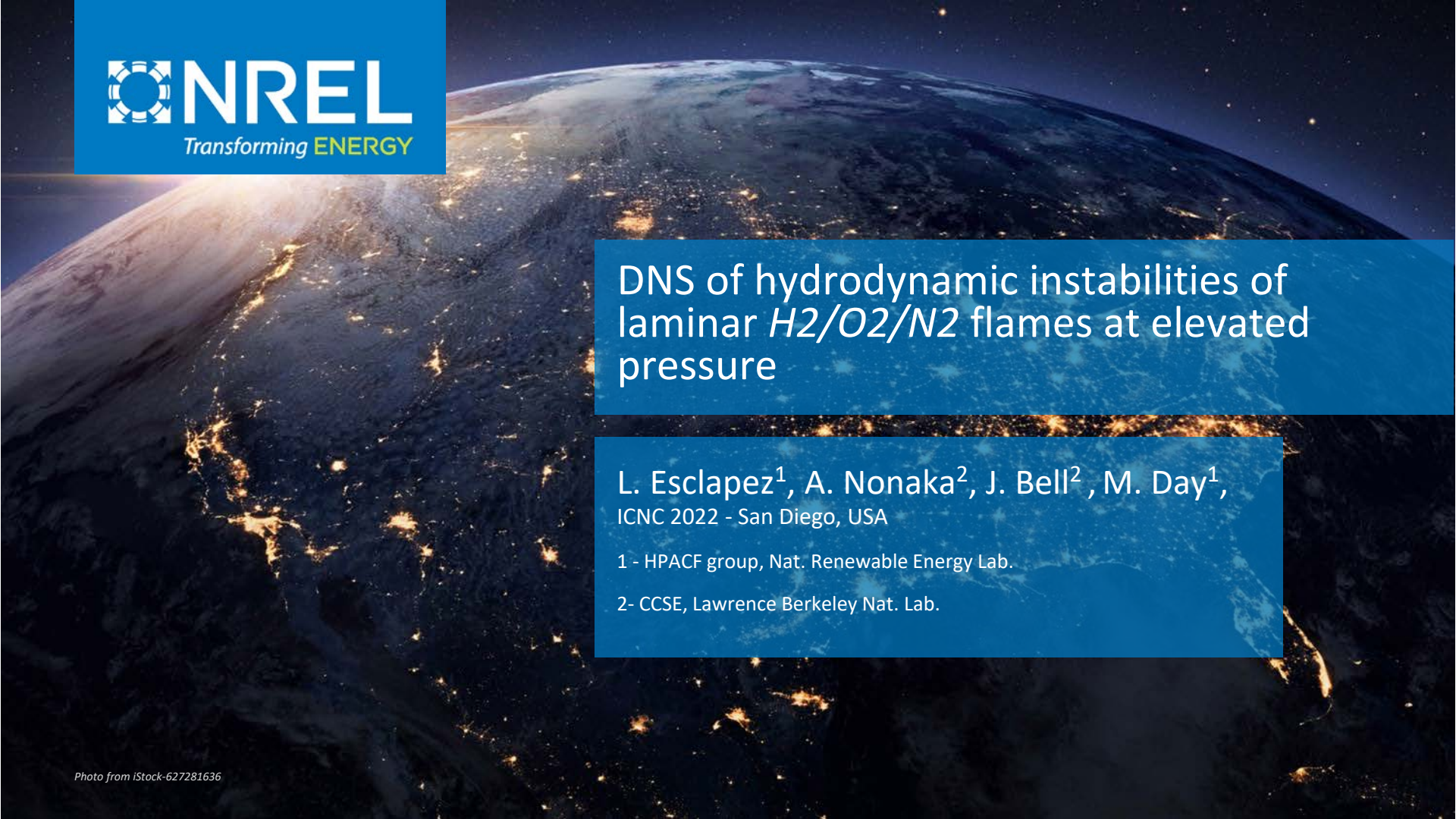

DNS of hydrodynamic instabilities of laminar *H2/O2/N2* flames at elevated pressure

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Motivation & Background

- Experimental studies of laminar propagating flames are essential to determine key flame properties (flame speed and thickness, flammability limits, …) and validate the development of chemical mechanisms

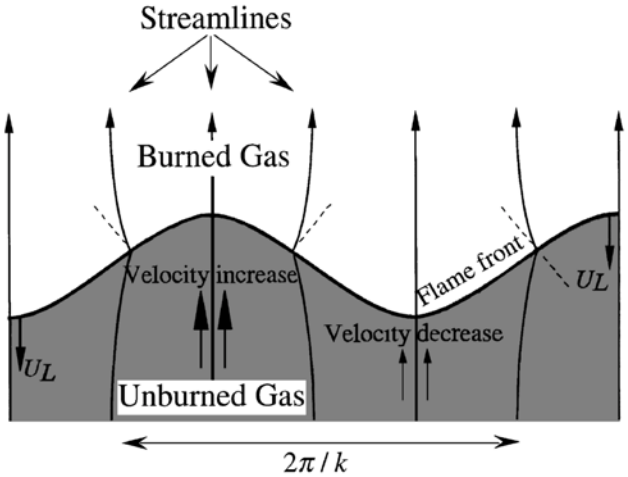
- Conducting experiments at engine relevant conditions is challenging because both flow and intrinsic flame instabilities are exacerbated, leading to large uncertainties in processing experimental data or even preclude the analysis entirely

- A better understanding of the flame behavior in these test devices could help reduce the experimental uncertainties and develop new processing methods

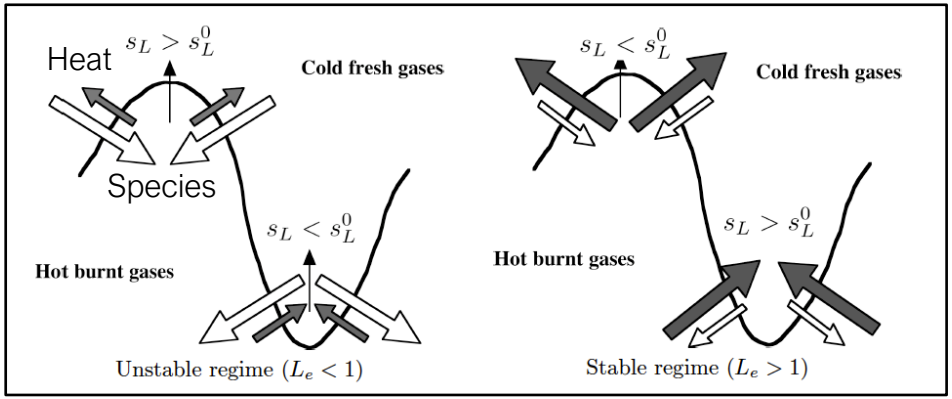
Motivation & Background

- At high pressure, spherically expanding flames (SEF) are the only possible experiments, optical access is not always available (Egolfopoulos ***et al.***, 2014)

- SEF are subjected to Darrieus-Landau (hydrodynamic) and thermo-diffusive instabilities:



Clanet & Searby, 1998



Poinsot & Veynante, 2011

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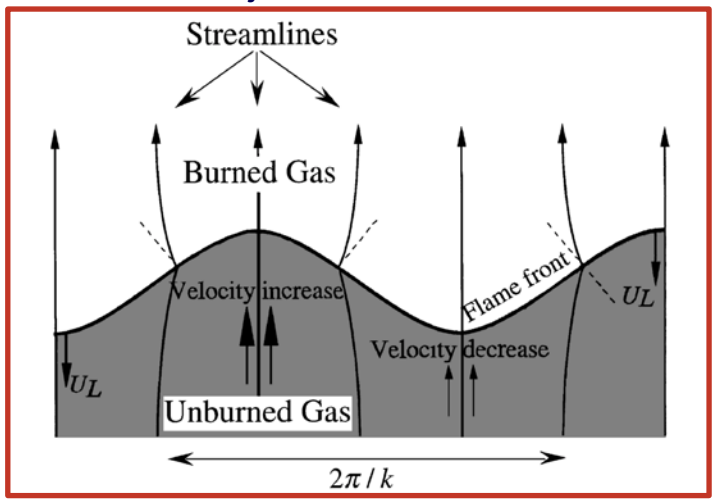

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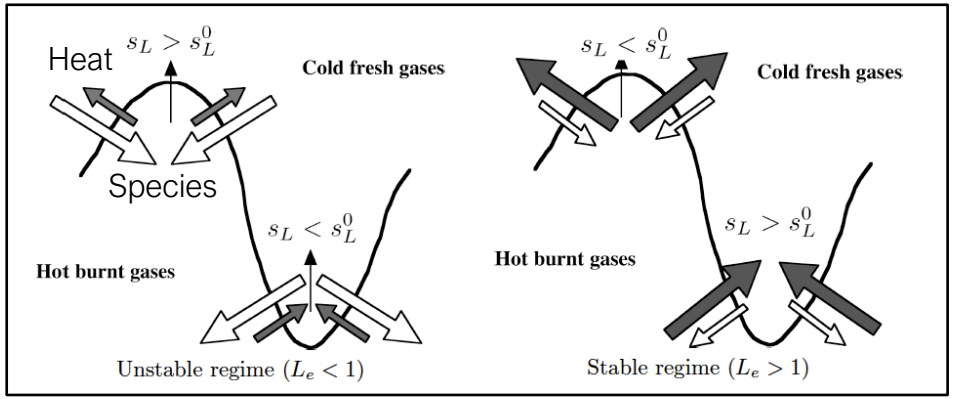


Poinsot & Veynante, 2011

Motivation & Background

- Bechtold & Matalon, 1987 theoretically showed that the onset DL instabilities in SEF is controlled by a Peclet number, the critical value of which was later corrected by Bradley and co-worker:

$$Pe = \frac{R(t)}{\delta_l} \qquad Pe_c = Pe_1(\sigma) + Ze(Le - 1)Pe_2(\sigma)$$

- Owing to the large disparity of scales between the flame thickness and its radius, DNS have remained elusive, and it is unclear how DL instabilities affect the flame morphology and its expansion rate (self-turbulization?)

- Most of the experiments done by C.K. Law and co-worker employed a constant-pressure vessel and the effect of rising pressure in constant-volume devices has not been fully characterized

Motivation & Background

Computational framework

- Multi-species Navier-Stokes equations, in the low Mach number limit (Day & Bell, 2000):

$$\frac{\partial(\rho Y_m)}{\partial t} + \boldsymbol{\nabla}\cdot(\boldsymbol{U}_{adv}\rho Y_m) = -\boldsymbol{\nabla}\cdot\boldsymbol{\Gamma}_m + \dot{\omega}_m \qquad m = 1:N$$

$$\frac{\partial(\rho h)}{\partial t} + \boldsymbol{\nabla}\cdot(\boldsymbol{U}_{adv}\rho h) = \boldsymbol{\nabla}\cdot\lambda\boldsymbol{\nabla}\boldsymbol{T} - \sum_m \boldsymbol{\nabla}\cdot(h_m\boldsymbol{\Gamma}_m) + \frac{dP_0}{dt}$$

$$\frac{\partial(\rho\boldsymbol{U}_{adv})}{\partial t} + \boldsymbol{\nabla}\cdot(\boldsymbol{U}_{adv}\rho\boldsymbol{U}_{adv}) = -\boldsymbol{\nabla}\boldsymbol{\pi} + \boldsymbol{\nabla}\cdot\boldsymbol{\tau}$$

ρ	: density
$\boldsymbol{U}_{adv}$	: velocity
Y_m	: species mass fraction
h	: enthalpy
$\dot{\omega}_m$	: chemical source term
$\boldsymbol{\tau}$	: stress tensor

where:

$$p(\boldsymbol{x},t) = P_0(t) + \pi(\boldsymbol{x},t) \quad \text{with} \quad P_0(\rho, Y_m, T) = \frac{\rho\mathcal{R}T}{W}$$

Uniform background pressure

Perturbational pressure

Computational framework

- Open (constant-pressure) domains:

$$\frac{D(P_0(t))}{Dt} = 0 \quad \Longrightarrow \quad \nabla \cdot \boldsymbol{U}_{adv} = \frac{1}{T}\frac{DT}{Dt} + W\sum_m \frac{1}{W_m}\frac{DY_m}{Dt} = S.$$

- Closed domains, the background pressure varies in time (Nonaka ***et al.***, 2018):

$$\nabla \cdot \boldsymbol{U}_{adv} + \theta\frac{dP_0}{dt} = S \qquad \theta = \frac{1}{\Gamma_1 P_0}$$

$$\nabla \cdot \boldsymbol{U}_{adv} + (\overline{\theta} + \delta\theta)\frac{dP_0}{dt} = (\overline{S} + \delta S)$$

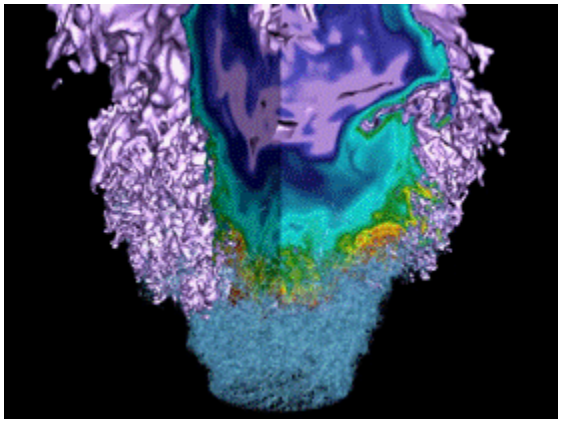
Mean Perturbation

Integrated over the computational domain:

$$\frac{dP_0}{dt} = \frac{\overline{S}}{\overline{\theta}} \quad \text{and} \quad \nabla \cdot \boldsymbol{U}_{adv} = \delta S - \delta\theta\frac{\overline{S}}{\overline{\theta}}$$

Computational framework

- Implemented in our open-source solver PeleLMeX
- Adaptive Mesh Refinement (AMR) using the AMReX library (Zhang ***et al***, 2019)
- Spectral deferred correction (SDC) to ensure coupling of the fast reaction/diffusion with advection, while enforcing the velocity divergence constraint (Nonaka ***et al.***, 2012)
- Advection treated with BDS scheme (May ***et al.***, 2013), classical 2nd-order diffusion stencil with GMG solver and CVODE (Balos ***et al.***, 2020) for the stiff chemistry implicit integration



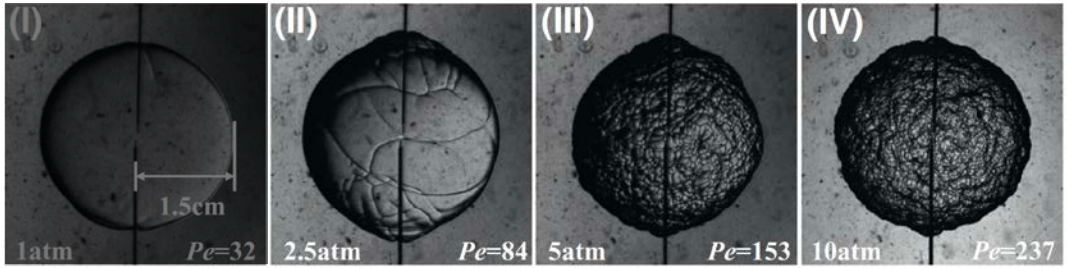
Swirled turbulent hydrogen flame (Day et al., 2015)

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

More details tomorrow in talk 3C11MS by M. Day ***et al.***

Content

DL instabilities of H2/O2/N2 flames



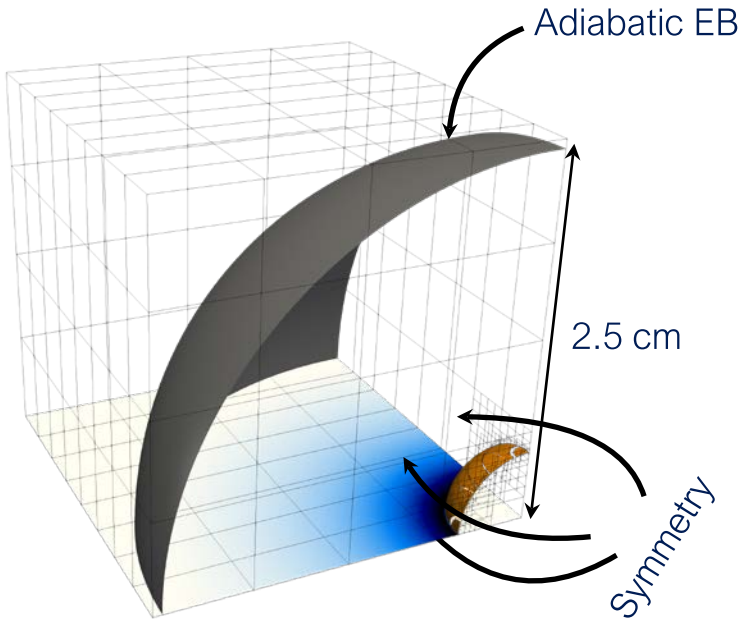
- Looking into Yang ***et al.*** 2016 flames, focusing on near stoichiometric mixtures with effective Lewis number close to one, σ ~ 5.47 —> hydrodynamic DL instabilities dominate

- Experiments observed a near constant critical Peclet number for all cases: Pe_c ~ 100
- Simulations will be performed in a closed chamber to extract a pressure trace

	2.5atm	5atm	10atm
∂l [μm]	178	98	63
Sl,b [m/s]	3.075	2.25	1.434
R_c [mm]	17.8	9.8	6.3

DL instabilities of H2/O2/N2 flames

- Burke-Dryer H2/Air mechanism
- Closed chamber, 5 cm in diameter, adiabatic no-slip walls
- Symmetry in all three directions is exploited: 1/8 fifth of the configuration
- 256^3 base grid, with up to 4 levels of refinement ($\Delta x \sim 6\mu m$), maintaining at least 10 grid cells within the thermal thickness
- Initial solution interpolated from a Cantera 1D flame at a radius of 5 mm

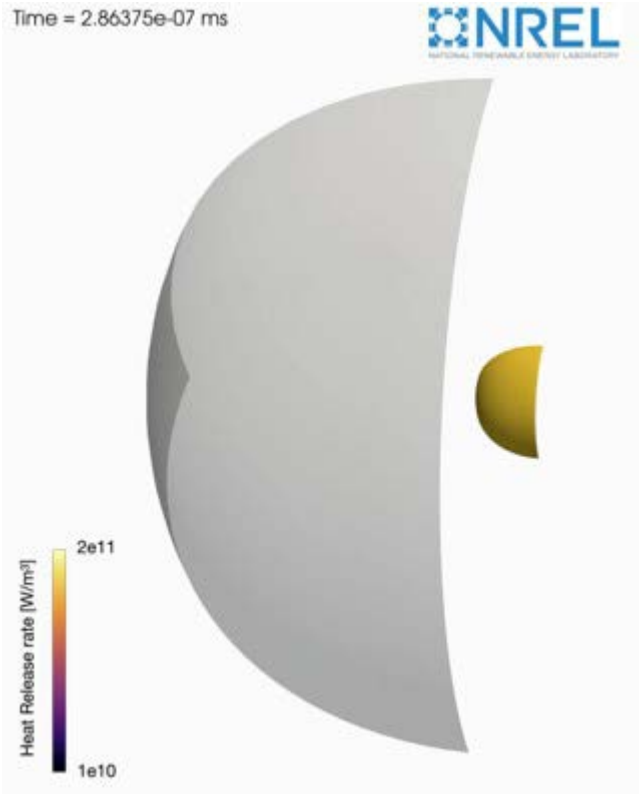


$$c = \frac{Y_{\mathrm{H2}_c} - Y_{\mathrm{H2}}}{Y_{\mathrm{H2}_c} - Y_{\mathrm{H2}_b}} \qquad S_f = \int_V |\nabla c|$$

DL instabilities of H2/O2/N2 flames

- Flame initially dominated by thermo-diffusive effects and is stable to small perturbations
- The flame radius increases and cells appear on the flame surface as DL instabilities develop
- As the flame further expands, growing cells destabilizes to form smaller cells

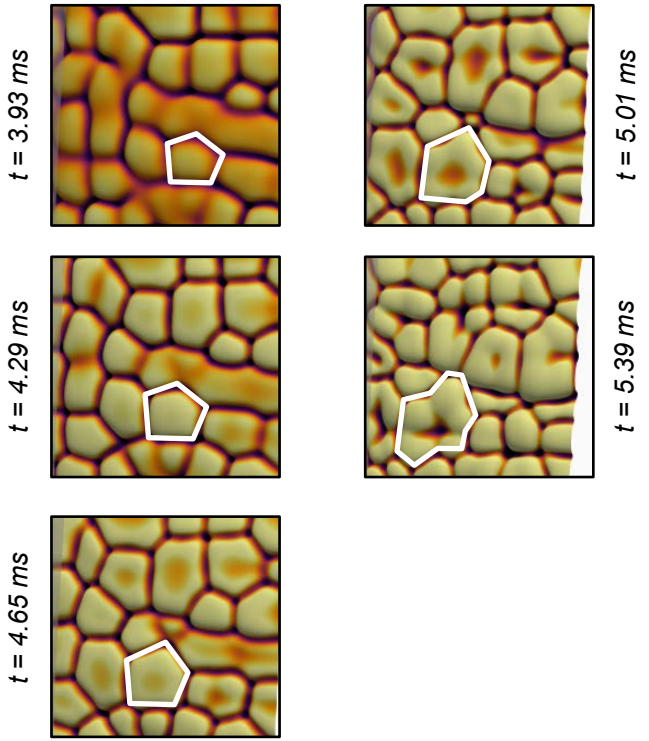
Note: the cell count goes from ~ 45M cells at t=0 to about 0.9B at t=5.2 ms.



10 atm, c = 0.7*

DL instabilities of H2/O2/N2 flames

- As the flame further expands, growing cells destabilizes to form smaller cells:
  - Streamlines diverge ahead of the cell, velocity increases in the cusps
  - Velocity deficit destabilize the cell center, eventually fragmenting it into smaller cells
- The process repeats as cells continuously expand with the flame mean radius



DL instabilities of H2/O2/N2 flames

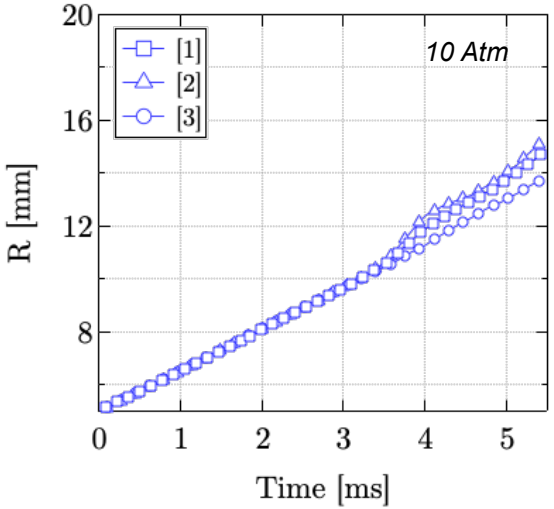
- Transition Peclet numbers:

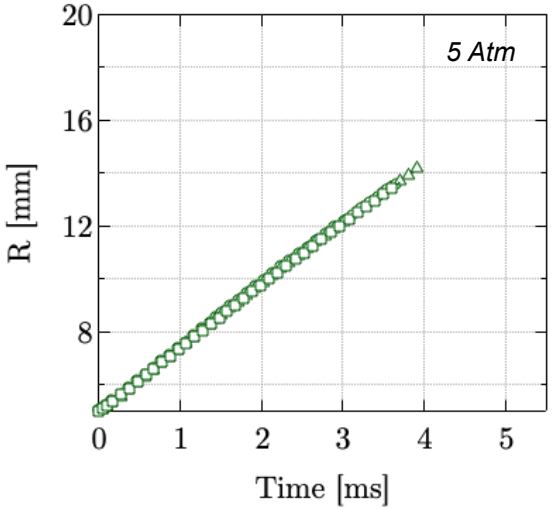
	2.5atm	5atm	10atm
Exp.	~ 100	~ 100	~ 100
DNS	Ongoing	~ 190	~ 140

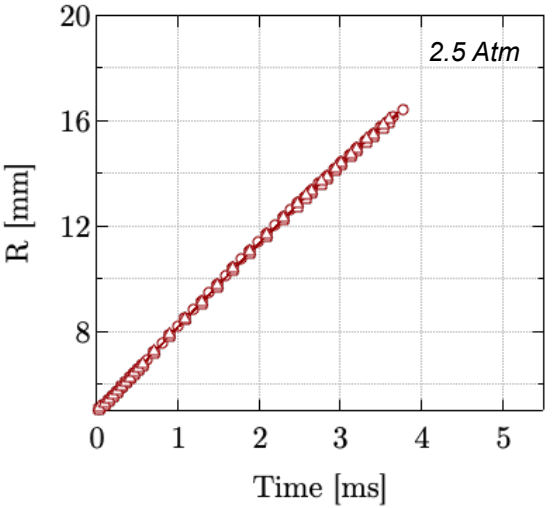
- DNS predictions are consistently larger than experimental observations:
  - Rising pressure have a stabilizing effect because the fresh gases temperature increases, resulting is smaller σ
  - DNS is initially free of perturbations naturally present in the experiments: instabilities are only triggered by numerical noise which can delay the onset
  - Most unstable azimuthal mode might be precluded by symmetry conditions

DL instabilities of H2/O2/N2 flames

- Extracting the averaged flame speed:
  - [1] : $S_f = \int_V |\nabla c|$ and $R_f = \sqrt{S_f \cdot 2/\pi}$
  - [2] : Area of iso-surface c*=0.7, $R_f = \sqrt{S_{iso} \cdot 2/\pi}$
  - [3] : Mean flame brush radius



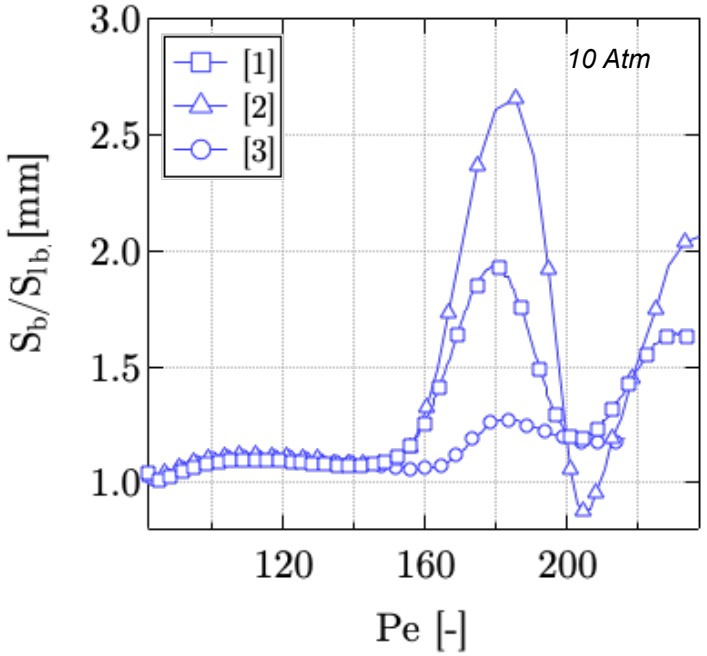




DL instabilities of H2/O2/N2 flames

- Extracting the averaged flame speed:
  - Differentiating the radius to get the flame speed
  - The flame speed appears to pulsate, also visible on the mean flame radius
  - Behavior previously observed in 2D-DNS, but more apparent here due to the coupled increase of pressure
- Self-turbulization often characterized by the self-acceleration exponent:

$$R = R_0 + At^{\alpha}$$



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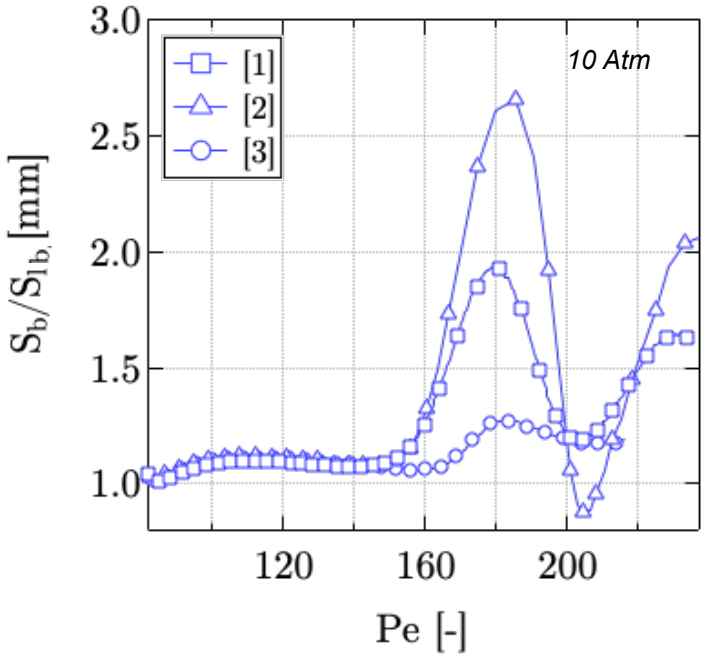
Currently investigating other way to estimate the fractal dimension



Contents

Conclusion and future work

- Developed a simulation framework able to tackle slow, high pressure laminar flames
- Onset of DL instabilities and cascade of cells reproduced in the DNS, albeit at larger critical Peclet number
- Simulations are still ongoing and subsequent analysis will focus on the flame front itself (fractal dimension, local/mean consumption rate, …) and its resulting effect on the flame acceleration
- Still interested in heavier hydrocarbon/hydrogen blends, especially at high pressure. Initial 2D results indicates minimal effects on the flame stability up to H2 volume fraction of ~80%.

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Early science allocation on NERSC Perlmutter and ORNL's Crusher

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