Conference or Workshop Item:

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Comparisons of Flame Surface Density Measurements with Direct Numerical Simulations of a lean Methane-air Flame in High-intensity Turbulence

Girish Nivarti , Ben Thorne,
Stewart Cant, Malcolm Lawes, and Derek Bradley

University of Cambridge and University of Leeds

Orlando: 5 April, 2017
16th International Conference on Numerical Combustion

Premixed turbulent flame propagation

The turbulent burning velocity

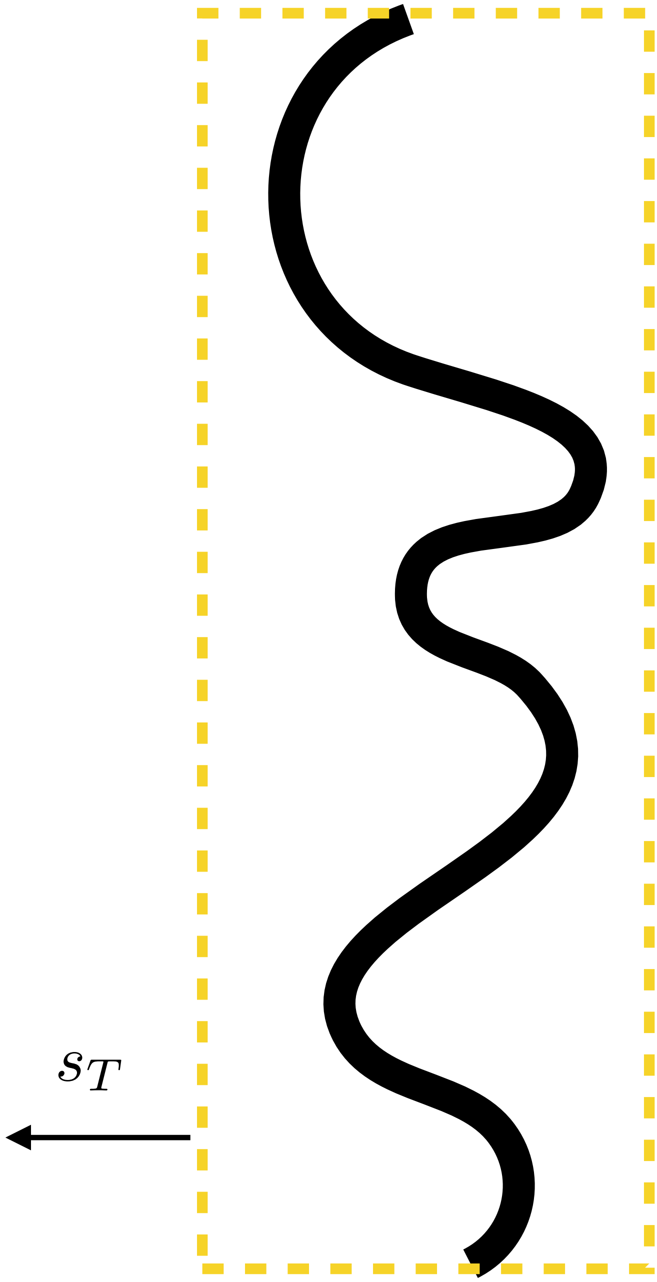
$$s_T \equiv -\frac{1}{\rho_u Y_{u,F} A_0} \int_V \dot{\omega}_F \, dV,$$

is a measure of the overall burning rate of a given fuel-air mixture.

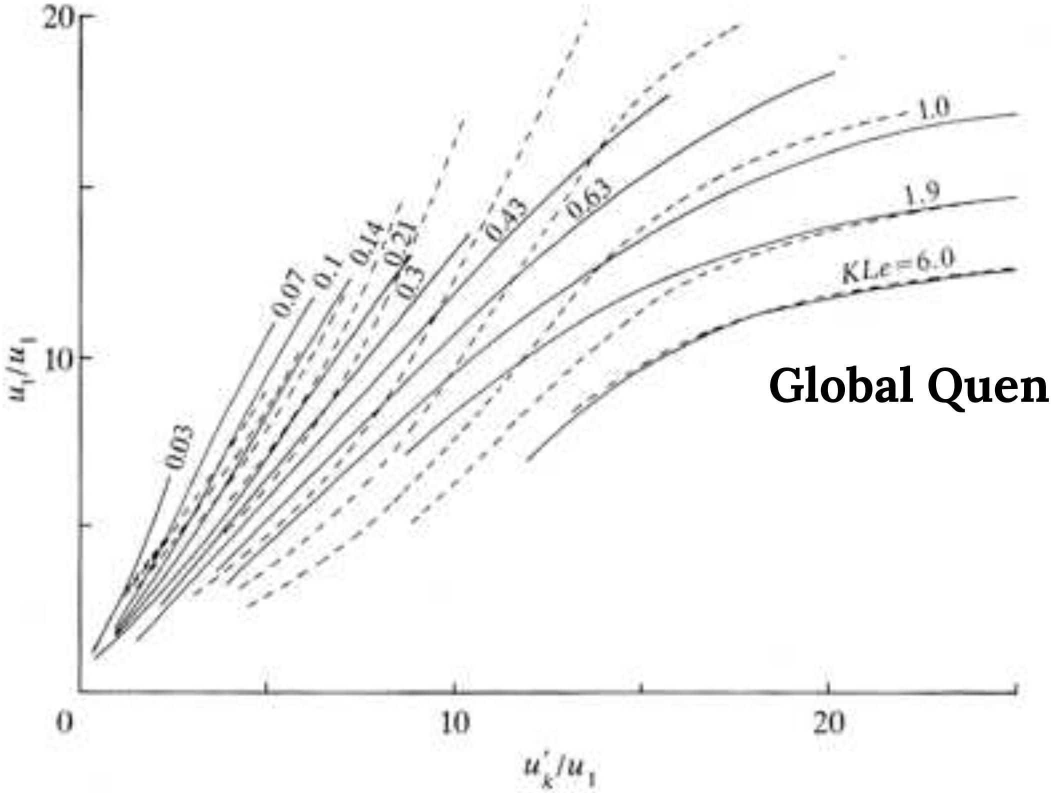
Damköhler's first hypothesis suggests that the enhancement in overall burning rate

$$s_T = s_L \frac{A_T}{A_L}$$

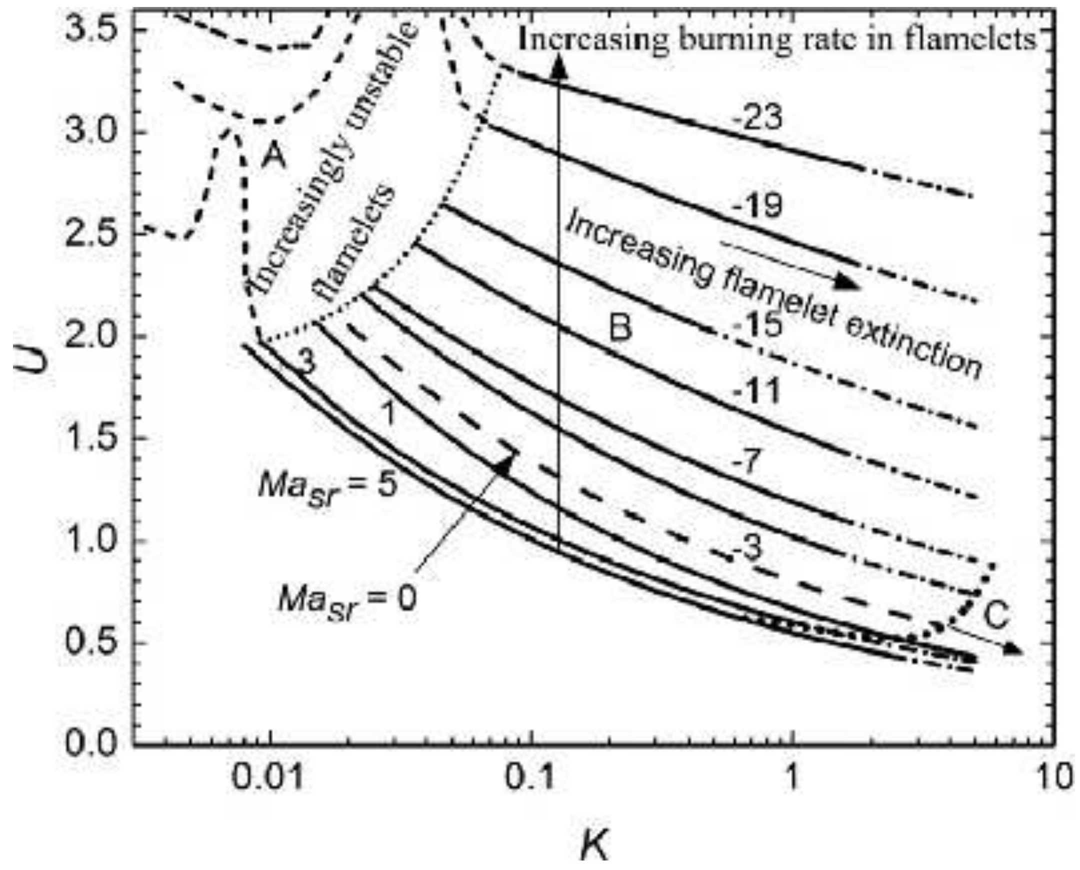
is due to enhanced flame surface area.



Bending effect: the Leeds hypothesis



Global Quenching



Experiments in Leeds have shown[1,2] that turbulent burning velocity shows a gradually **diminishing enhancement** with increasing levels of turbulence.

Eventually, at high enough intensities the entire flame is extinguished.

The Leeds group suggested that the **increased extensive strain** expected in high intensity turbulence governs the local and global extinction.

Damköhler's hypothesis needs to be modified to determine the burning velocity

$$s_T = \underline{I_0} s_L \frac{A_T}{A_L} = I_0 s_L \frac{1}{A_L} \underline{\int \Sigma dV}$$

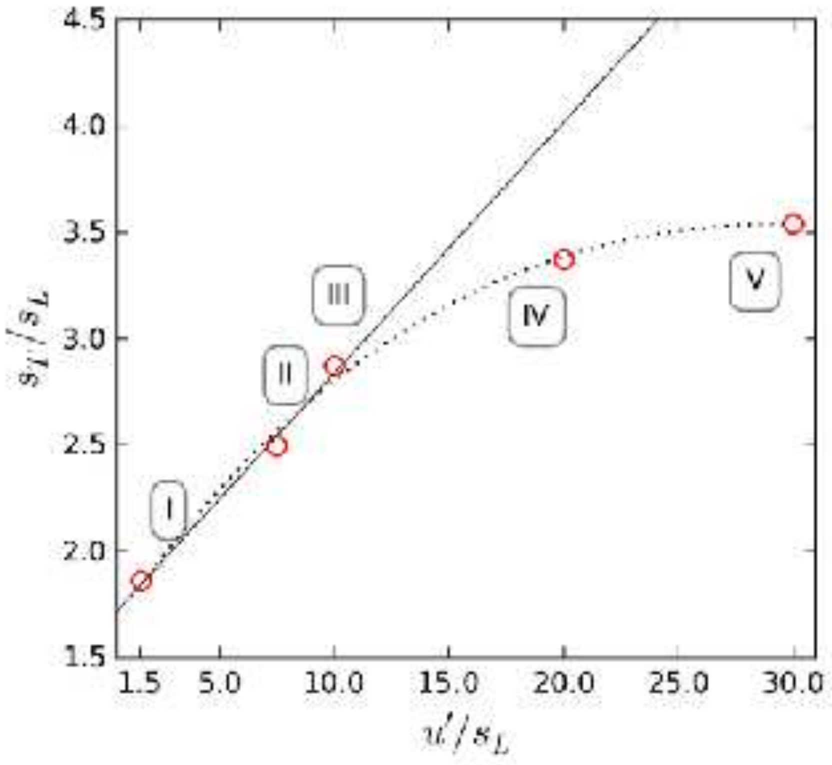
[1] Bradley, Lau and and Lawes (1992) Phil. Trans. R. Soc. London

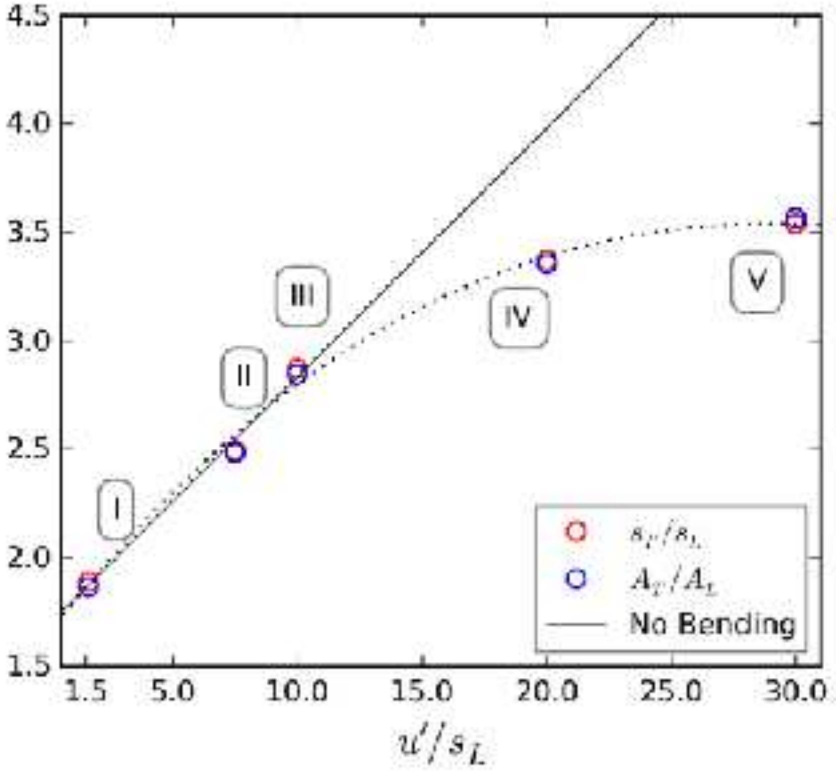
[2] Bagdanavicius et al. (2015) Combustion and Flame

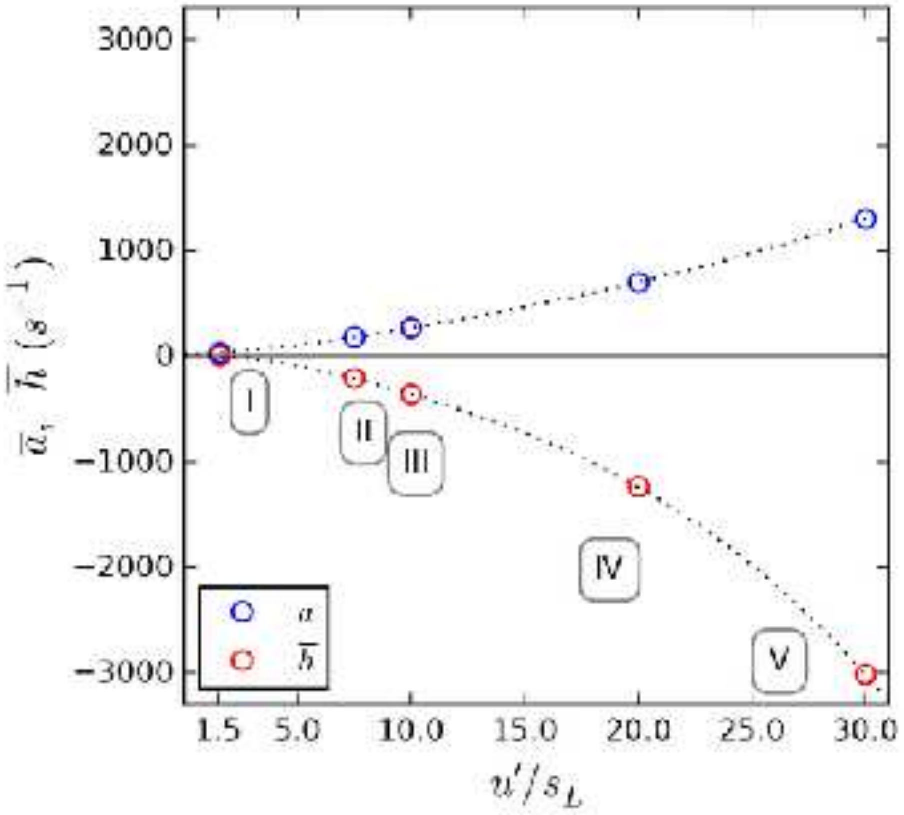
Bending effect: the Cambridge argument

More recently, experimental measurements obtained by several researchers[1] have failed to record local extinctions – alternative explanations have since been proposed[2].

One such explanation has emerged from a parametric DNS investigation conducted in Cambridge[3].







The Cambridge DNS investigation[3] shows that **negative mean curvatures** outweigh the effects of positive ones and of the overall extensive strain at increased levels of turbulence.

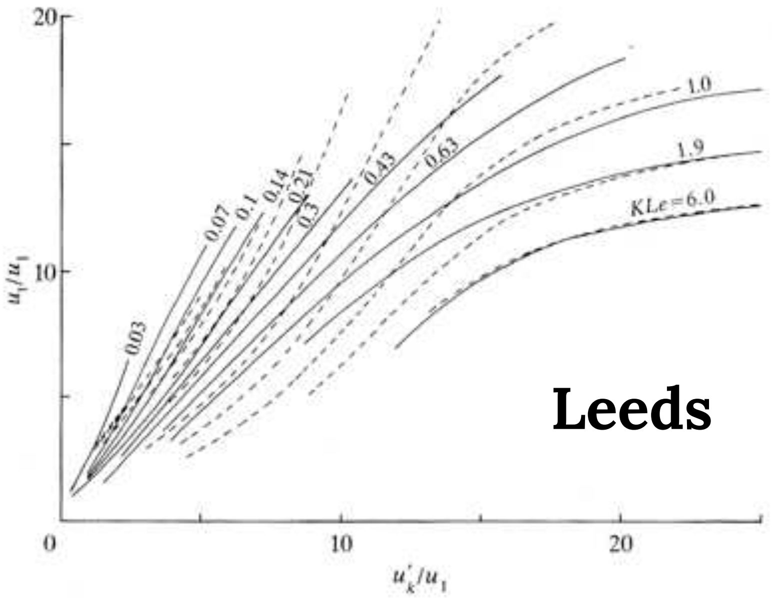
[1] Driscoll, J. (2008) *Progress in Energy and Combustion Science*

[2] Wabel et al. (2017), Proceedings of the Combustion Institute 36

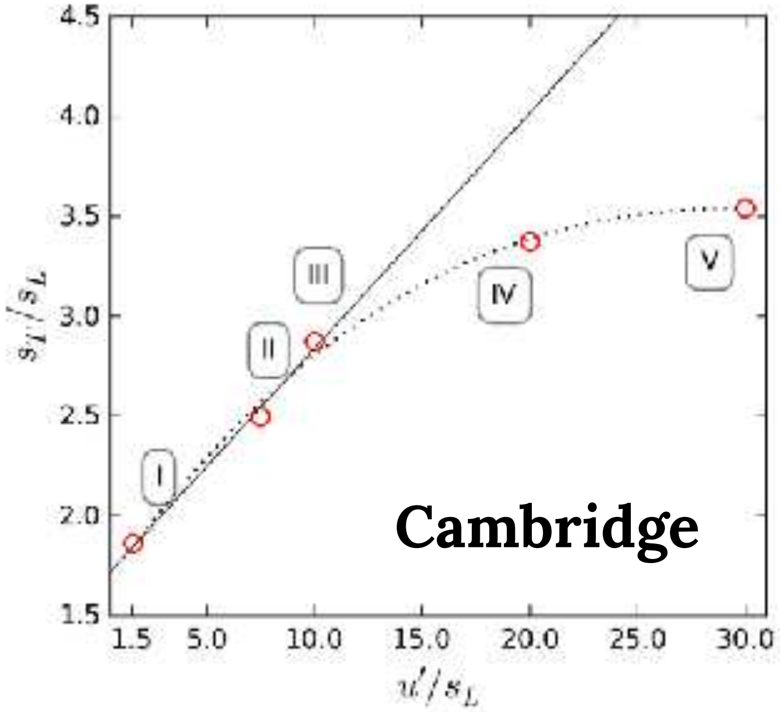
[3] Nivarti, G. V. and Cant, R. S. (2017) Proceedings of the Combustion Institute 36

Bending effect: open questions

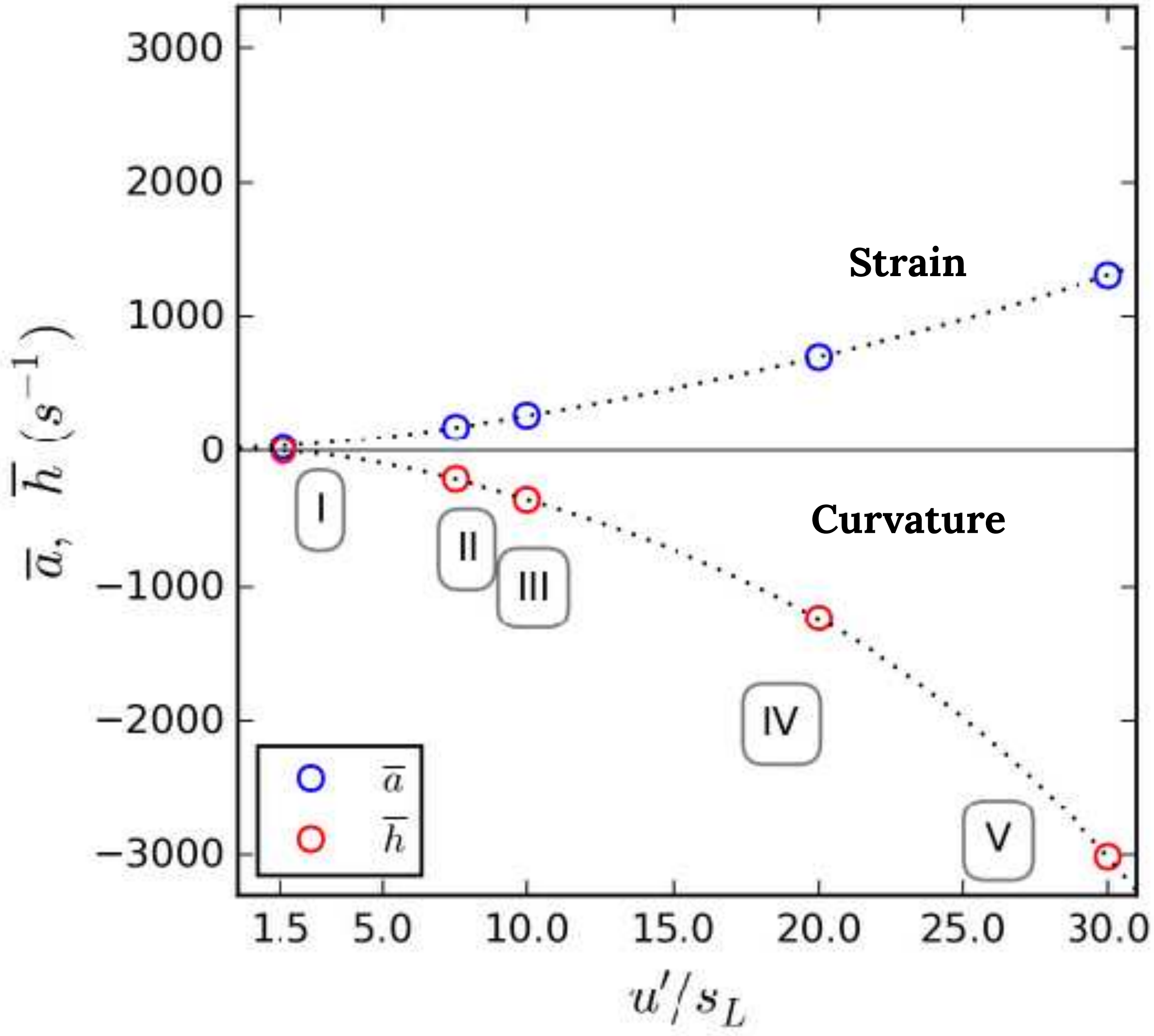
What initiates bending?



Leeds



Cambridge

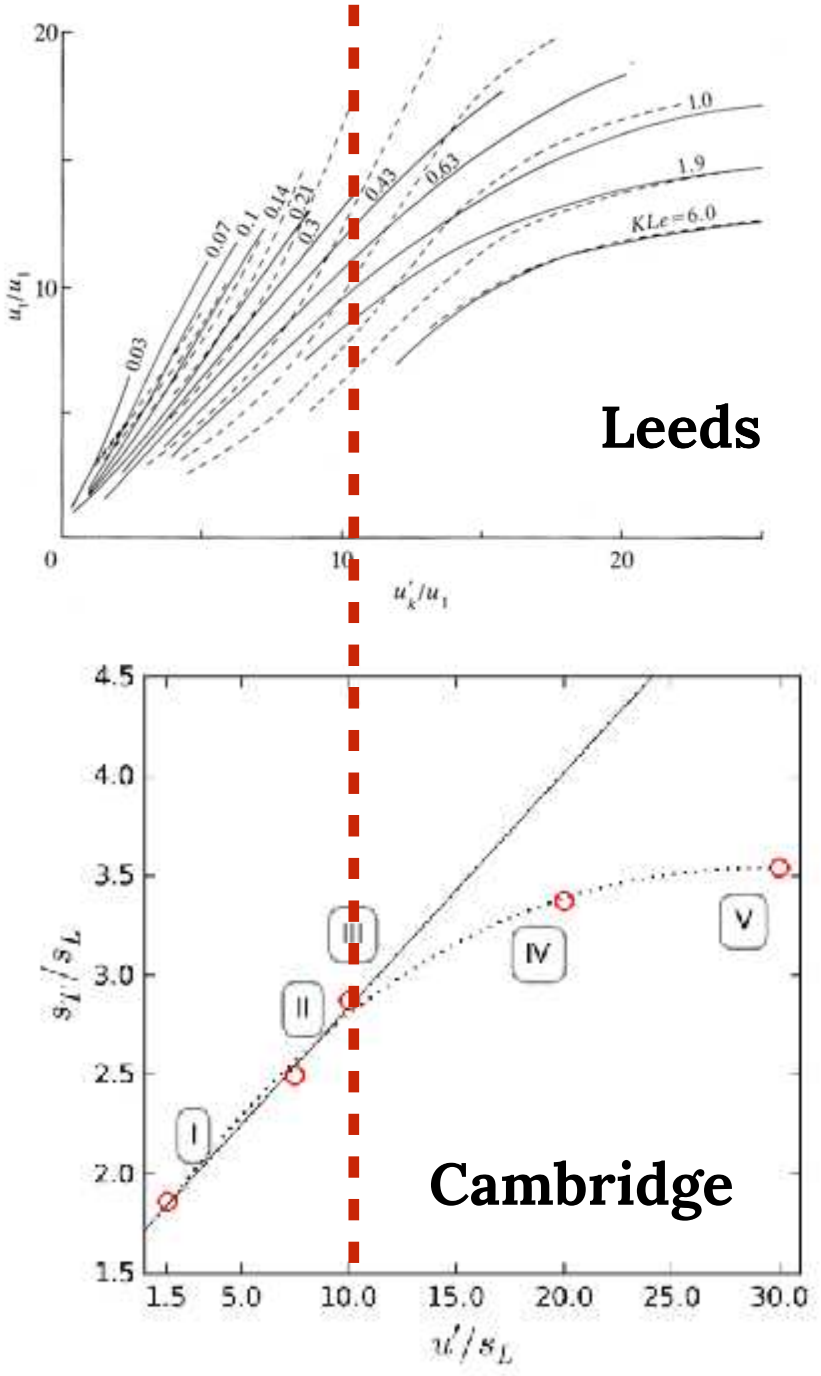


Strain

Curvature

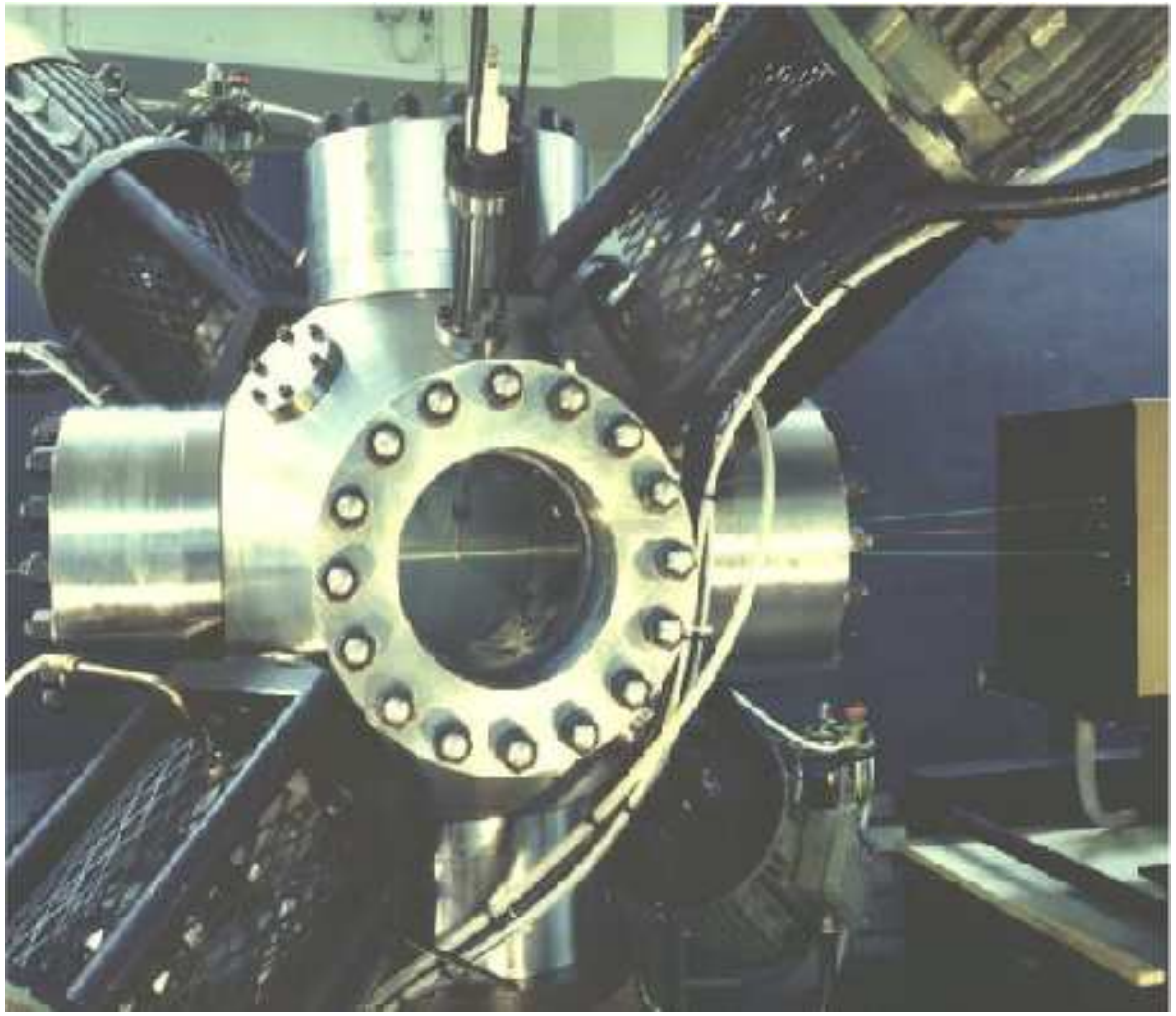
Is bending a result of local extinctions from excessive straining
or does it result from flame surface destruction due to increased negative curvature?

Bending Effect: Leeds-Cambridge comparison

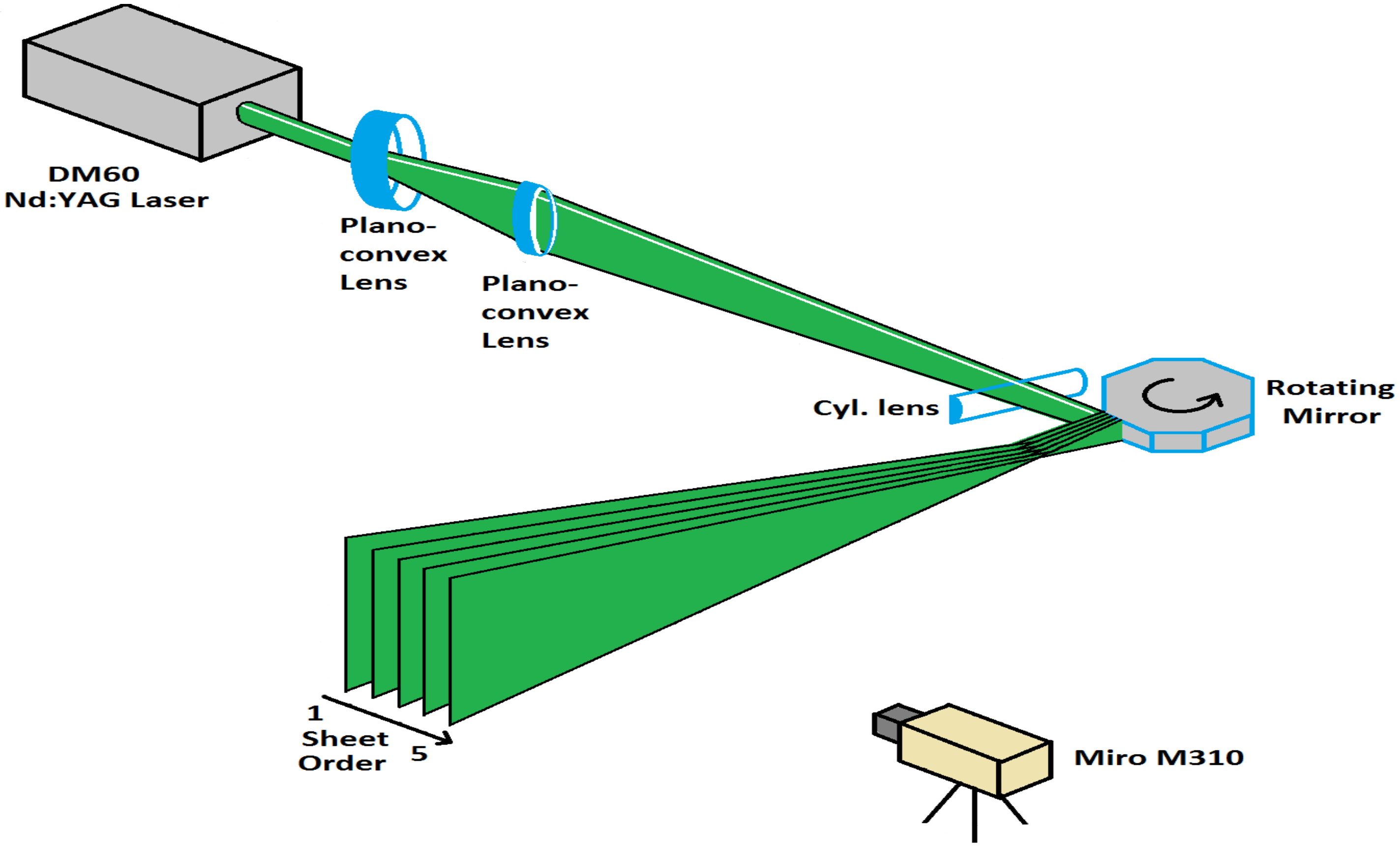


In order to resolve this question, flame propagation behaviour as observed in experiments is compared with DNS results at similar turbulence levels.

Leeds-Cambridge comparison: fan-stirred bomb

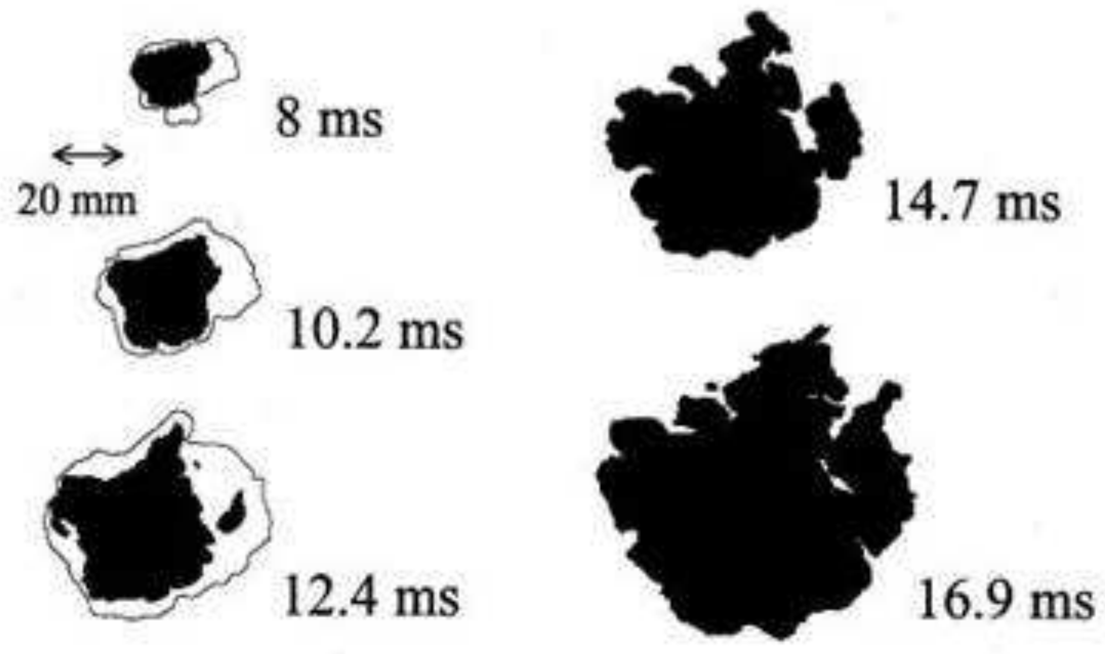


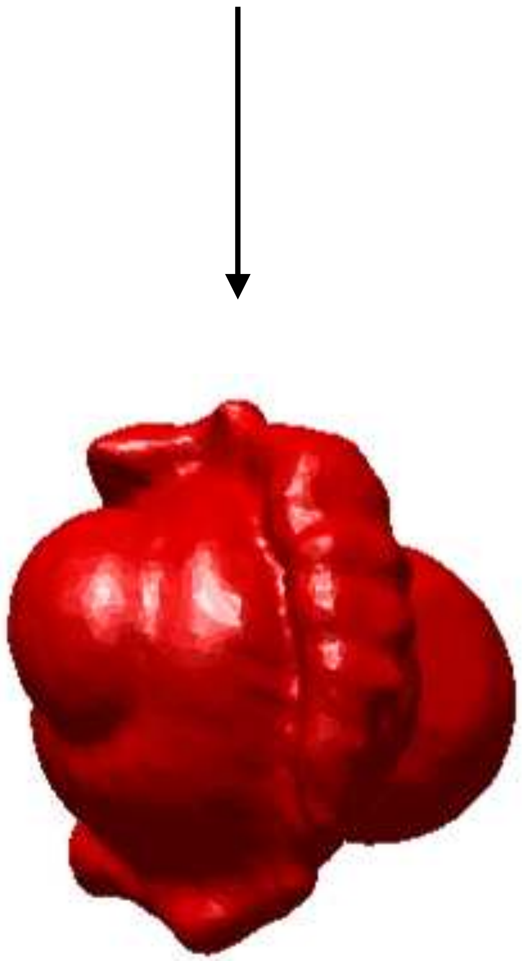
Bomb with multiple quartz windows



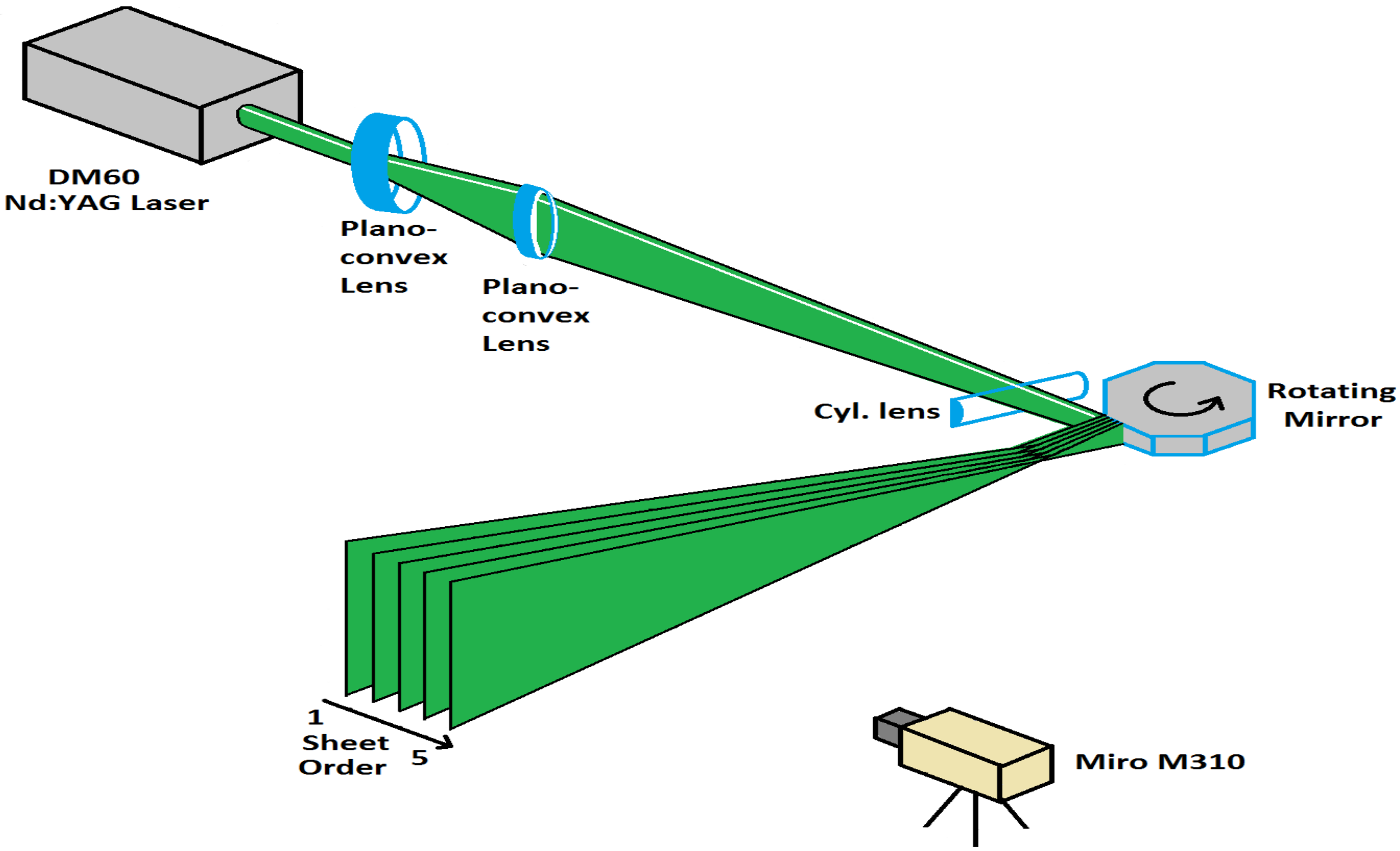
Swinging Laser Sheet for 3D imaging

Leeds-Cambridge comparison: fan-stirred bomb



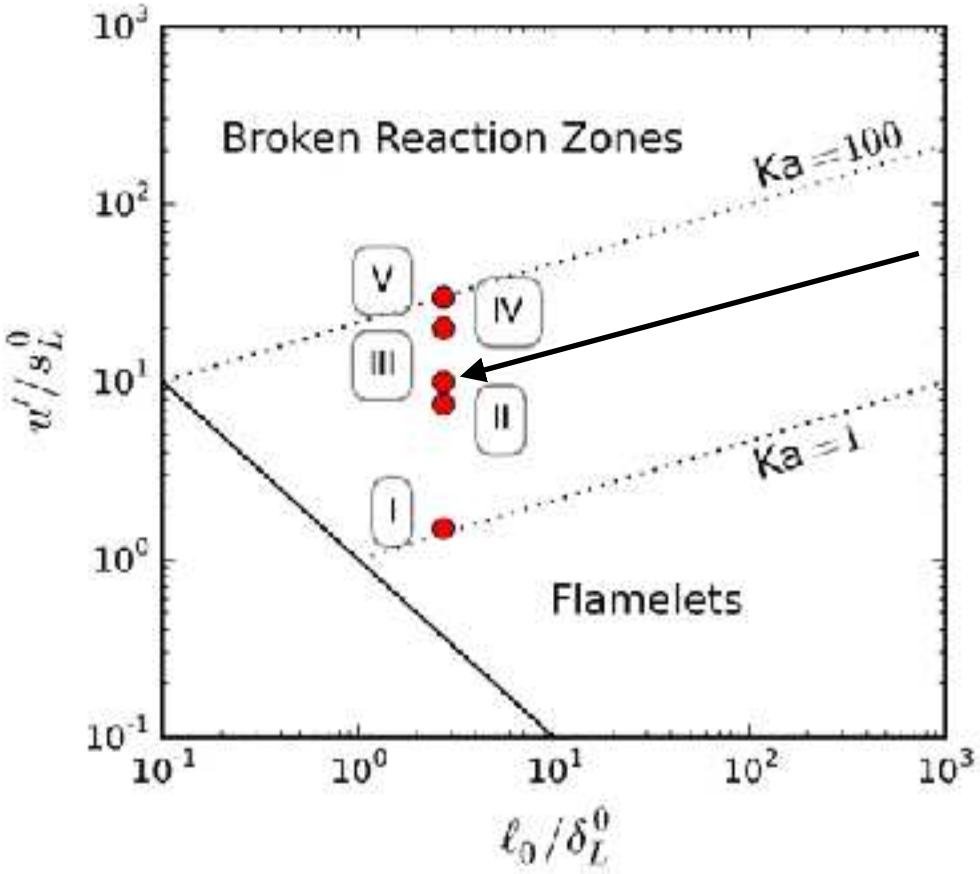


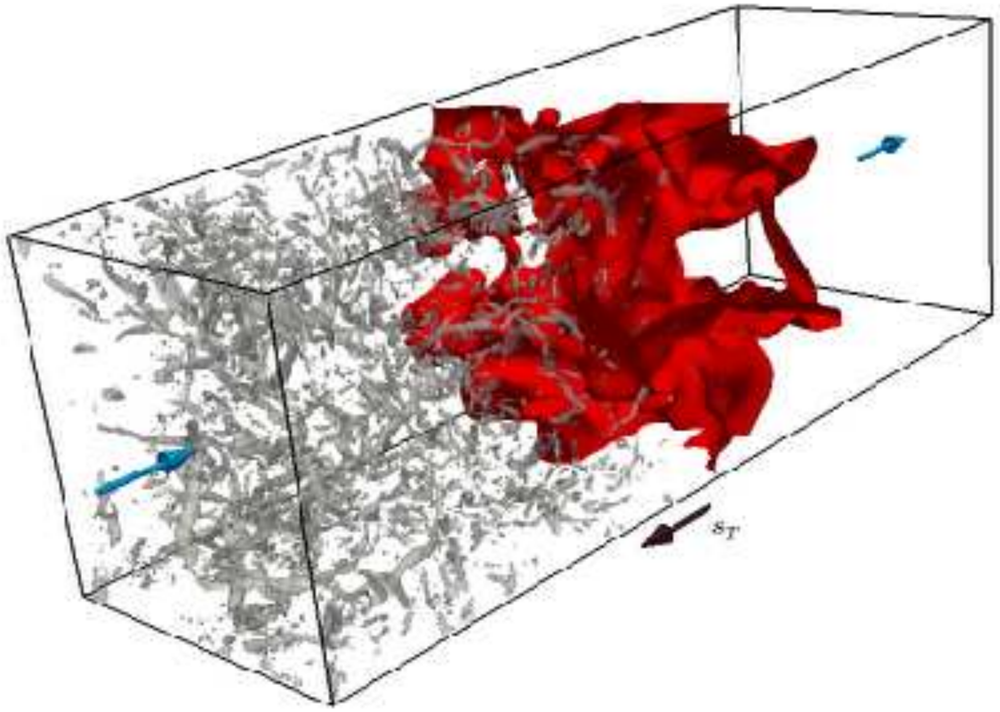
Laser excited particles in unburned mixture obtaining multiple slices at the same stage of flame propagation.



The slices obtained at a given instant are processed to reconstruct the 3D flame surface.

Leeds-Cambridge comparison: old DNS study





DNS code: Senga2

Compressible Navier-Stokes equations with no forcing

Difference Scheme: 10^{th} order finite difference

Time-marching: 4^{th} order explicit Runge-Kutta

Adaptive time-step size PID controller

Boundary conditions: NSCBC with LODI assumption

Grid: 288 x 96 x 96 in 0.015m x 0.005m x 0.005m

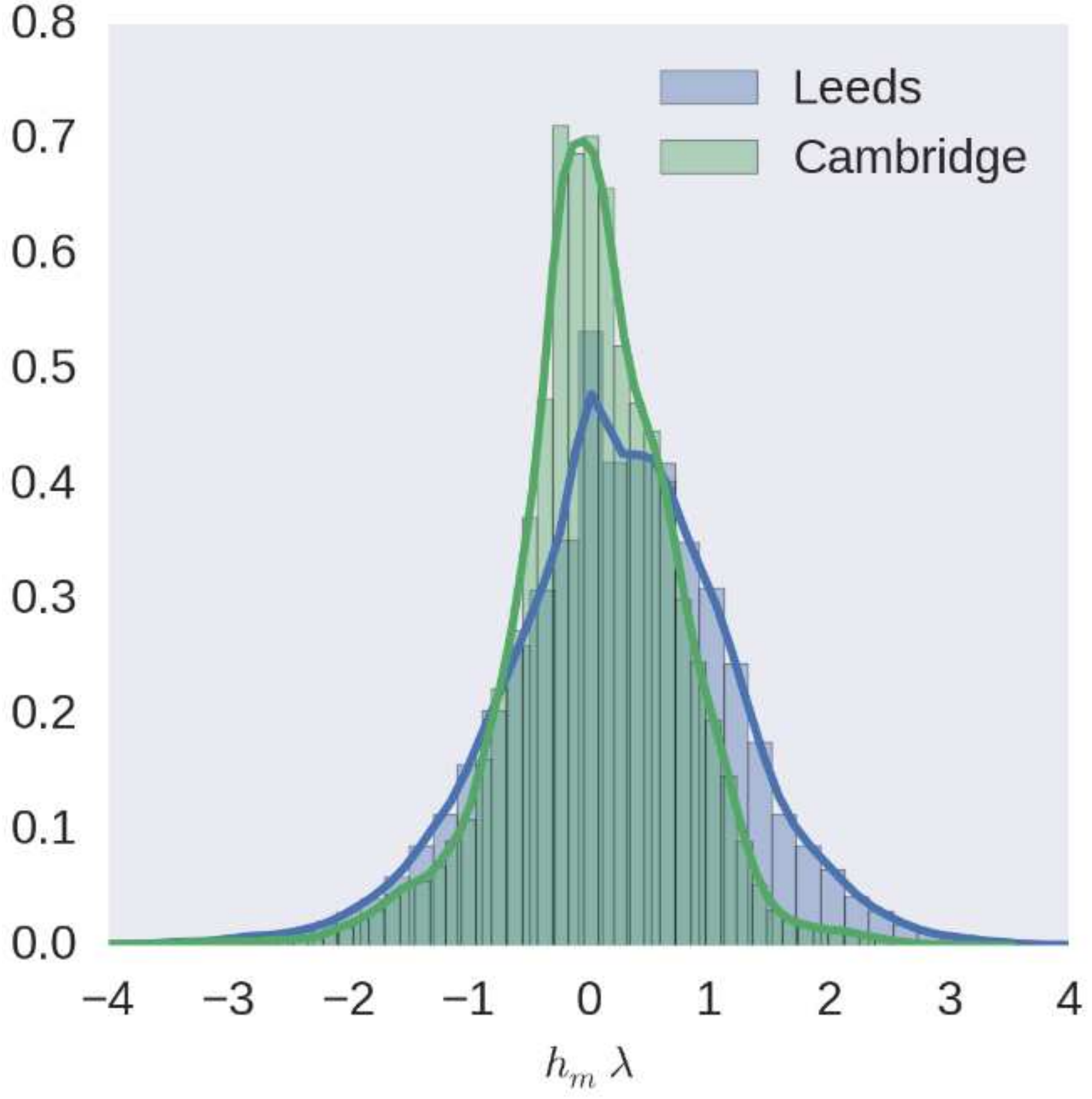
Chemistry: single-step Arrhenius, stoichiometric mixture

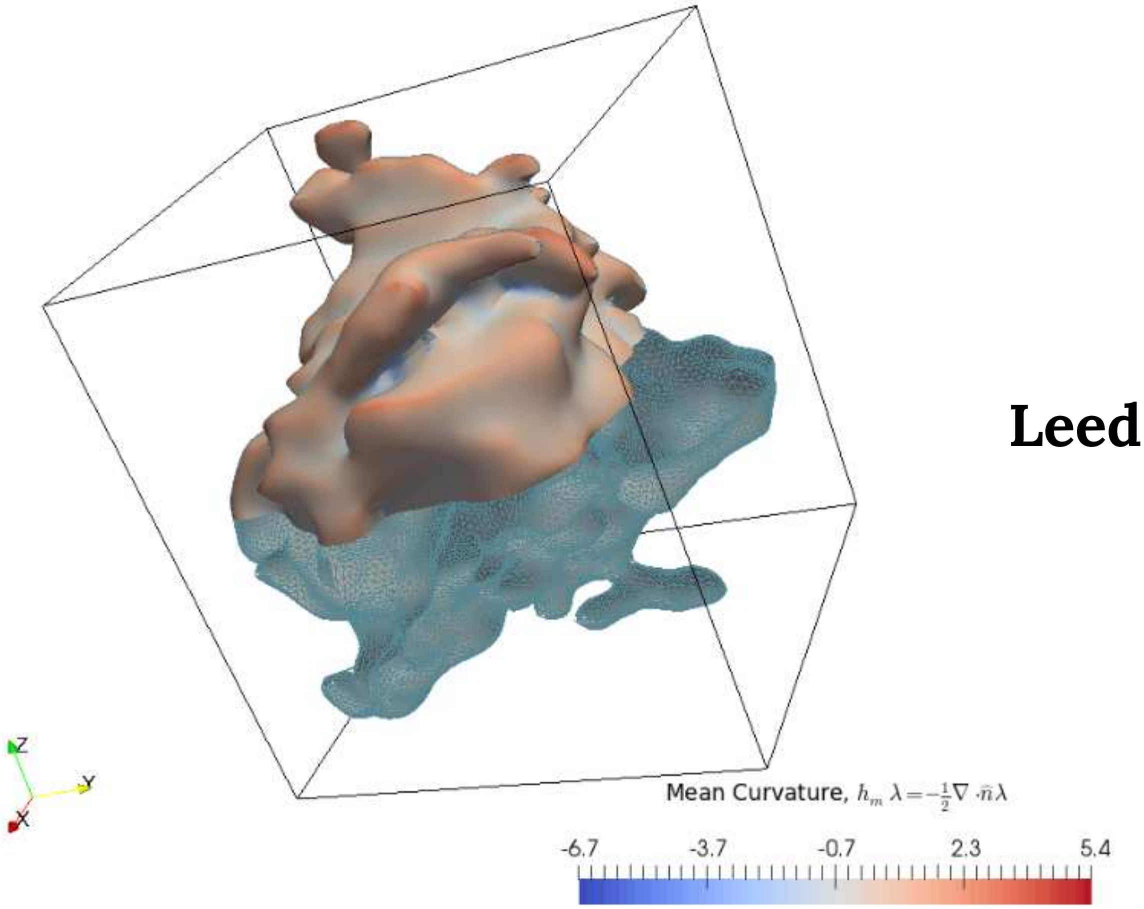
Nivarti, G. V. and Cant, R. S. (2017) Proceedings of the Combustion Institute 36

Leeds-Cambridge comparison: reconstructed iso-surfaces

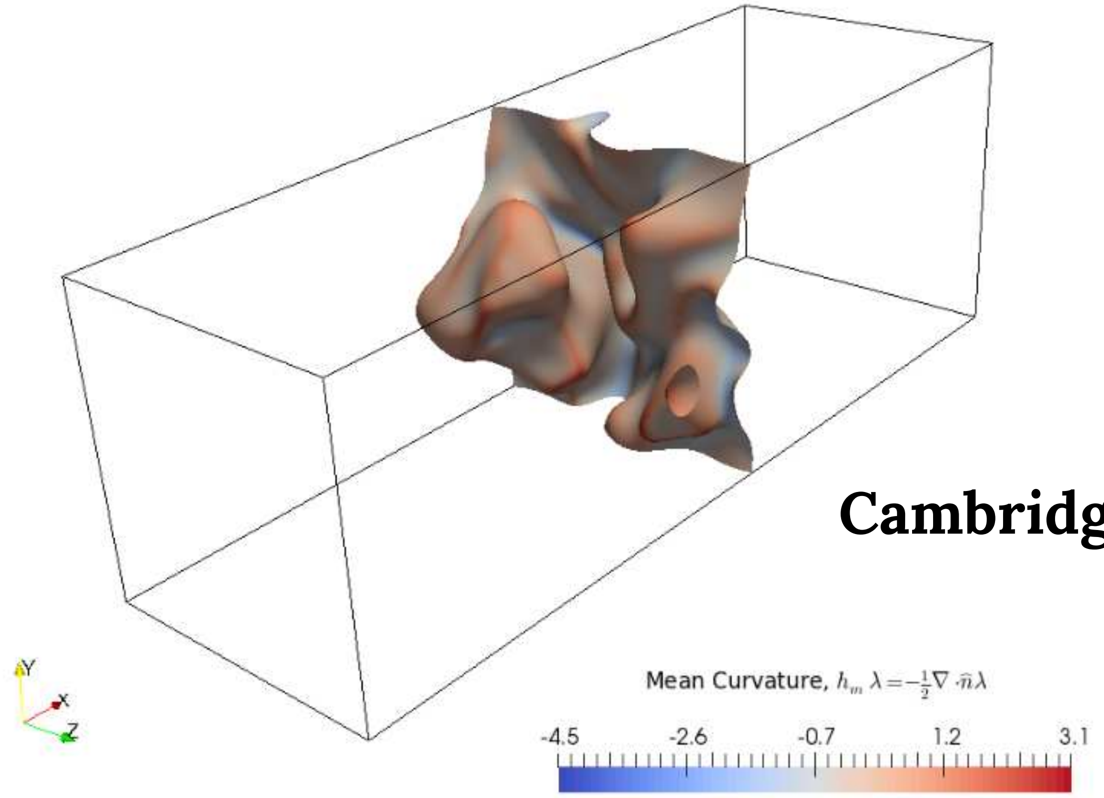
$u' = 10 s_L$

stoichiometric flames



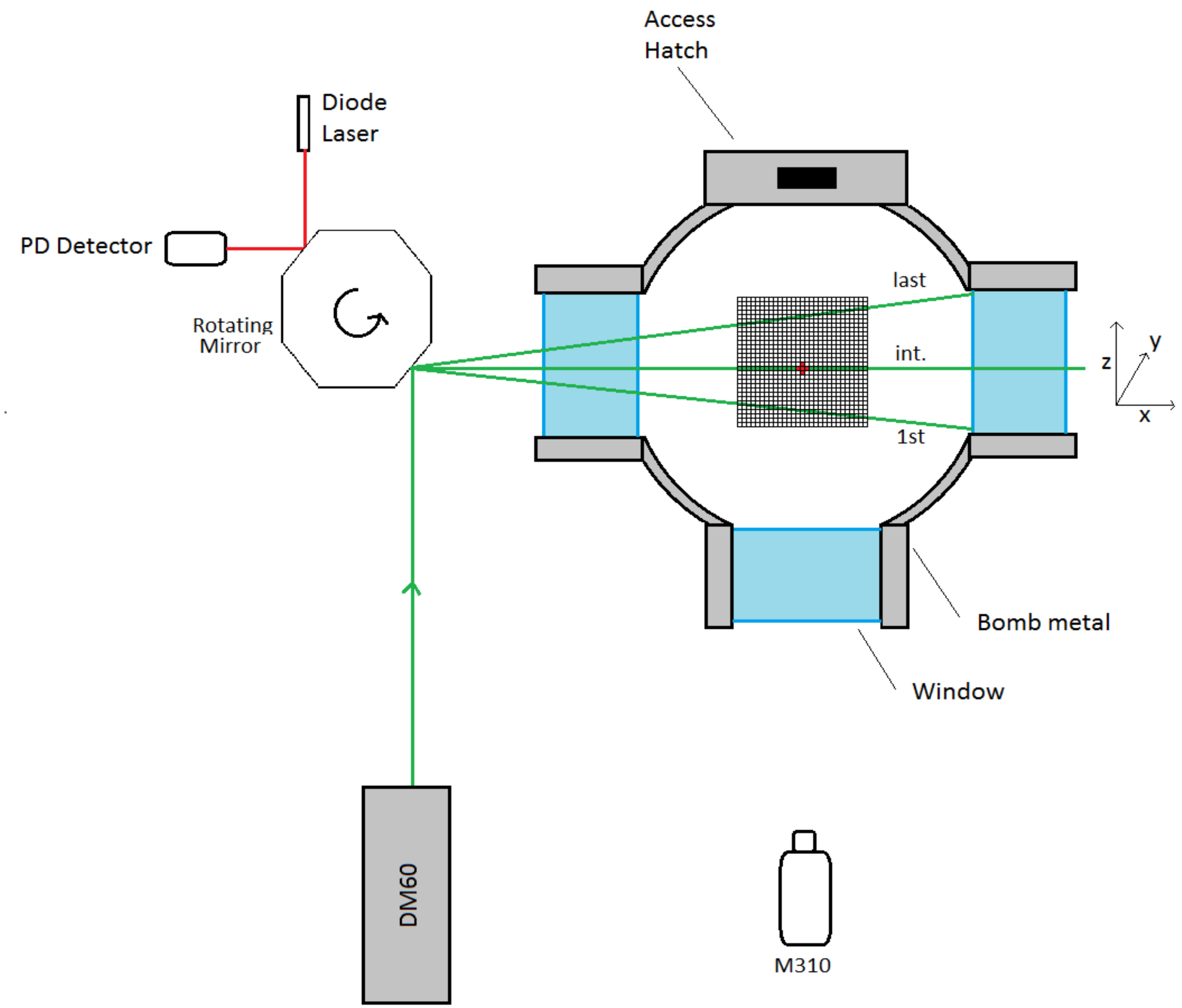


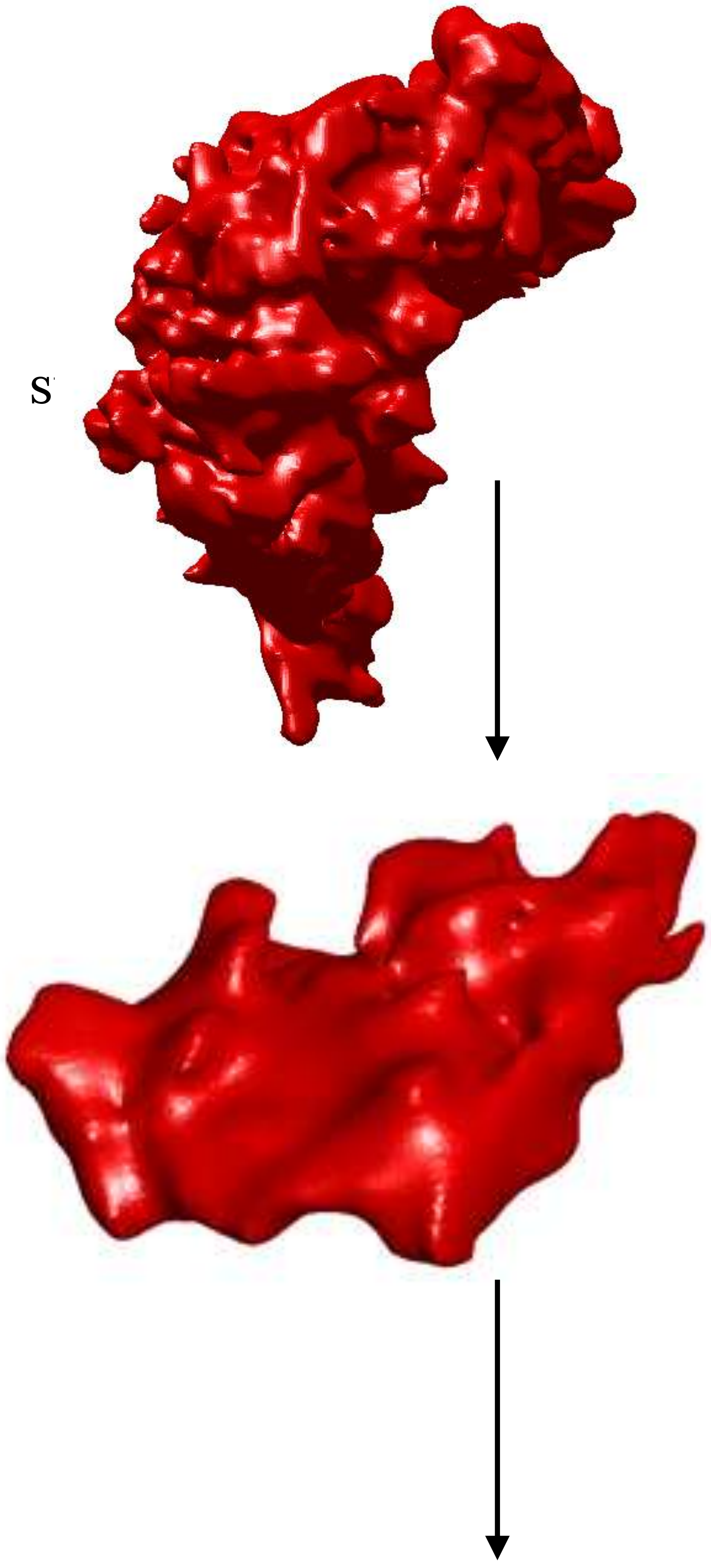
Leeds



Cambridge

Leeds-Cambridge comparison: reconstructed iso-surfaces

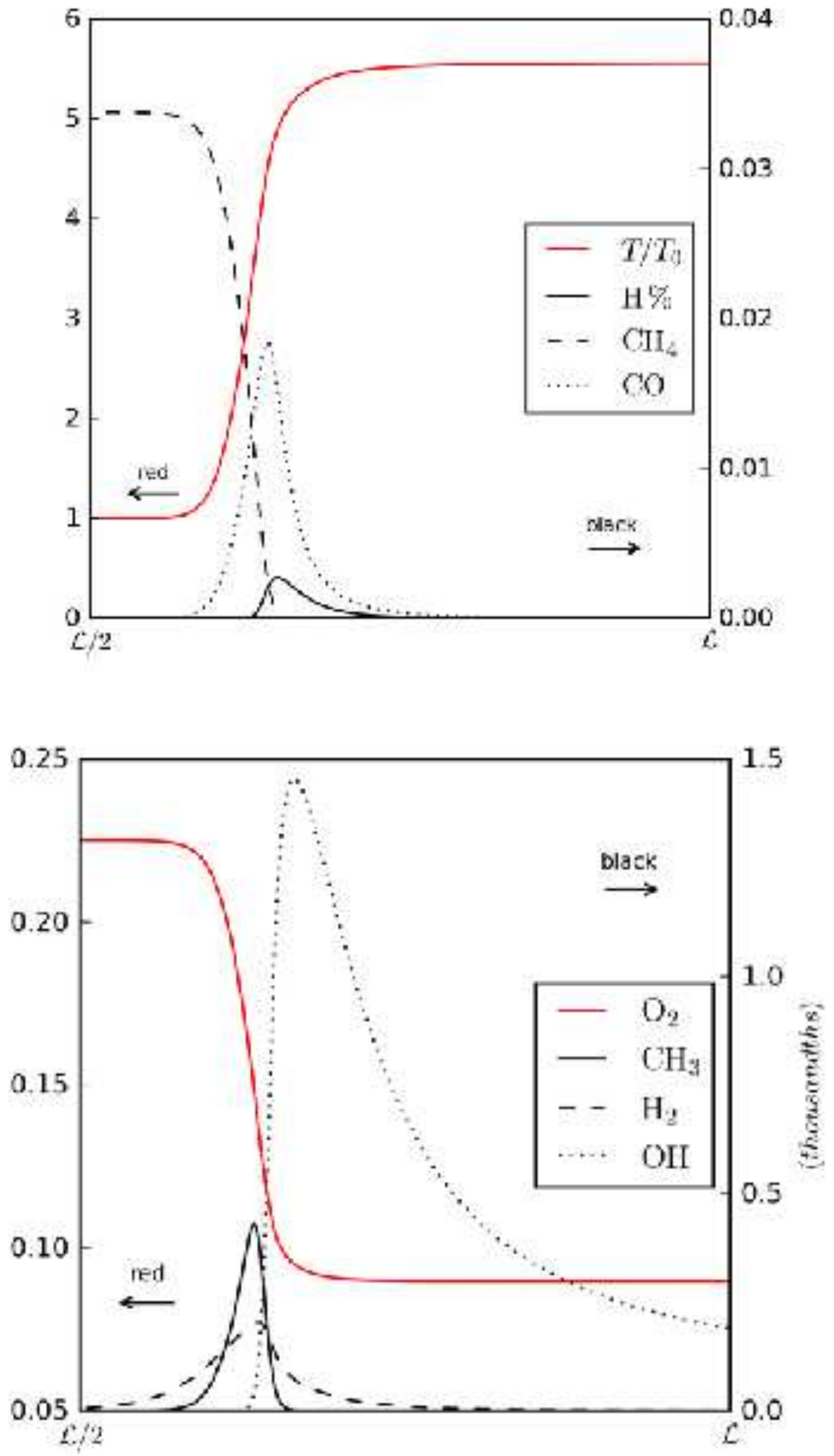




Stoichiometric methane-air flames are too fast for faithful reconstruction of 3D isosurfaces. Hence, a slower lean flame with methane-air ER = 0.6 is studied instead.

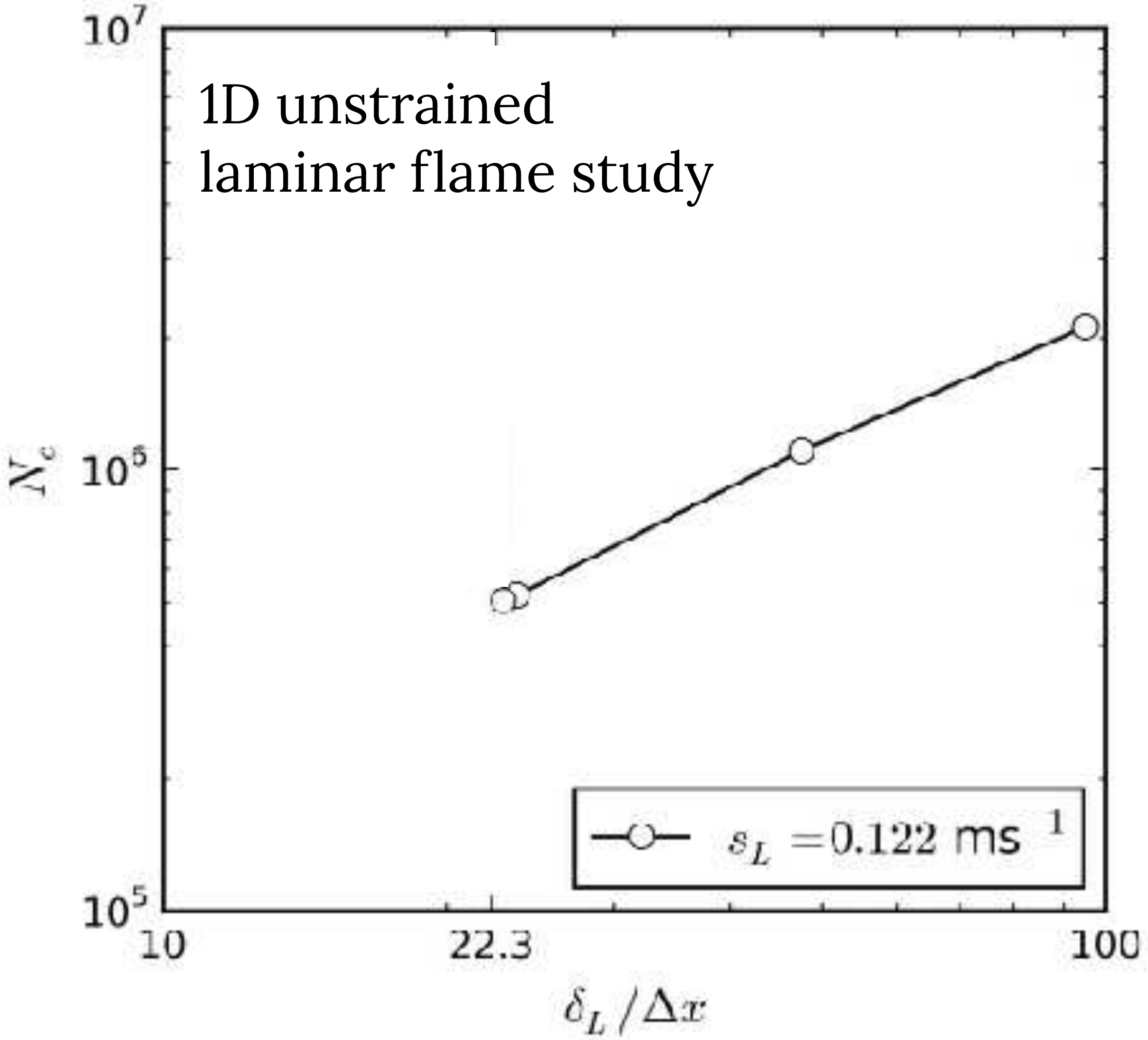
no image

DNS modifications: (1) multi-step chemistry



Chemical kinetic pathways modelled using a 25-step, 16 species mechanism[1].

The mechanism allows chemical structure of a lean methane-air flame to be represented faithfully when resolved using more than ~23 points within the flame.


1D unstrained laminar flame study

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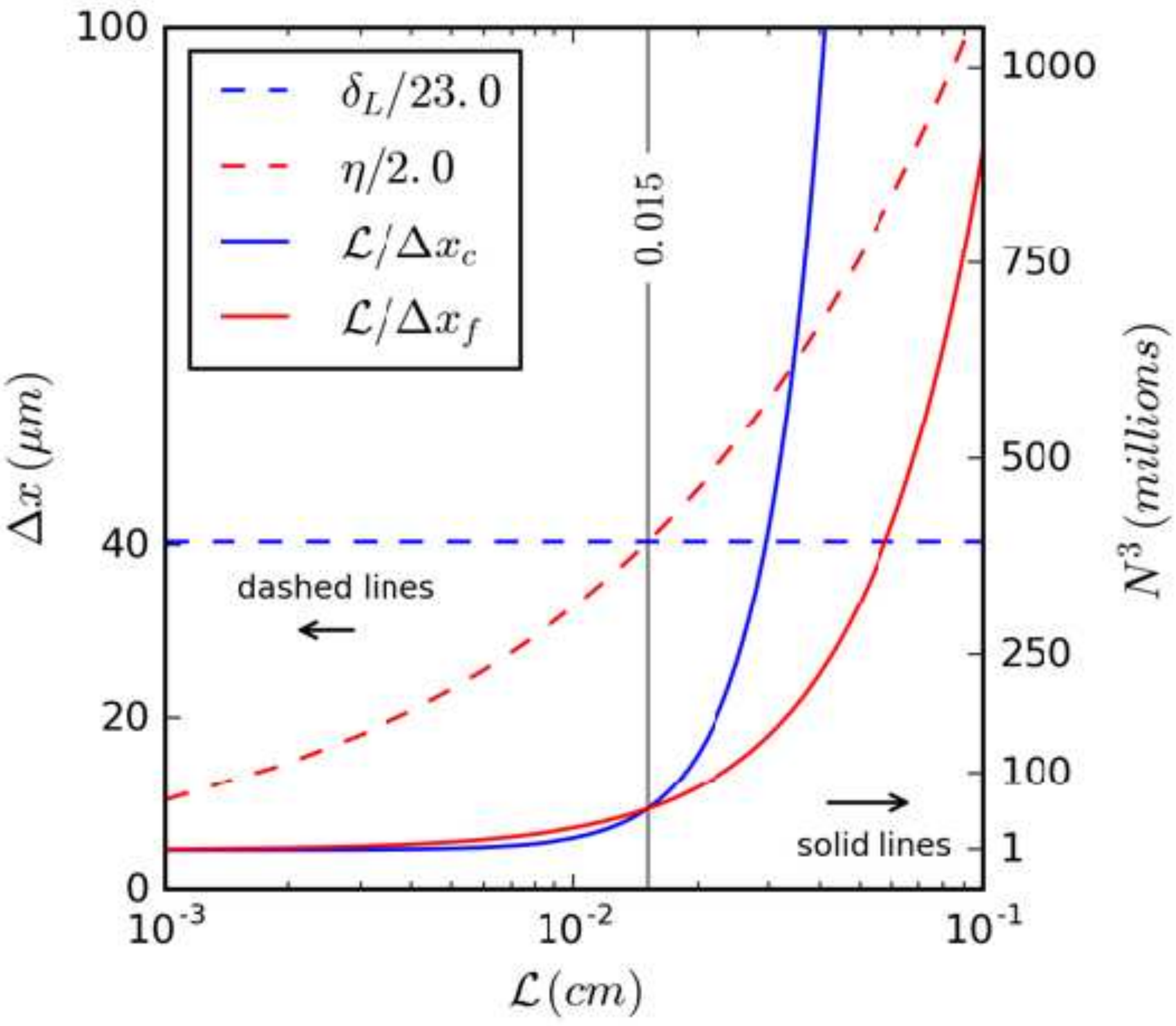
[1] Smooke, M. and Giovangigli, V (1991) Lecture Notes in Physics 384

DNS modifications: (2) domain and grid size



Dashed lines show resolution constraints due to **chemistry**, and due to **turbulence microsclaes**.

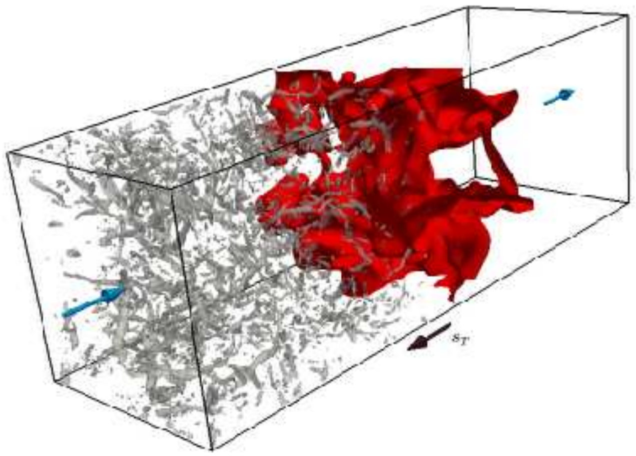
Solid lines show computational costs incurred upon resolving these constraints respectively.

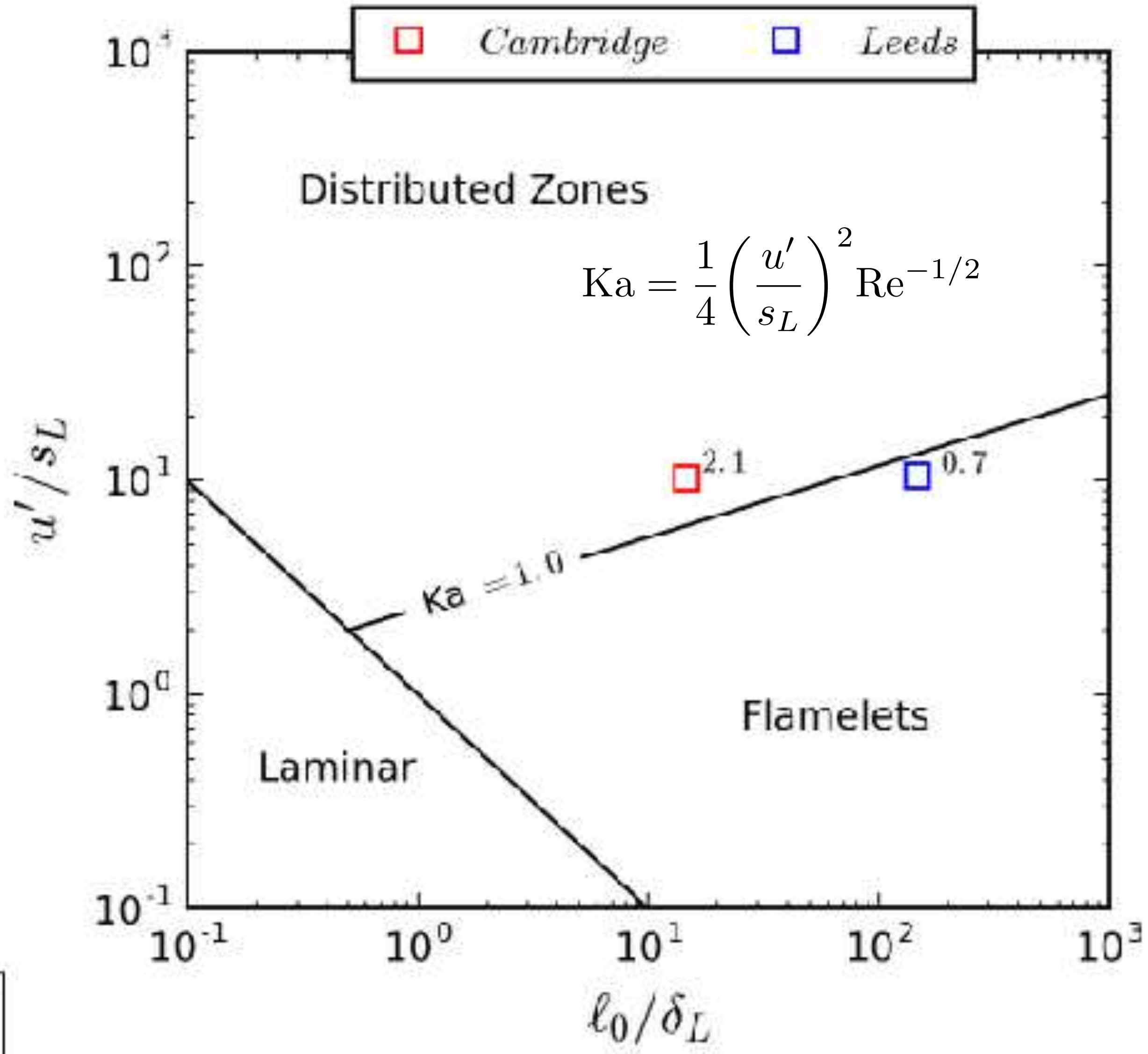
The largest size of the domain that allows feasible computations is 1.5 cm (width). This corresponds approximately to 2mm integral length scale.

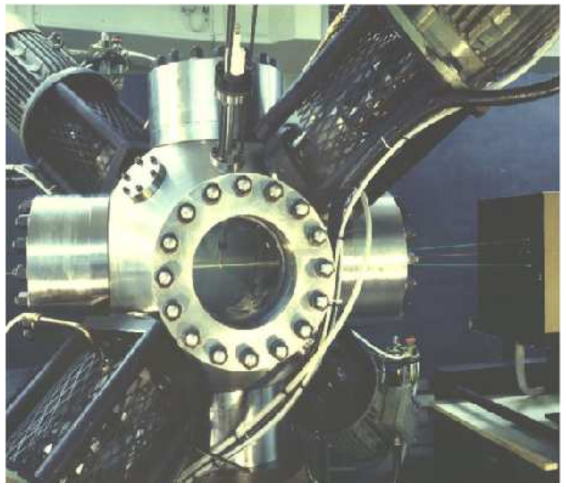
As large a domain size as possible is chosen so as to

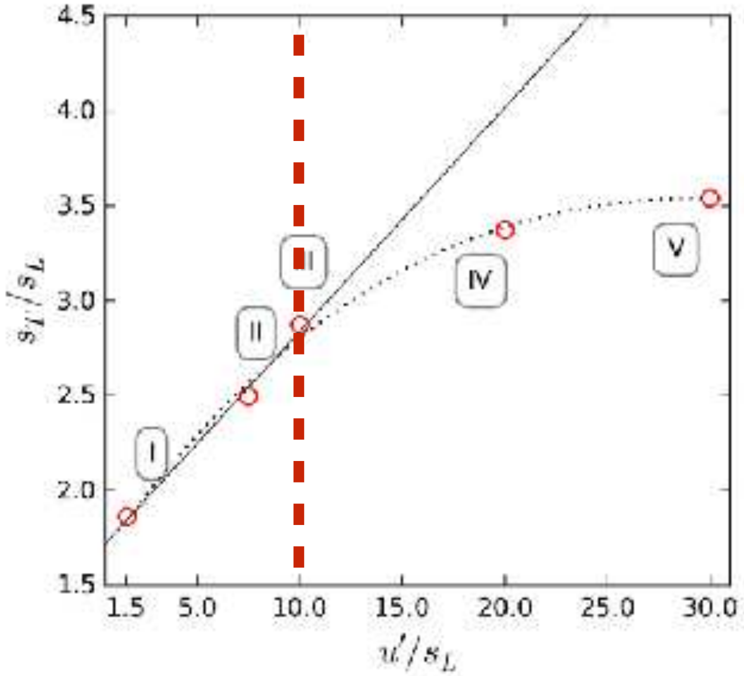
a) increase size of integral length scale with respect to flame thickness
b) have multiple such integral length scales in the domain interact with the flame

Leeds-Cambridge comparison: present DNS study









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Boundary conditions: NSCBC with LODI assumption

Grid: 816 x (408 x 408) in **3** cm x (1.5 cm)^2

Chemistry: 25-step, 16 species with ER = 0.6 (lean)

DNS modifications: (3) adaptive time-step control

PID Control[1]

$$\Delta t^{(n+1)} = \Delta t^{(n)} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n+1}}\right)^{\alpha} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n}}\right)^{\beta} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n-1}}\right)^{\gamma}$$

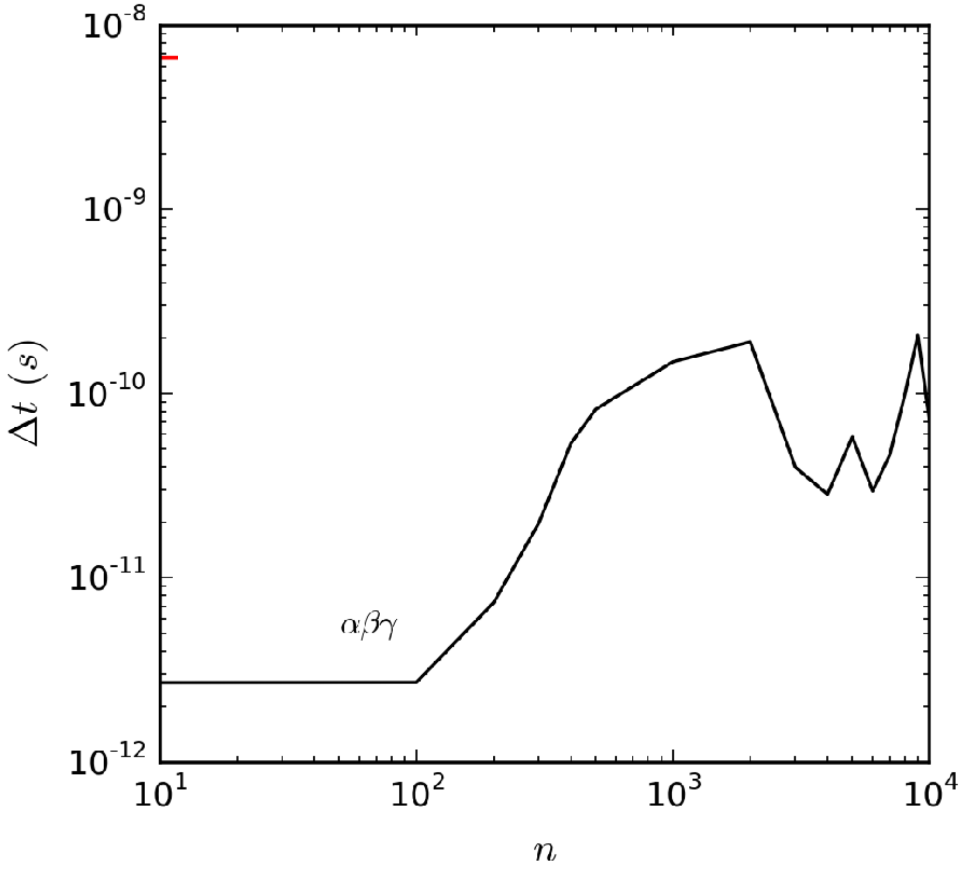
$\widehat{\epsilon}$	pre-specified error **tolerance**
$\widehat{r}_n$	solution **error estimate**
$\alpha\beta\gamma$	controller **exponents**

An adaptive time-stepper is used to ensure that the solution error is retained within a pre-specified tolerance.

This comes with the problem of providing error estimates for the global solution.

Time steps are inhibitive still.

3D flame simulation



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[1] Kennedy, C. A. and Carpenter, M. H. (2003) Applied Numerical Mathematics

DNS modifications: (3) adaptive time-step control

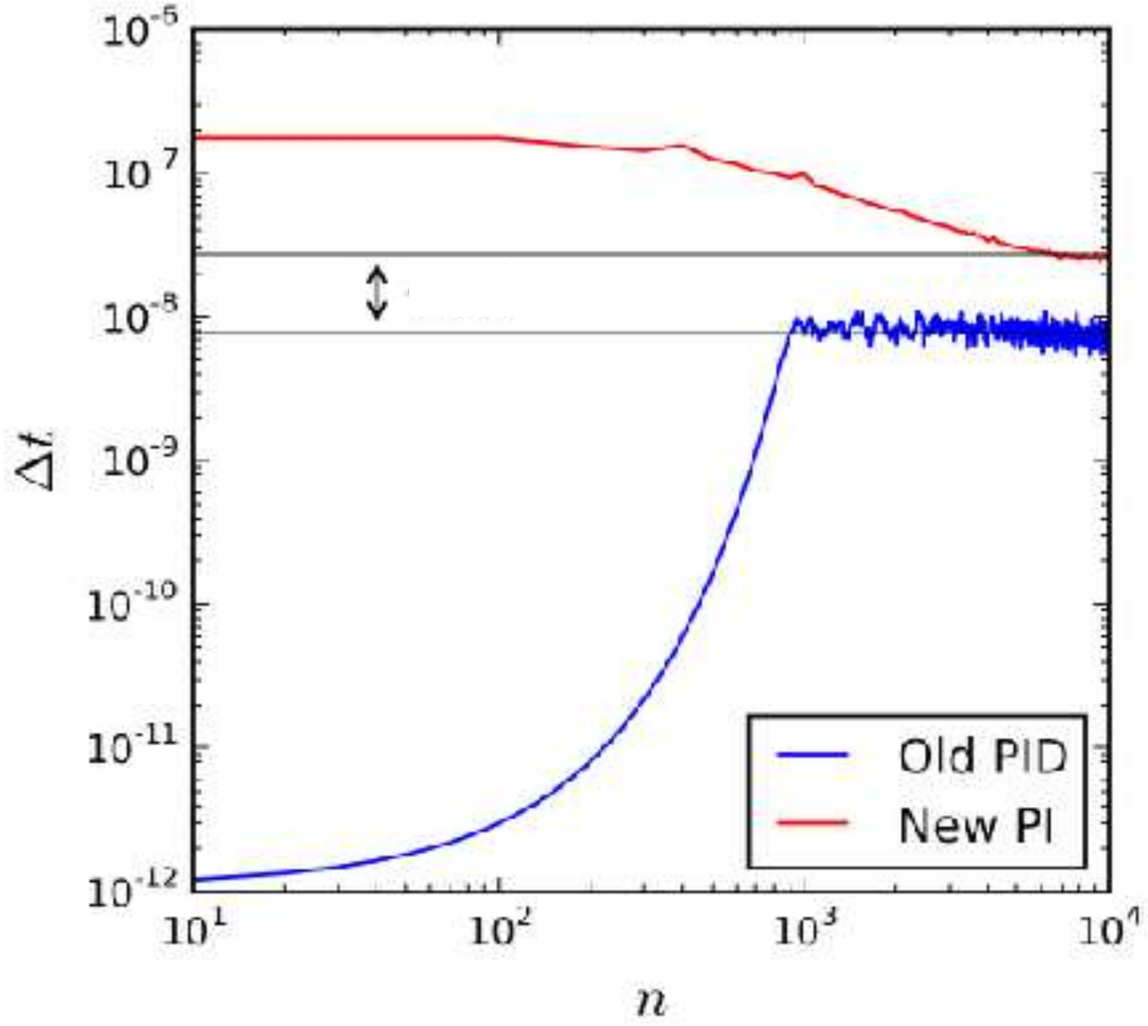
Old PID Control

$$\Delta t^{(n+1)} = \Delta t^{(n)} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n+1}}\right)^{\alpha} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n}}\right)^{\beta} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n-1}}\right)^{\gamma}$$

New PI Control

$$\Delta t^{(n+1)} = \Delta t^{(n)} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n}}\right)^{\beta *} \left(\frac{\widehat{\epsilon}}{\widehat{r}_{n-1}}\right)^{\gamma *}$$

1D laminar flame study



$\widehat{r}_n$ the error estimate is an un-normalised maximum of local error vector norms.

$\widehat{\epsilon}$ solution tolerance is maintained

initial time step is maintained,
but no bounds on maximum step ratios.

$\beta \gamma$ exponents 0.6 and -0.2

[1] Kennedy, C. A. and Carpenter, M. H. (2003) Applied Numerical Mathematics **44**

[2] Söderlind, G and Wang, L. (2006) J. Comp and Appl. Math. **185**

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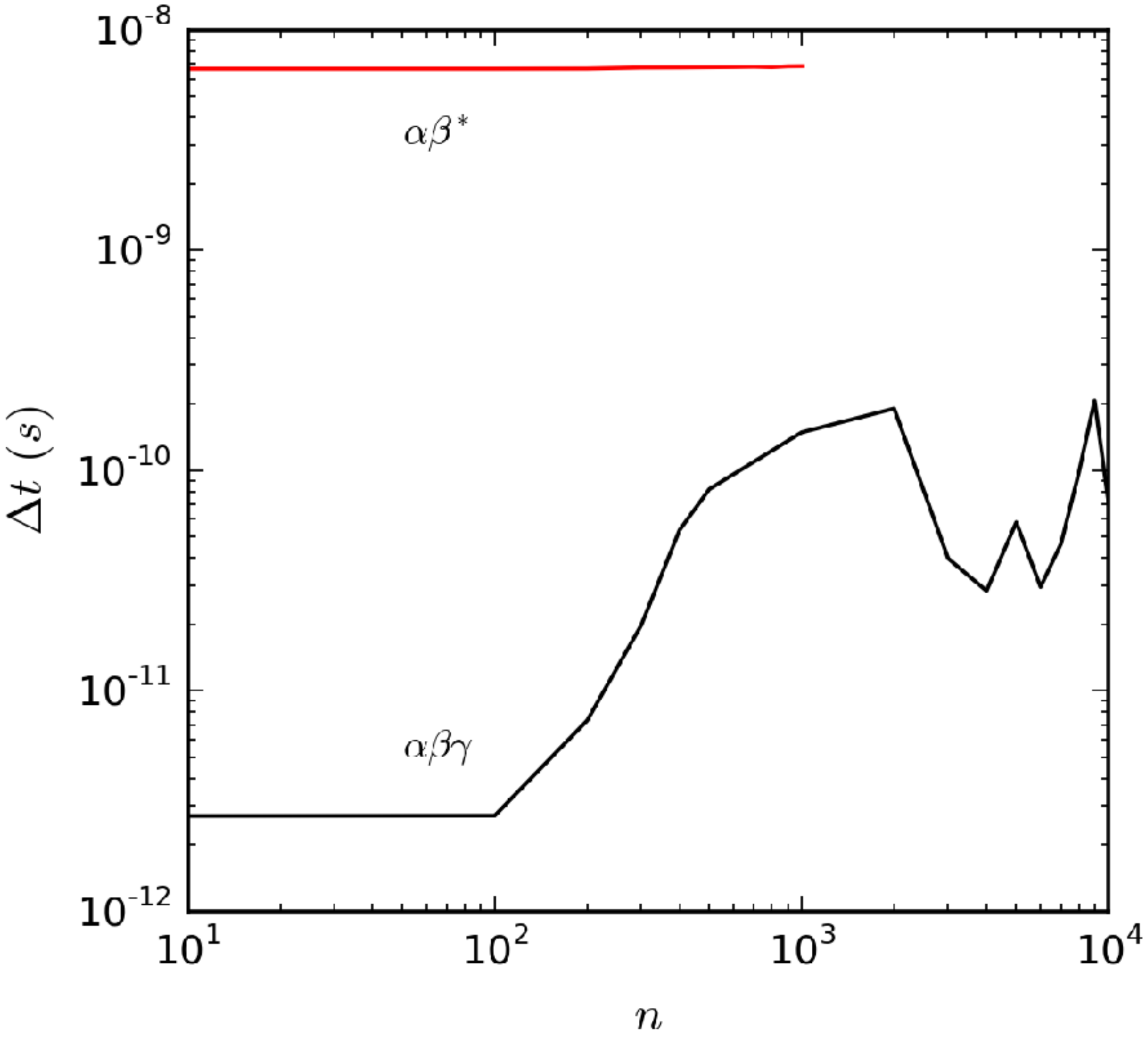
3D flame simulation



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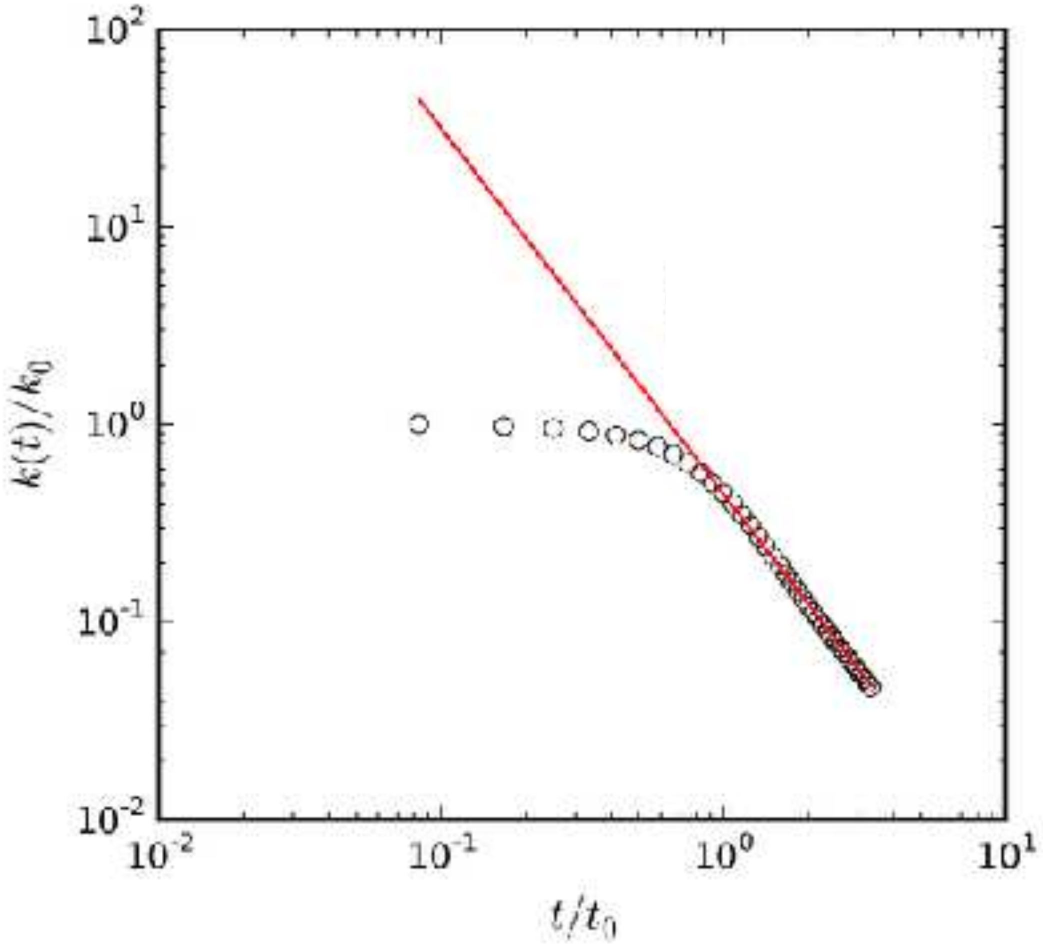
DNS modifications: (4) linear turbulence forcing

In the absence of any turbulence forcing
the turbulent kinetic energy
decays exponentially in a homogeneous
isotropic turbulence case

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho\langle u_k u_k\rangle\right) = -\rho\epsilon$$



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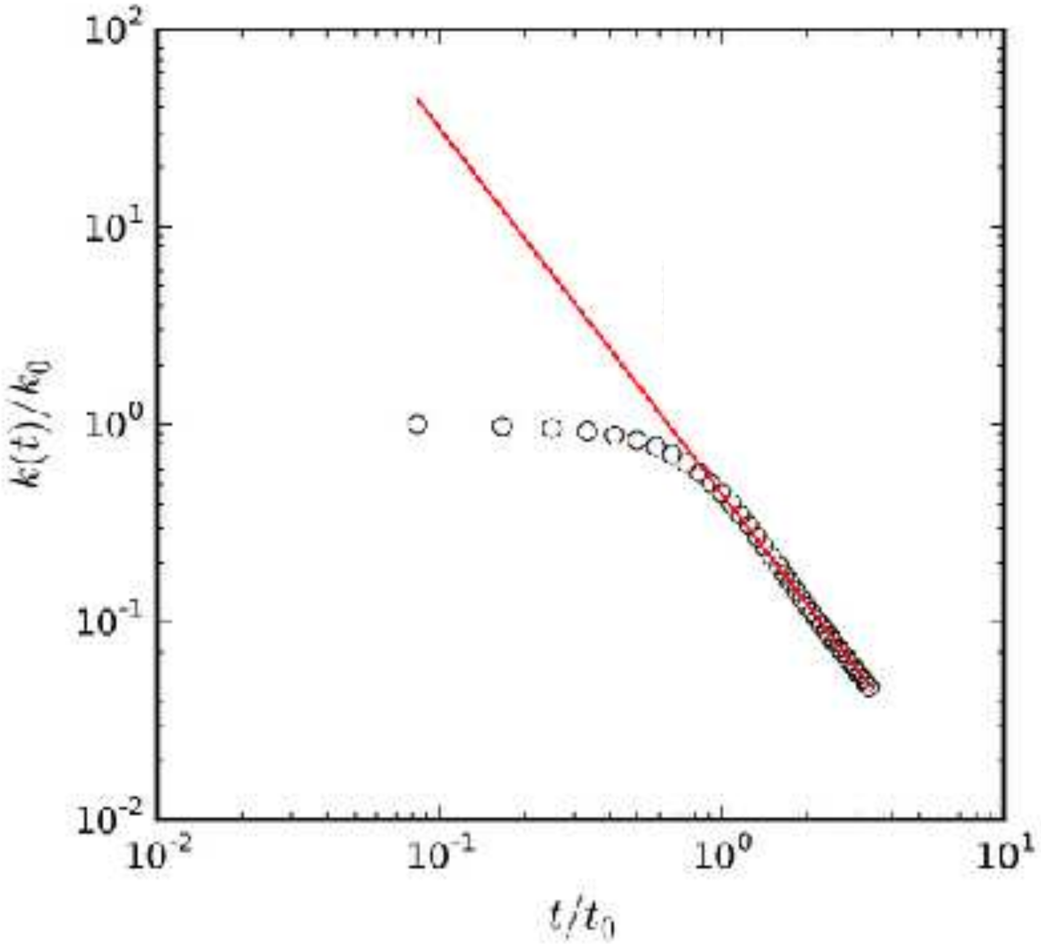
Chemistry: 25-step, 16 species with ER = 0.6 (lean)

DNS modifications: (4) linear turbulence forcing

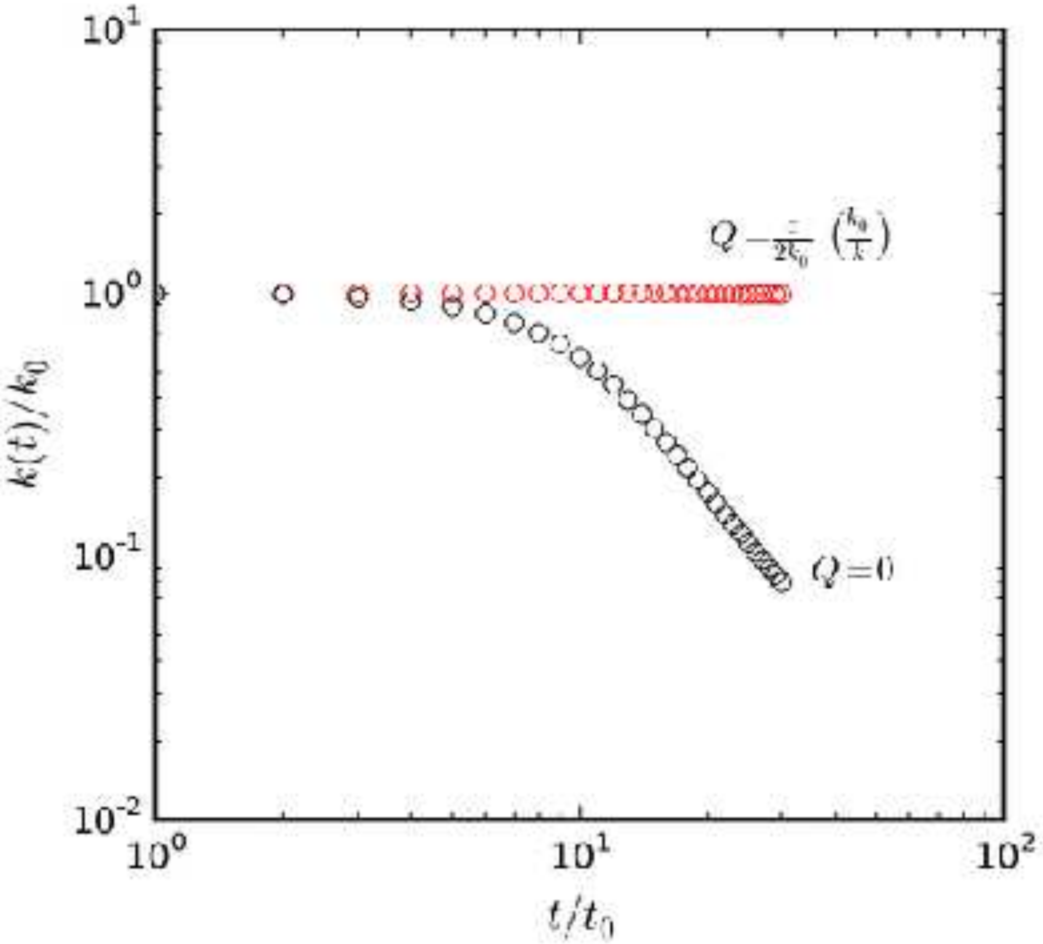
In the absence of any turbulence forcing the turbulent kinetic energy decays exponentially in a homogeneous isotropic turbulence case

$$\frac{\partial}{\partial t}\left(\cancelto{\sim 0}{\frac{1}{2}\rho\langle u_k u_k\rangle}\right) = -\rho\epsilon + Q\rho\langle u_k u_k\rangle$$



A forcing strategy was proposed by Lundgren[1] and refined later[2] to accommodate for dampen kinetic energy oscillations.

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial}{\partial x_i}(p) + \frac{\partial}{\partial x_j}(\tau_{ji}) + Q\rho u'$$



[1] Lundgren, T. S. (2003) CTR Annual Research Briefs

[2] Caroll, P. and Blanquart, G. (2015) Physics of Fluids **25**

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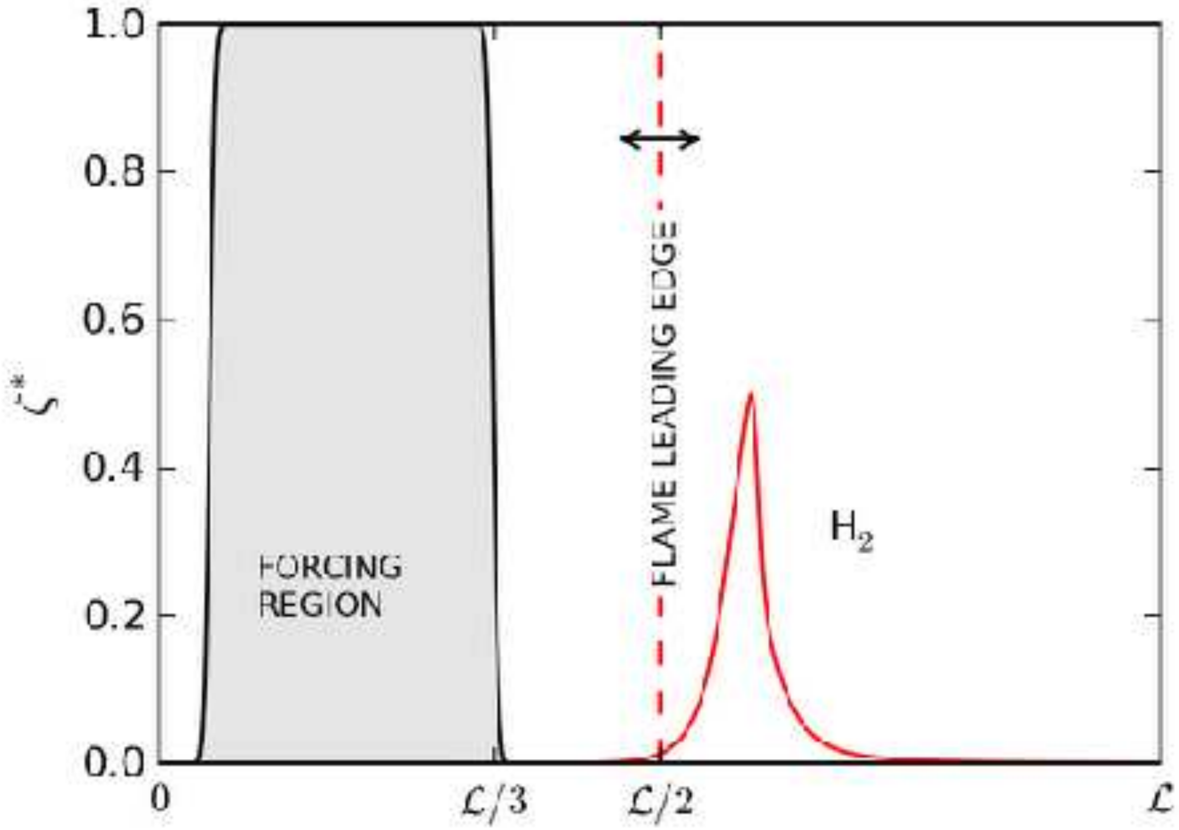

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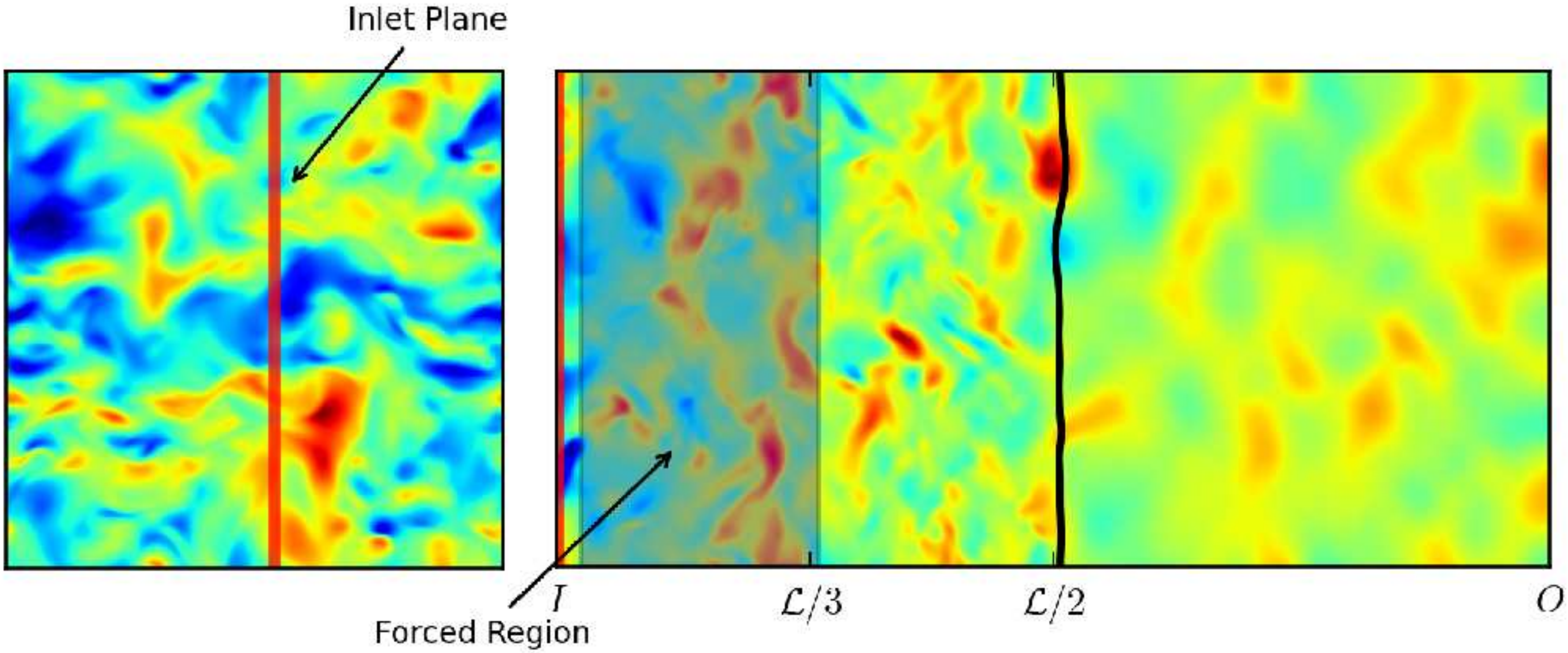
[1] Lundgren, T. S. (2003) CTR Annual Research Briefs

[2] Caroll, P. and Blanquart, G. (2015) Physics of Fluids **25**

Present Cambridge DNS: a snapshot



Summary: lean premixed turbulent flame comparisons

DNS code: Senga2

Compressible Navier-Stokes equations with forcing

Difference Scheme: 10th order finite difference

Time-marching: 4th order explicit Runge-Kutta

Adaptive time-step size PI controller

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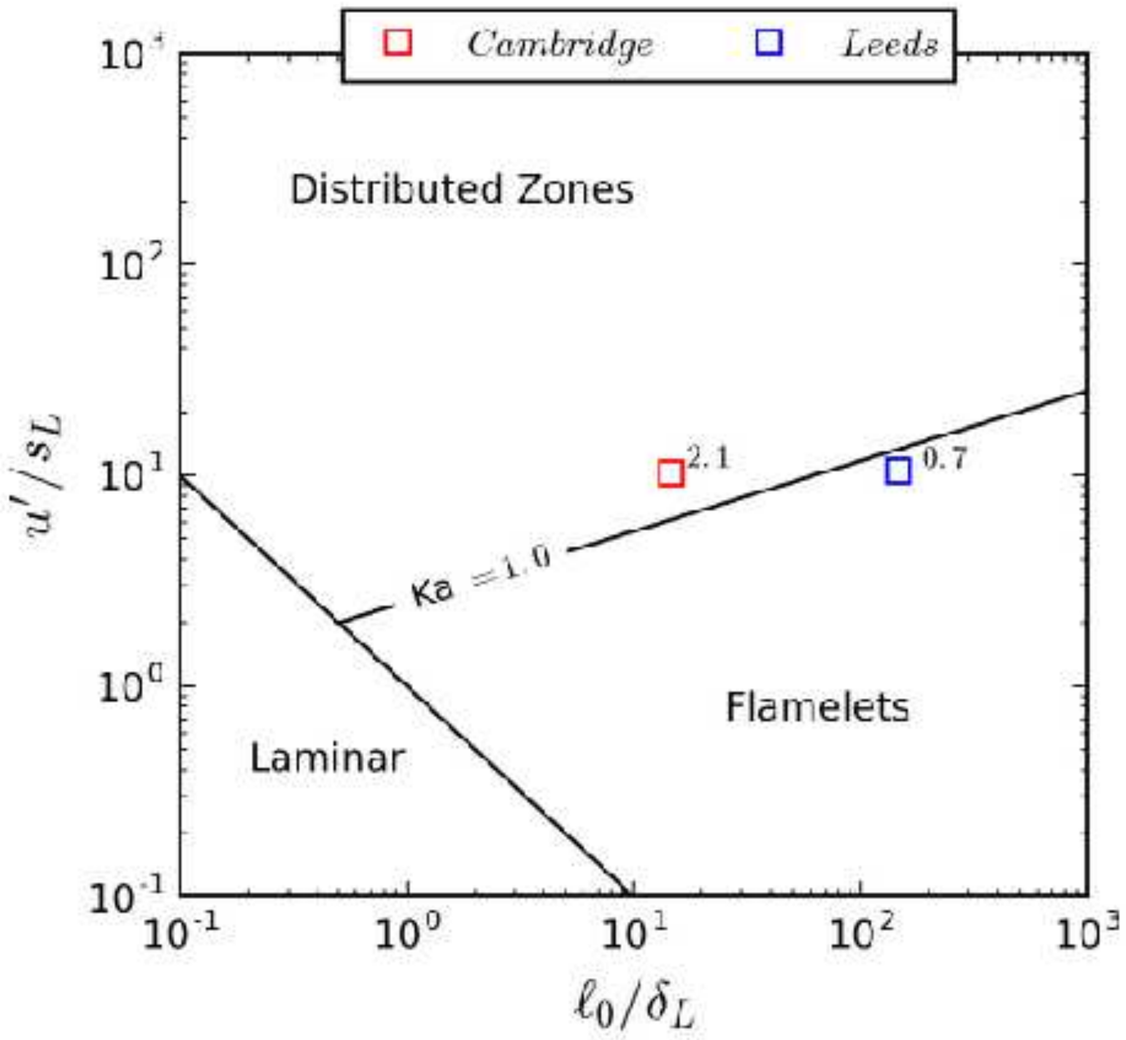

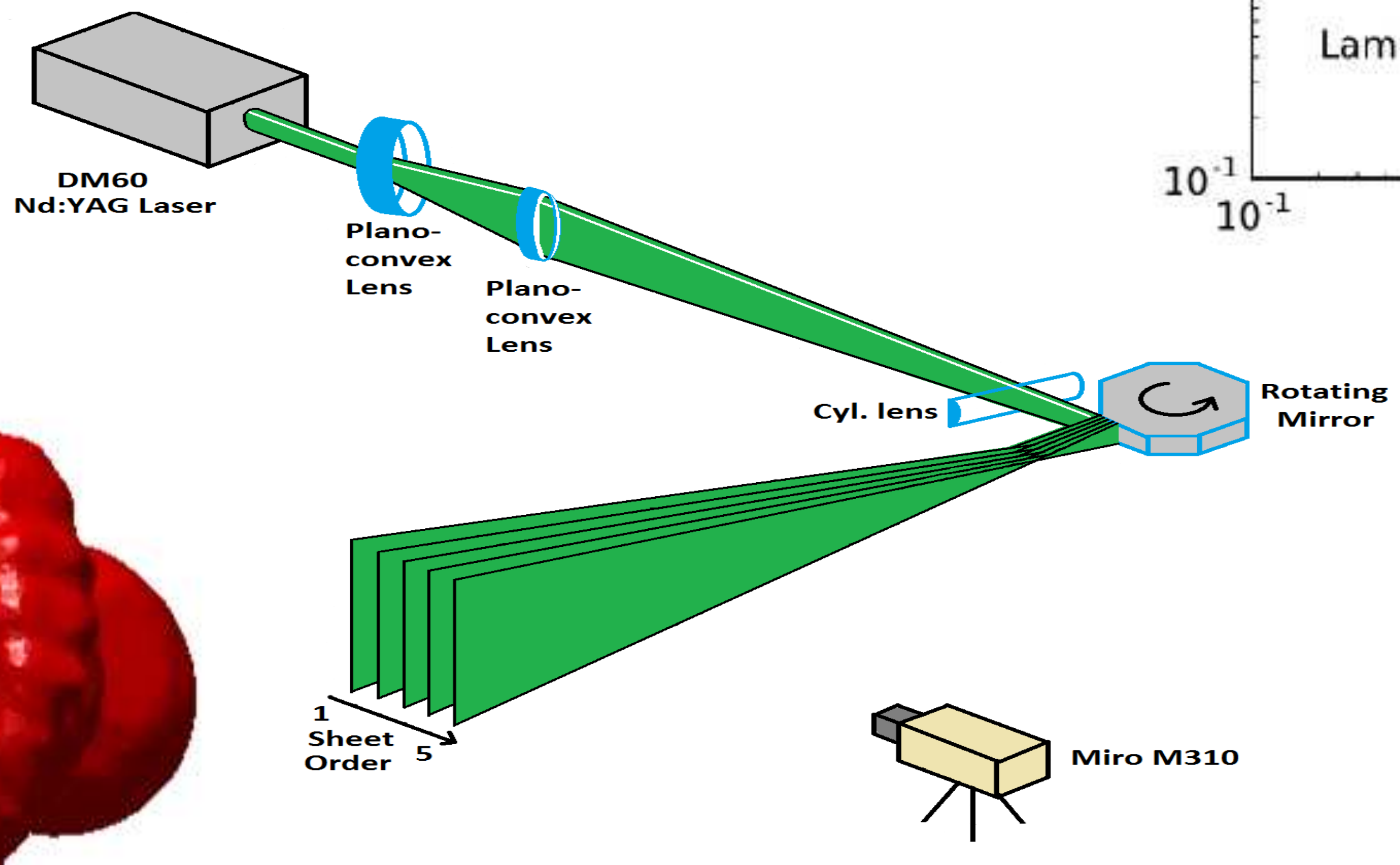

Questions:

Girish (DNS): gvn22@cam.ac.uk

Ben (Bomb): mnbjt@leeds.ac.uk