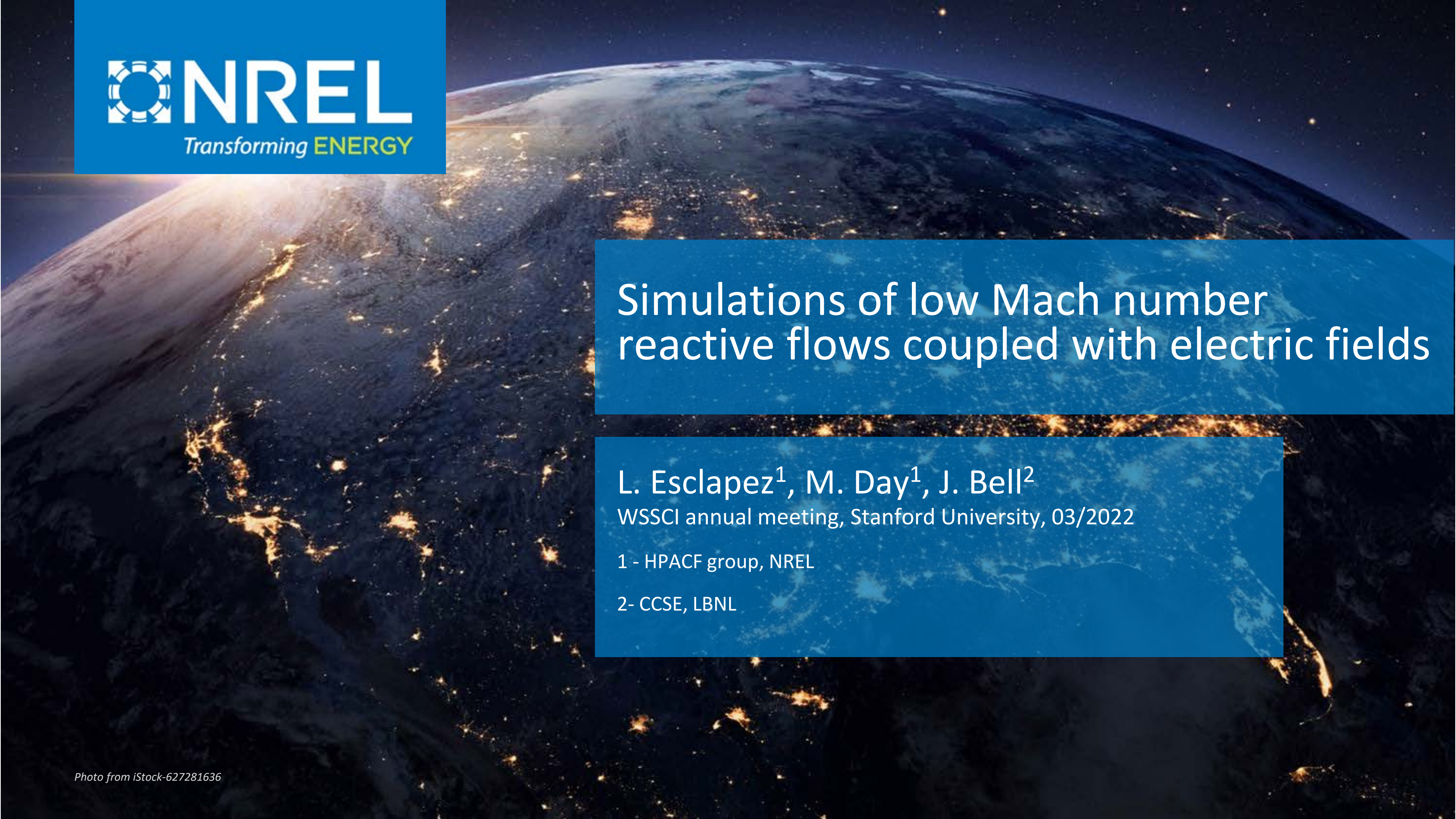


Simulations of low Mach number reactive flows coupled with electric fields

L. Esclapez[1], M. Day[1], J. Bell[2]

WSSCI annual meeting, Stanford University, 03/2022

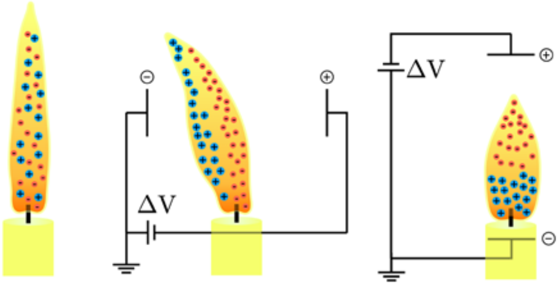
1 - HPACF group, NREL

2- CCSE, LBNL

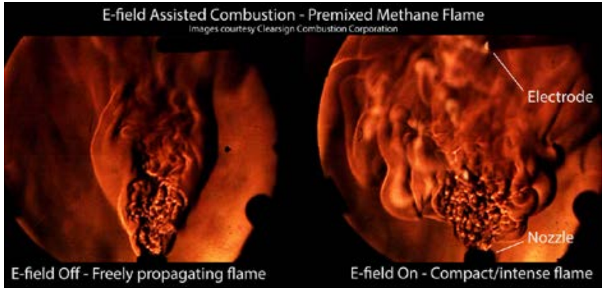
Photo from iStock-627281636

Motivation

- Charged particles naturally appear in flame during the chemical decomposition of hydrocarbons
- An electric field (e-field) can be used to apply a force on these particles
- The interactions of the charged particles with the surrounding gas result in a flame global response to electric fields called ion wind
- It can be use to provide an active control over the flame, in order to:
  - increase the flame speed
  - improve the flame stabilization
  - reduce NOx and soot emissions
  - …



Schematics of the interactions between a flame and an external electric field

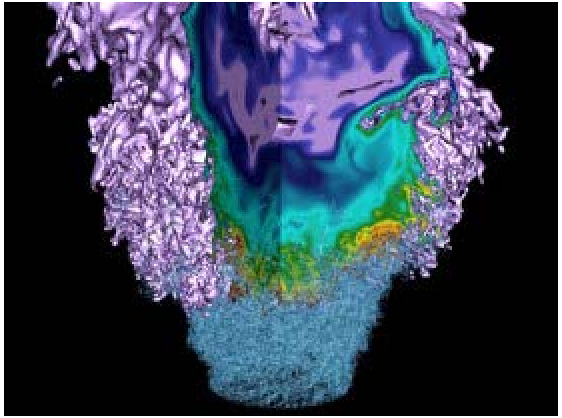


Turbulent flame subjected to e-field (courtesy of ClearSign Combustion)

Content

Computational framework

- Multi-species Navier-Stokes equations, in the low Mach number limit
- Spectral deferred correction (SDC) to ensure coupling of the fast reaction/diffusion with advection, while enforcing the velocity divergence constraint
- Adaptive Mesh Refinement (AMR) using the AMReX library (Zhang *et al*, 2019)
- Implemented in the open-source solver PeleLM, developed under the ExaScale Computing Program



Swirled turbulent hydrogen flame (Day et al., 2015)

https://amrex-combustion.github.io/PeleLM/

Computational framework

- To enable flow/electric field coupling:
  - Navier-Stokes augmented with electron transport and electro-static Poisson equation:

$$\frac{\partial(n_e)}{\partial t} + \boldsymbol{\nabla}\cdot(\boldsymbol{U}_{adv} n_e) = -\boldsymbol{\nabla}\cdot\boldsymbol{\Gamma}_e + \dot{\omega}_e$$

$$\boldsymbol{\nabla}^2\phi = -\frac{\overline{n}_c}{\epsilon_0\epsilon_r}$$

  - Charged species transport includes to a drift flux: $\boldsymbol{\Gamma}_m = -\rho D_m \boldsymbol{\nabla}\boldsymbol{X}_m - \rho Y_m \kappa_m \boldsymbol{\nabla}\boldsymbol{\phi}$
  - Momentum and energy equations include source terms for Lorentz forces and Ohmic heating, resp.:

$$\rho\sum_m z_m Y_m \boldsymbol{E} \qquad \rho\sum_m z_m Y_m \boldsymbol{\Gamma}_m\cdot\boldsymbol{E} \qquad \text{with} \qquad \boldsymbol{E} = -\boldsymbol{\nabla}\boldsymbol{\phi}$$

Lorentz forces   Ohmic heating

Computational framework

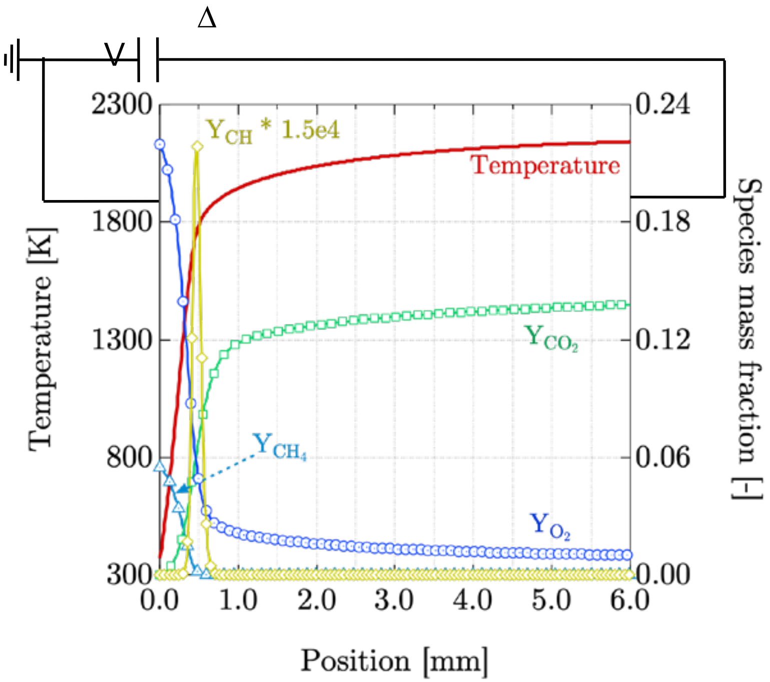
- The electron motion and tight electron/electric field coupling introduces very fast time scales
- We implemented the non-linear implicit solve presented in Esclapez et al, 2019 into the PeleLM solver
- To enable the implicit solve in an AMR context, a non-subcycling (all the AMR level advance at the same time) version of PeleLM was developed

https://amrex-combustion.github.io/PeleLMeX/

Content

1D premixed flame

- Burner-stabilized methane/air flame of Speelman *et al.*, 2015
- GRI3.0 mechanism + chemi-ionization submechanism of Belhi *et al.*, 2018 (9 ions + electrons)
- Local field approximation: electron transport properties tabulated as function of the reduced electric field |E|/N
- Varying the external electric voltage ΔV to covers the range of engineering applications

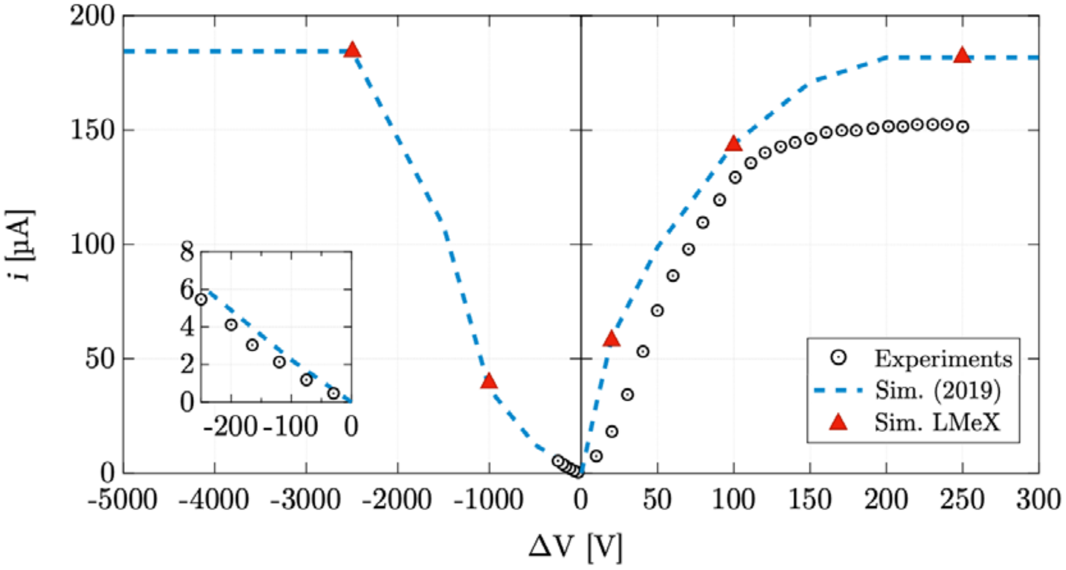


1D premixed flame

- Experimental data consist of ***i***-V curves, measuring the current across the flame as function of the imposed electric field:

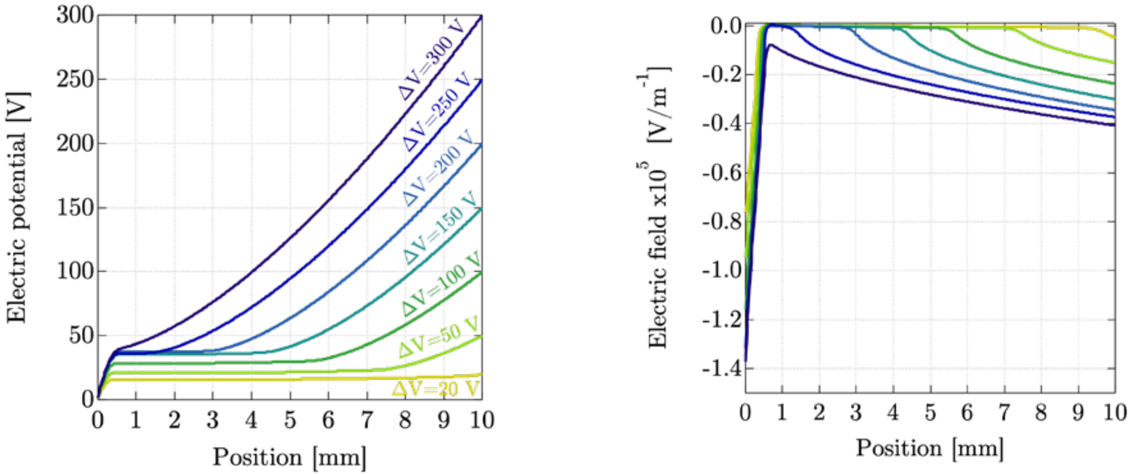
- PeleLMeX is able to reproduce experimental trends and match our initial, purely 1D, implementation

- The large differences observed between positive and negative polarity are related to the asymmetric position of the flame in the domain



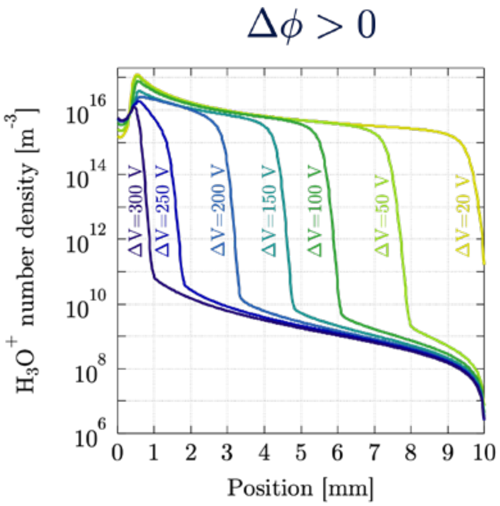
1D premixed flame

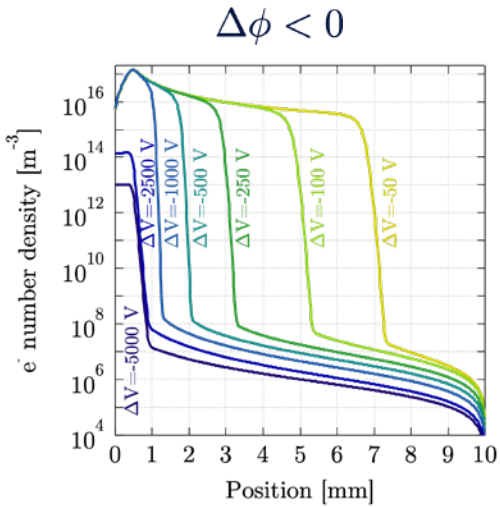
- Effect of increasing external forcing on the electronic structure of the flame:
  - The electric field is able to penetrate further into the flame, driving a flux of the charged particles to the electrodes



1D premixed flame

- Effect of increasing external forcing on the electronic structure of the flame:
  - Progressively sweeping the charged particles, creating steep gradients

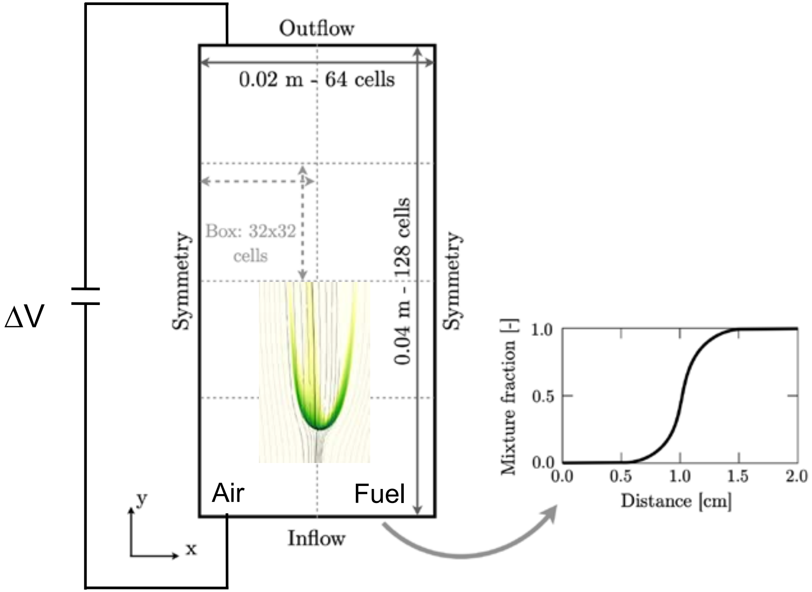

$\Delta\phi > 0$


$\Delta\phi < 0$

Content

2D propagating edge flame

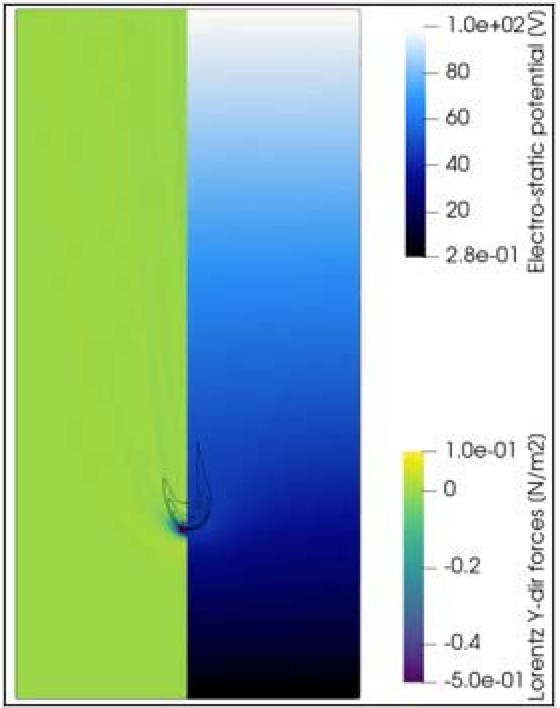
- Edge flames are a essential feature of flame stabilization and propagation in many combustion devices.
- They exhibit a flame complex structure with combustion occurring in both premixed and non-premixed mode.
- Their propagation speed is the key characteristic we are interested in.



Schematics of the computational domain

2D propagating edge flame

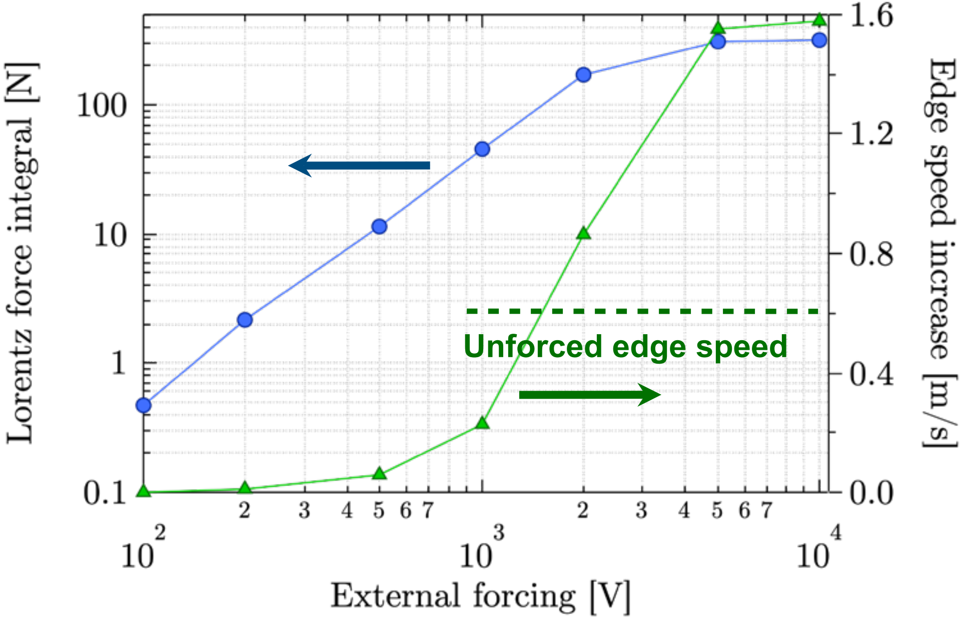
- What happens when we start applying the external voltage ?
  - Electrons rapidly move across the domain and establish the electro-static potential (right)
  - The slower positive ions are pulled towards the bottom, resulting in a downward Lorentz force (left)
  - The edge flame accelerates !



Transient Lorentz forces (left) and electro-static potential (right) upon applying external ΔV

2D propagating edge flame

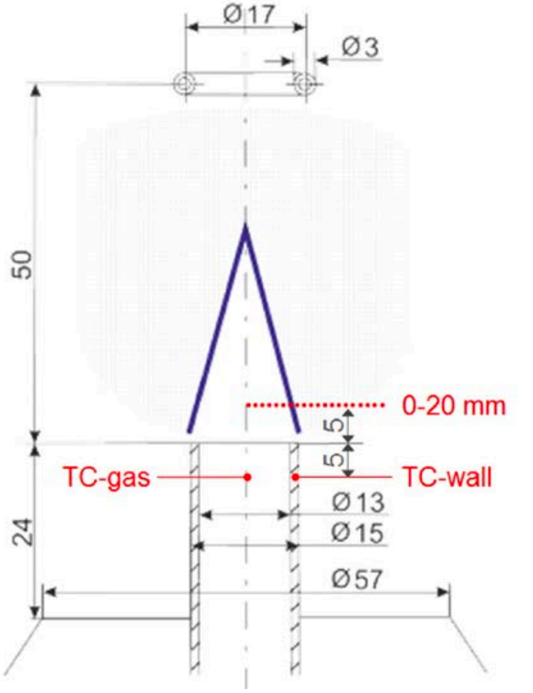
- Effect of increasing external forcing:
  - Integral of the Lorentz forces initially increases with external electro-static voltage intensity and eventually plateau
  - A more practical measure: how much the flame speed increases when submitted to this force for 2 ms
  - Ionic wind (effect of the Lorentz forces) can be used to modify flame stabilization



Content

3D premixed bunsen flame

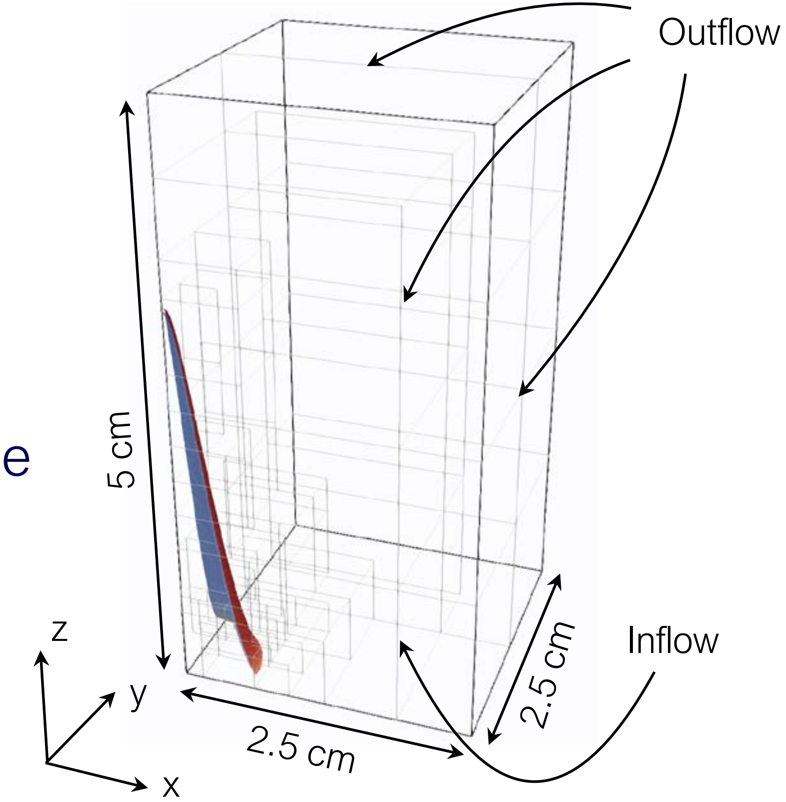
- Methane/air premixed burner of Kuhl *et al.*, 2017
- Three different equivalence ratio, maintaining a constant inlet flow speed
- Forced axially with a constant mean electric field of 120kV/m between a downstream electrode and the bunsen tube
- Available measurement of current, local temperature, velocity field and OH luminescence



Experimental setup of Kuhl et al.. Distances in mm

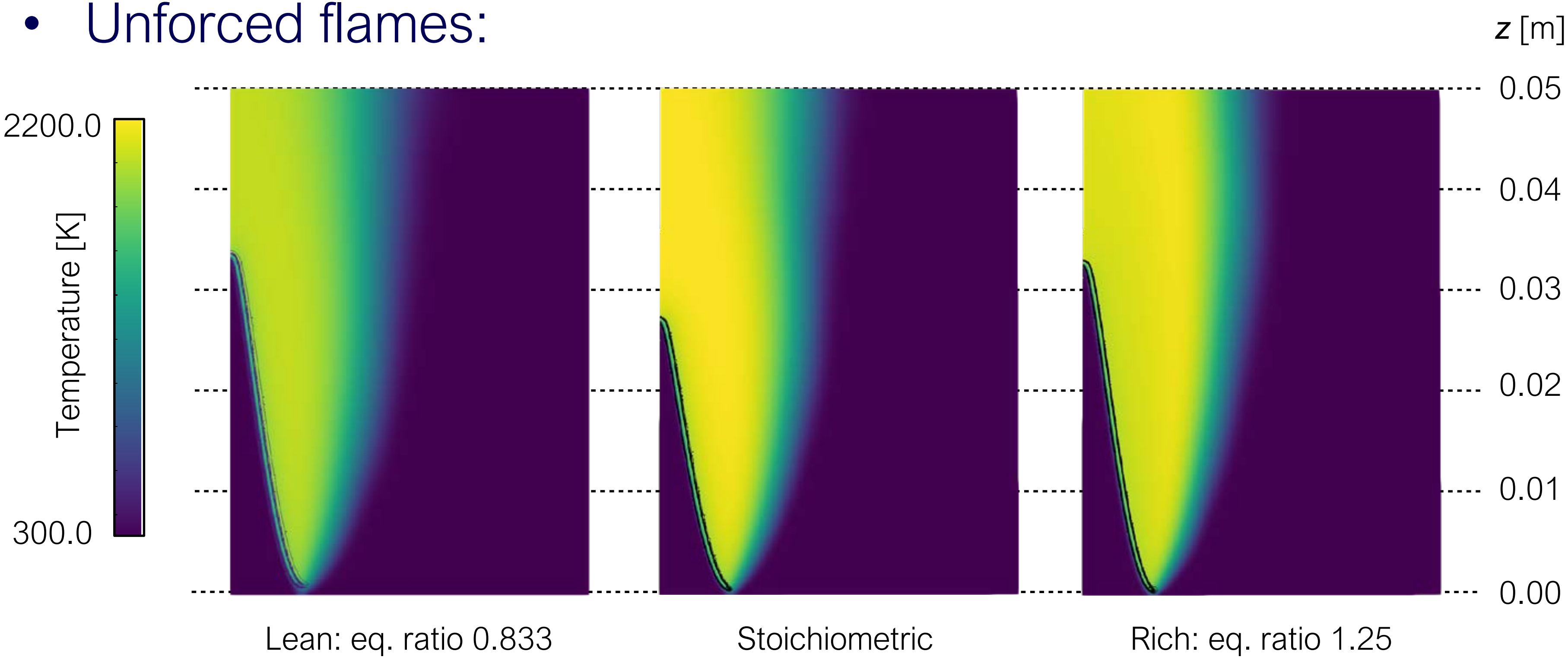
3D premixed bunsen flame

- 1/4 domain with lateral symmetry employed in the simulation
- Parabolic laminar profile in the bunsen inlet, 0.1 m/s coflow
- Burner lip represented on the inflow face
- Ambient conditions
- levels of refinement, Δx = ~25μm



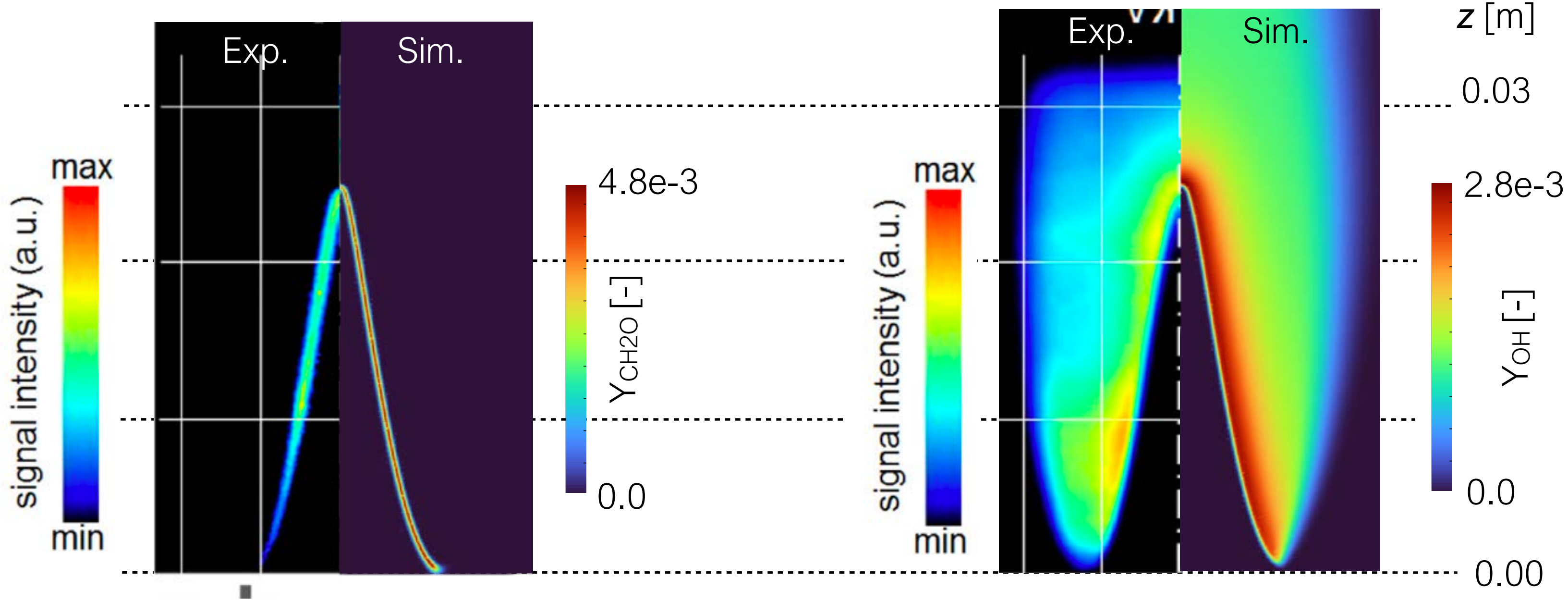
3D premixed bunsen flame

- Unforced flames:



3D premixed bunsen flame

- Unforced flames:



CH_2O-fluorescence

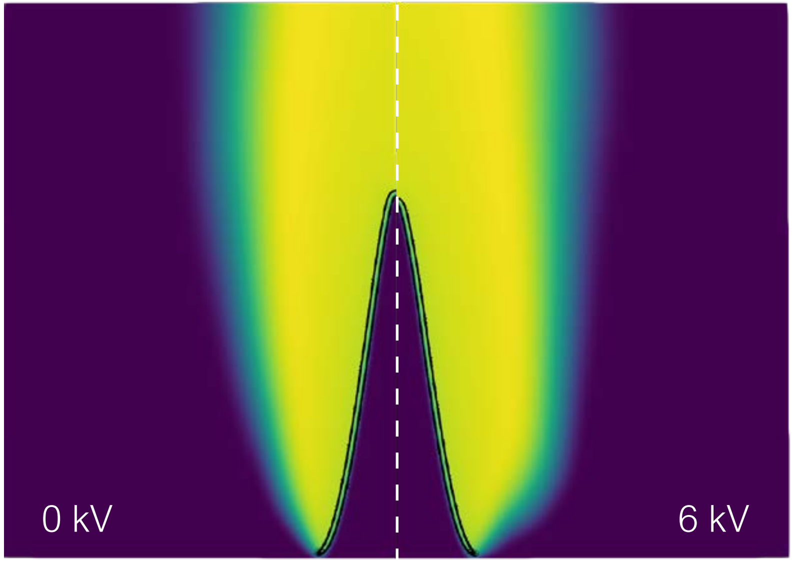
OH-fluorescence

Stoichiometric

3D premixed bunsen flame

- Applied external forcing: slow process, inducing small changes in the overall flame and plume shapes:

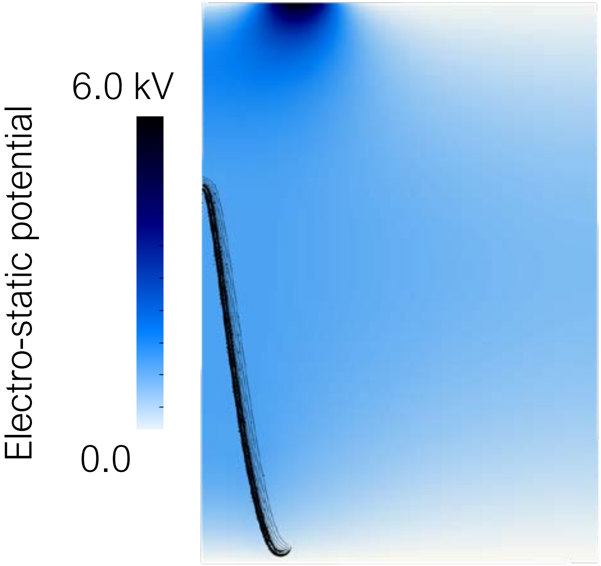
- Slight shortening of the flame length
- Widening of the hot gas region close to the grounded burner lip
- No significant changes in the flame thickness or major species distribution

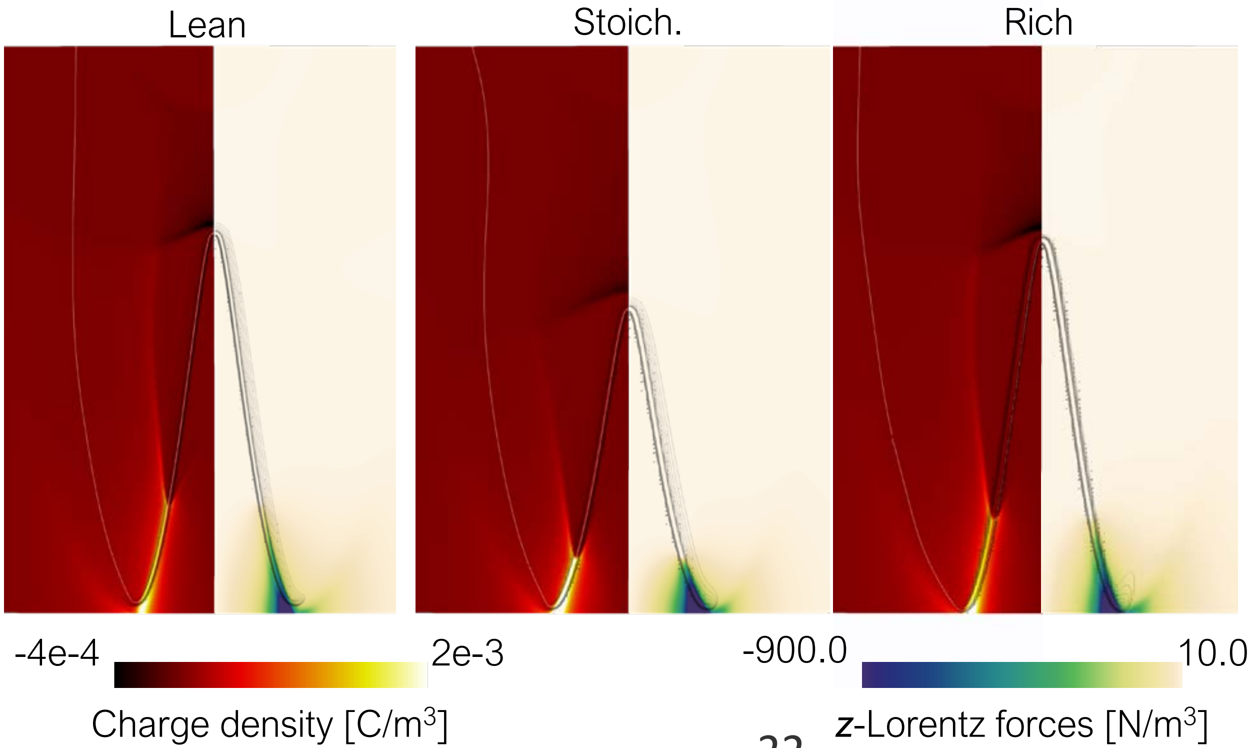


Rich conditions

3D premixed bunsen flame

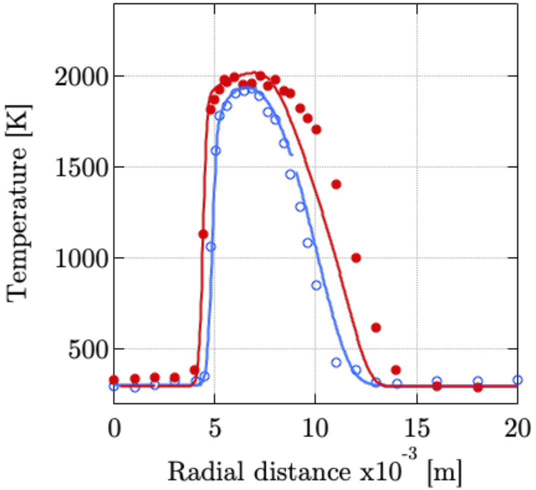
- Applied external forcing: electronic structure

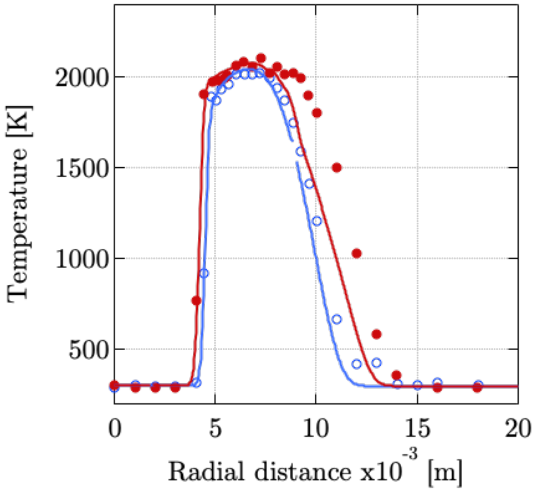


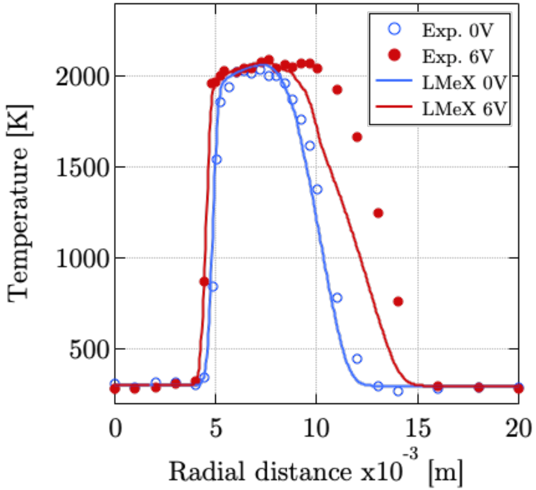


3D premixed bunsen flame

- Applied external forcing: temperature measurements


Lean


Stoich.


Rich

	Lean	Stoichiometric	Rich
Experiments	0.12	0.16	??
Simulations	0.135	0.178	0.231

Current measurements [mA]

3D premixed bunsen flame

- The trends appear to be captured, but simulations and further analysis are still ongoing
- Experiments show an increase of the burner lip temperature with the applied voltage, not accounted for in the simulations
- The simulation remains expensive:
  - Convective time scale of the burner of ~10 ms, but time step size constrained to ~0.1µs —> 1e6 steps !

Conclusion

- Successfully extended our initial SDC-JFNK method to multi-dimensional AMR simulations

- Time step size 2 order of magnitude larger than explicit constraint, but still relatively small compared to advection scales

→ Further improvements are under considerations

- Starting a collaboration with UCI to explore their micro-gravity experimental data (NASA-PSI project) with PeleLM

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EXASCALE COMPUTING PROJECT

U.S. DEPARTMENT OF
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Office of
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