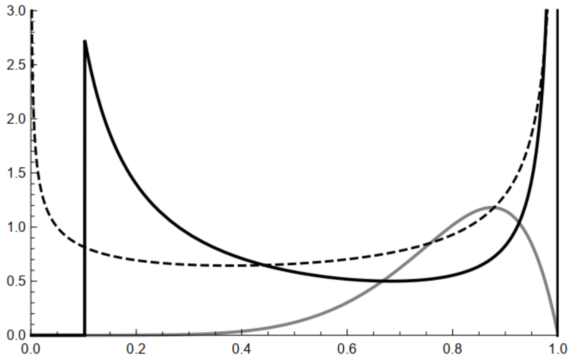
Multidimensional PDF modelling of turbulent premixed combustion



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Overview

Introduction – LES of turbulent premixed flames

Premixed laminar flame structure

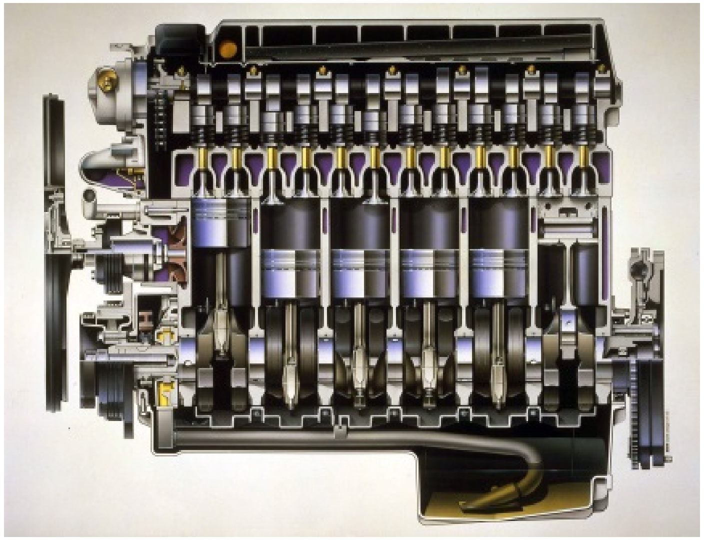
Laminar flame pdf

Multidimensional effects

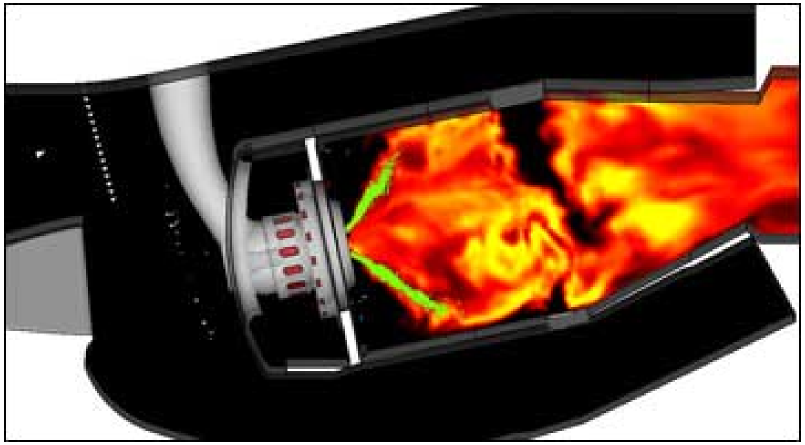
Valididation with DNS data

Conclusions and future work

Premixed turbulent combustion in industrial applications



Internal combustion engines



Stationary gas turbines

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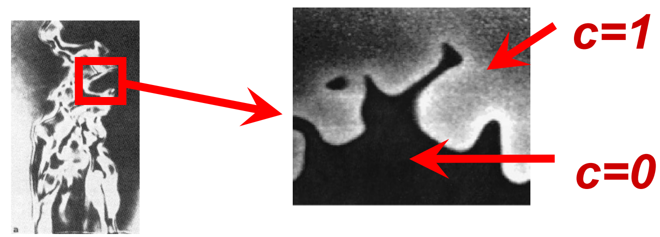
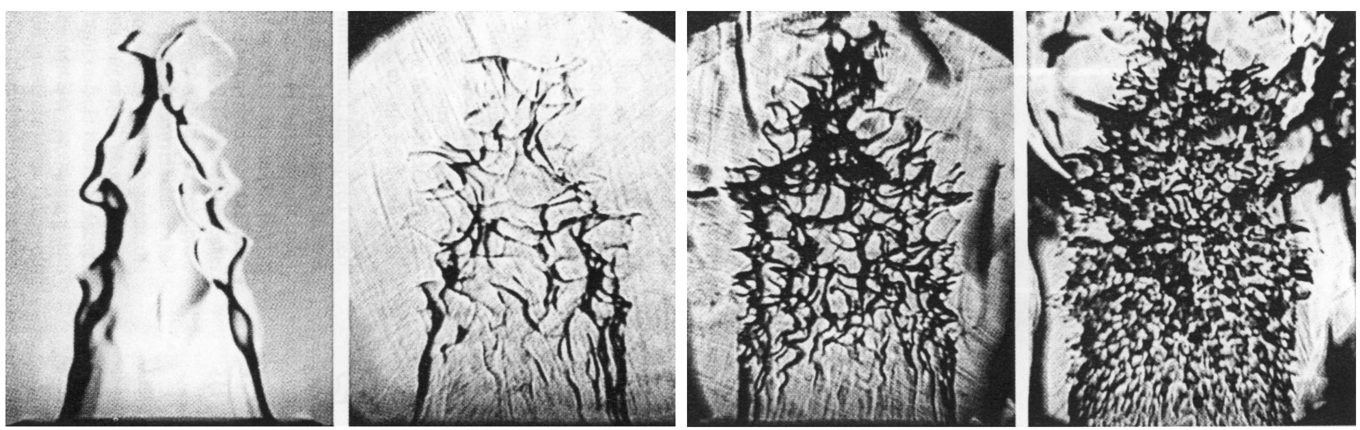
Fully premixed turbulent flames - experiment



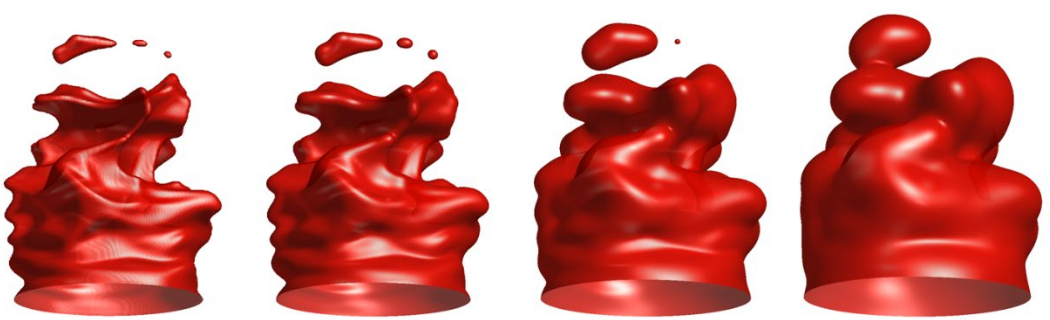


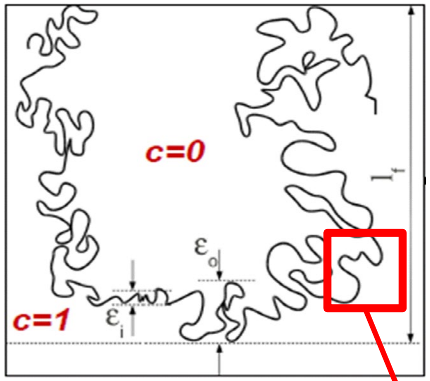
0.1 MPa | 0.25 MPa | 0.5 MPa | 1 MPa

Thinner flame / more flame wrinkling with increasing pressure

Fully premixed turbulent flames - DNS

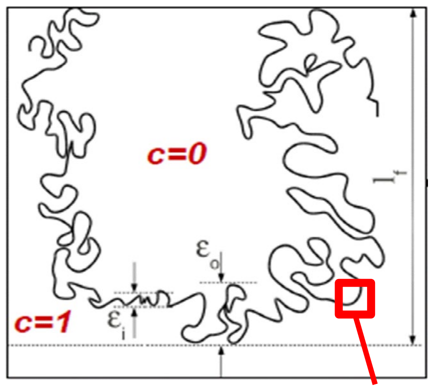
p = 1 bar   p = 5 bar   p = 10 bar





DNS flame shape

LES cell (coarse)



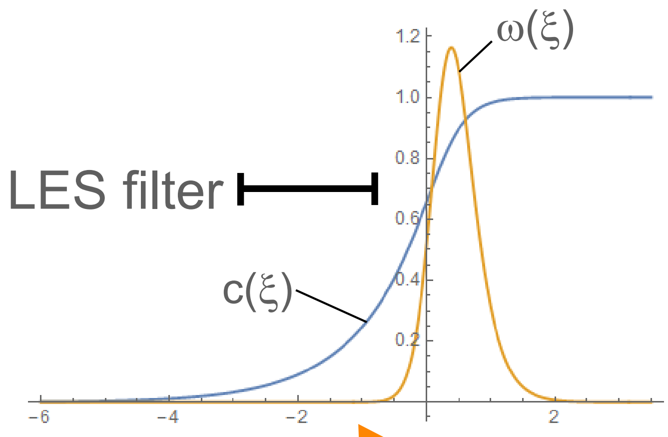
Result of LES filtering

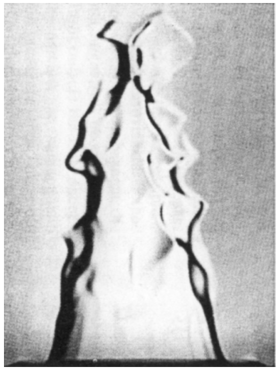
LES cell (fine)

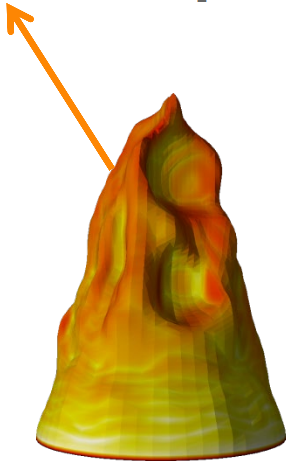
→ Subgrid flame folding – increases with filter width / pressure

Premixed LES modelling

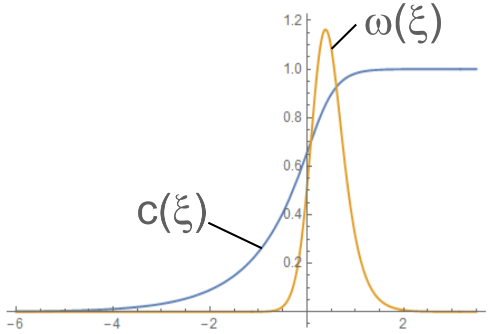
- LES model needed for mean reaction source term
- PDF methodology – multidimensionally valid
- Fokus on wrinkled / thickened flame regime (low Ka)




Experiment


LES

Laminar premixed flame (1-D)



Progress variable $$c(x,t) = (T - T_u)/(T_b - T_u)$$

1D c transport equation $$\rho \frac{\partial c}{\partial t} + \rho u \frac{\partial c}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\lambda}{c_p}\frac{\partial c}{\partial x}\right) - \omega(c)$$

Transformation $$\xi = \int_0^x \rho_u s_L C_p/\lambda dx$$

Steady-state, u = s_L $$\frac{\partial c}{\partial \xi} = \frac{\partial^2 c}{\partial \xi^2} + \omega(c)$$

ξ: canonical coordinate

Flame profiles / source terms

Arrhenius source term:

$$\omega(c) = \Lambda\left(1-\alpha(1-c)\right)^{\beta_1 - 1}(1-c)exp\left(-\frac{\beta(1-c)}{1-\alpha(1-c)}\right)$$

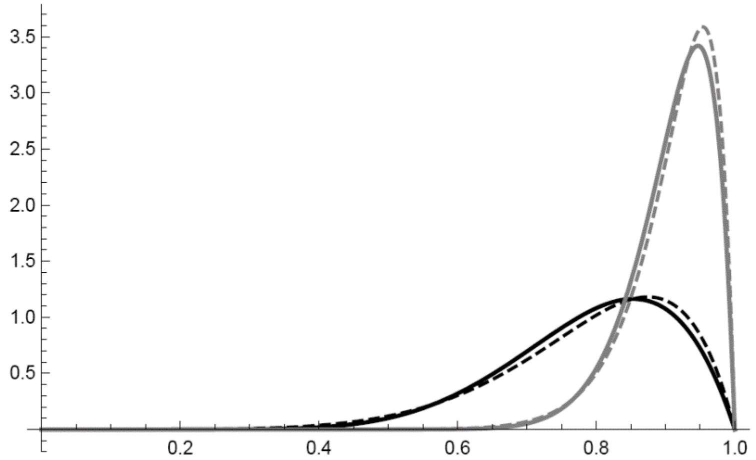
$\alpha = \frac{T_b - T_u}{T_b}$ β: activation energy

Analytic source term:

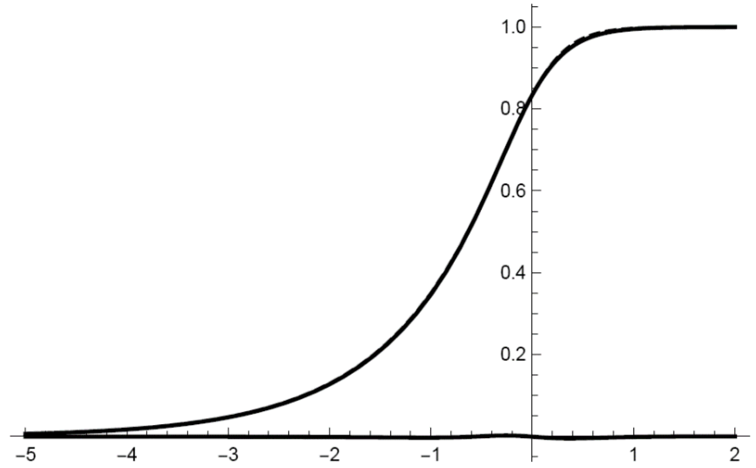
$$\omega_m(c) = (m+1)(1-c^m)c^{m+1}$$

$$c_m(\xi) = [1+exp(-m*\xi)]^{-1/m}$$

$$\xi_m(c) = \frac{1}{m}ln\left(\frac{c^m}{1-c^m}\right)$$



Arrhenius / analytic ω(c)



c(ξ) profiles

$c_A(\xi)$ solved numerically

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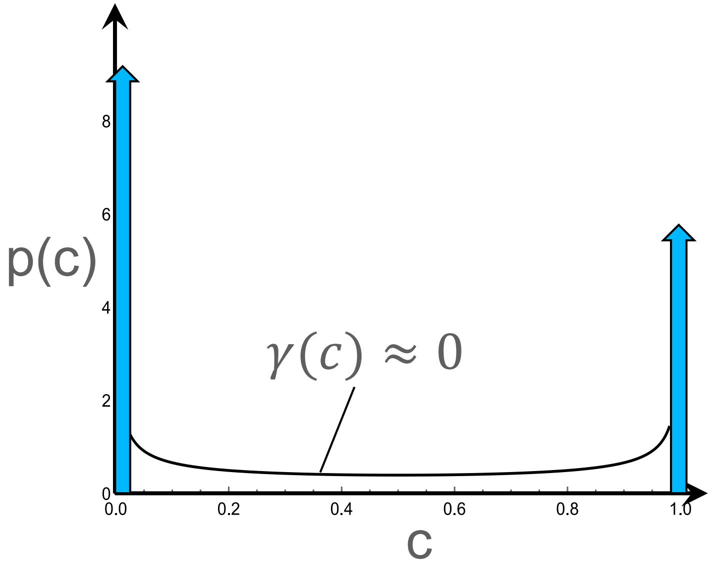
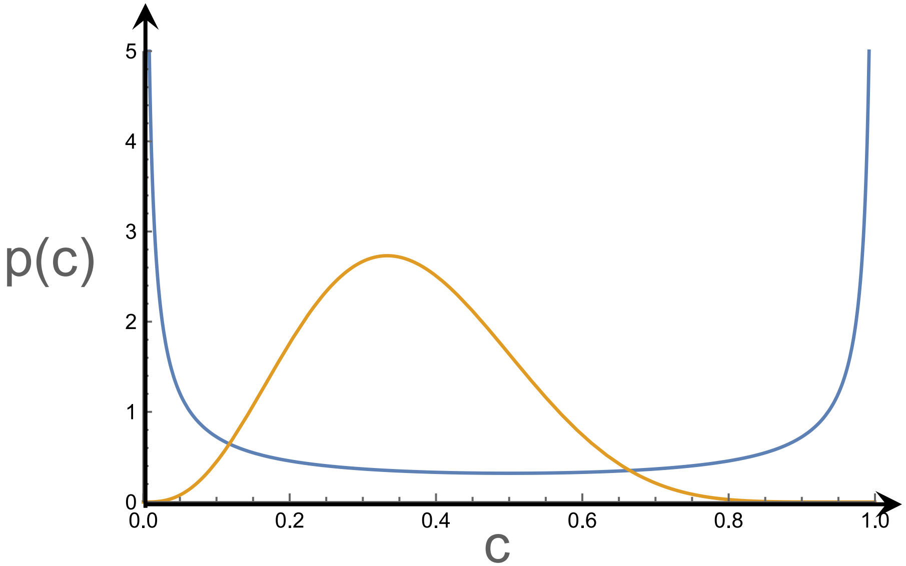
Popular presumed premixed pdf's

$$\bar{f} = \int_0^1 f(c)p(c)dc$$



Bray-Moss-Libby pdf

(thin flame limit)



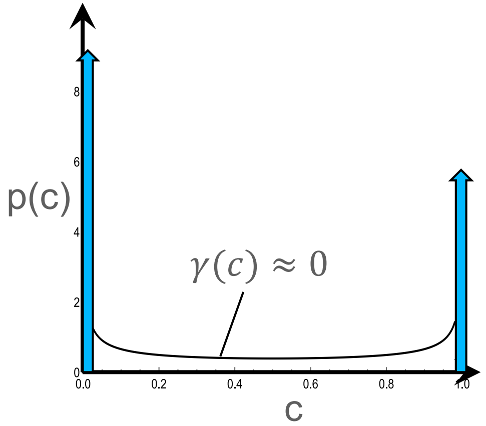
Beta pdf

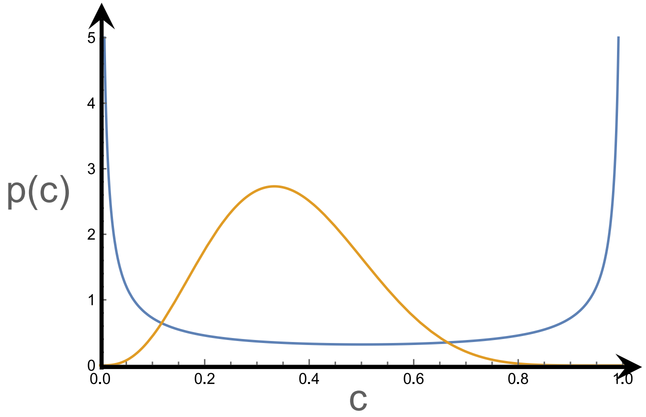
(diffusion process)

$$p_{BML}(c) = (1-\tilde{c})\delta(c) + \tilde{c}\delta(1-c)$$

$$p_\beta(c) = \frac{c^{(\alpha-1)}(1-c)^{(\beta-1)}}{N}$$

Features BML / Beta pdf's





BML pdf:

- accurate means for quantities f(c) in thin flame limit
- only applicable to f(c) with $f(c) \neq 0$ for $c=(0,1)$

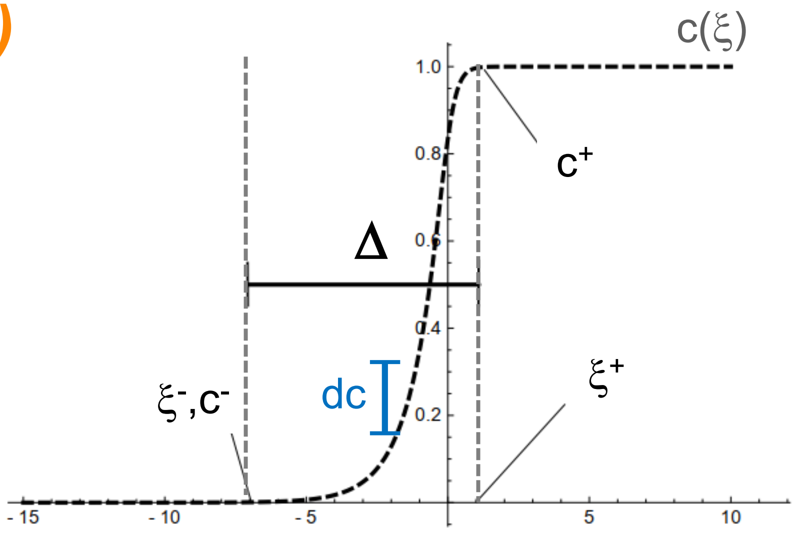
→ not applicable to calculate $\overline{\dot{\omega}}$

Beta pdf:

- good results for variables in diffusion processes
- successful in non-premixed combustion
- needs second variable for α,β e.g. scalar dissipation rate
- $\overline{\dot{\omega}}$ not accurate for large filters

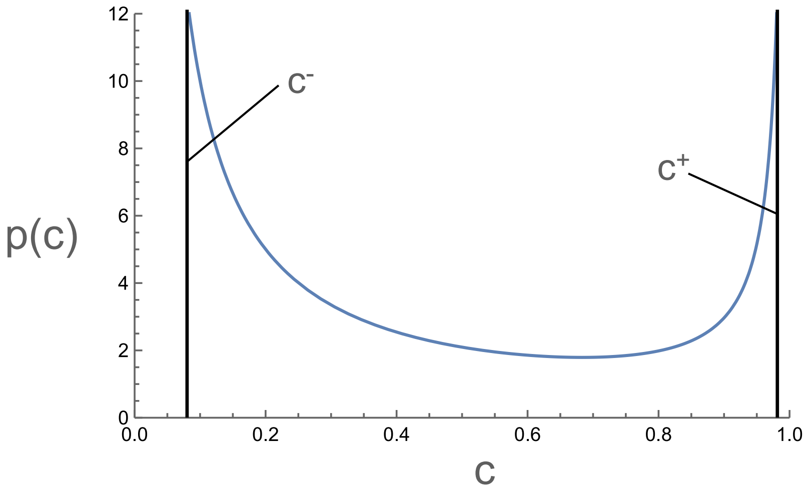
Flamelet pdf (laminar 1-D flame)

$$p(c) = \begin{cases} 0 & : c < c^- \\ \frac{1}{N}\frac{1}{dc/d\xi} & : c^- \leqslant c \leqslant c^+ \\ 0 & : c > c^+ \end{cases}$$

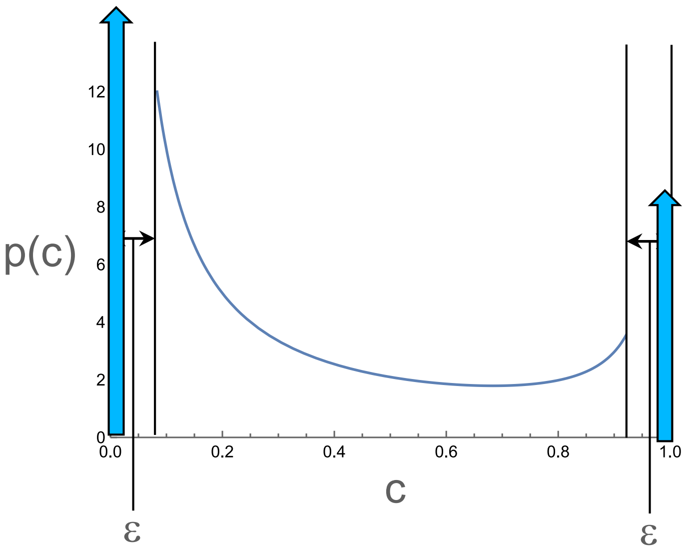


$$\int p(c)dc \overset{!}{=} 1 \rightarrow N=\Delta$$

$$\int \frac{1}{\partial c/d\xi} dc$$ diverges at c→0,1



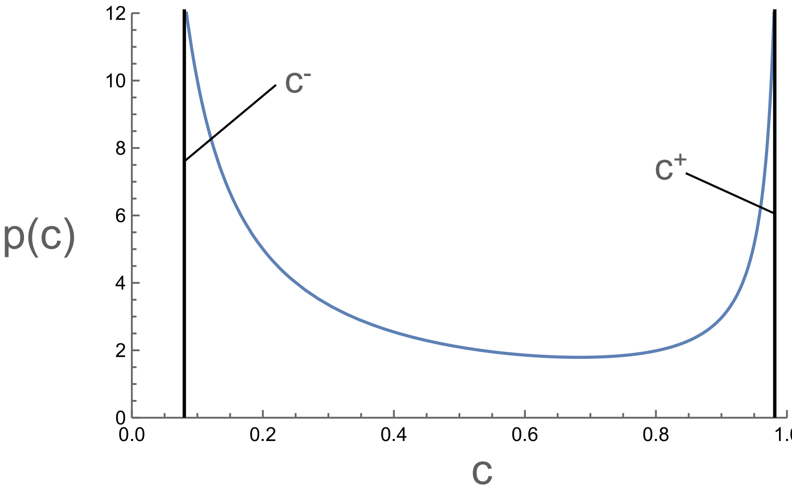
Flamelet pdf implementations



$$\bar{f} = Af(0) + Bf(1) + \int_{\varepsilon}^{1-\varepsilon} f(c)p_f(c)dc$$

- Negative A,B possible (constant ε)

→ Domingo: replace by β pdf there



$$\bar{f} = \int_{c^-}^{c^+} f(c)p_f(c)dc$$

- No need for delta functions at c=(0,1)
- accurate c^-, c^+ required

Comparison flamelet / beta pdf

Beta pdf:

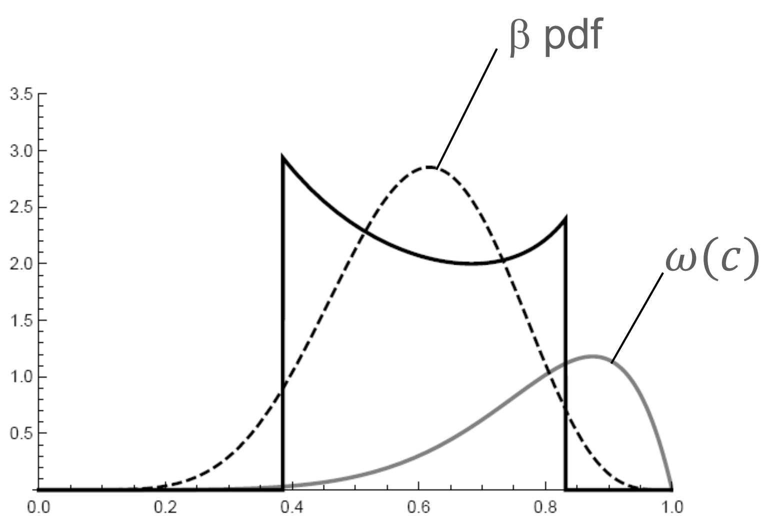
$$p_\beta(c) = \frac{c^{a-1}(1-c)^{b-1}\Gamma(a+b)}{\Gamma(a)\Gamma(b)}$$

a,b determined from $\bar{c}, \overline{c'^2}$

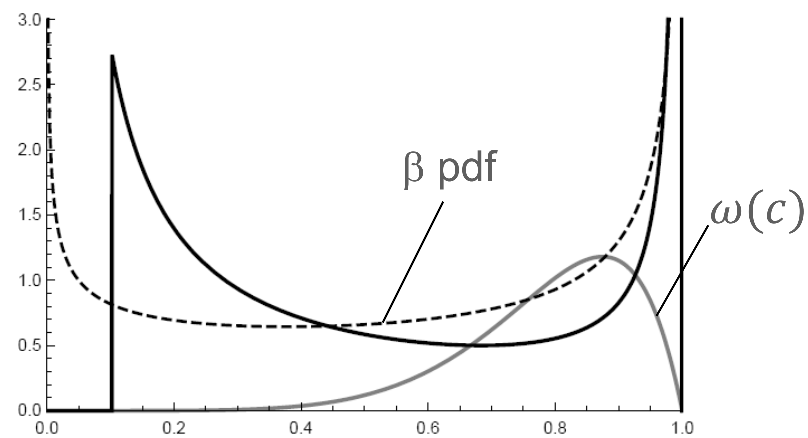
Analytic flamelet pdf:

$$p_m(c) = \frac{1}{\Delta c(1-c^m)}, \quad c^- \leq c \leq c^+$$

c^-, c^+ determined from $\bar{c}, \Delta$

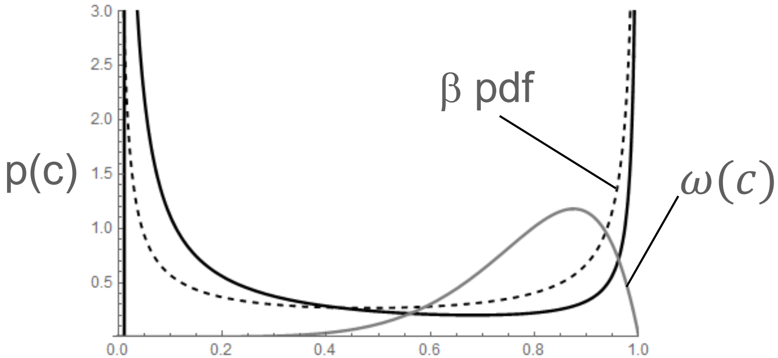


small $\Delta = 0.5^*\delta_f$, $\bar{c} = 0.6$

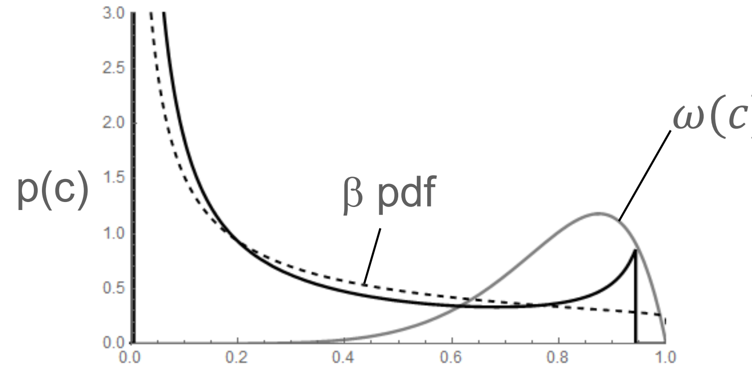


large $\Delta = 2^*\delta_f$, $\bar{c} = 0.6$

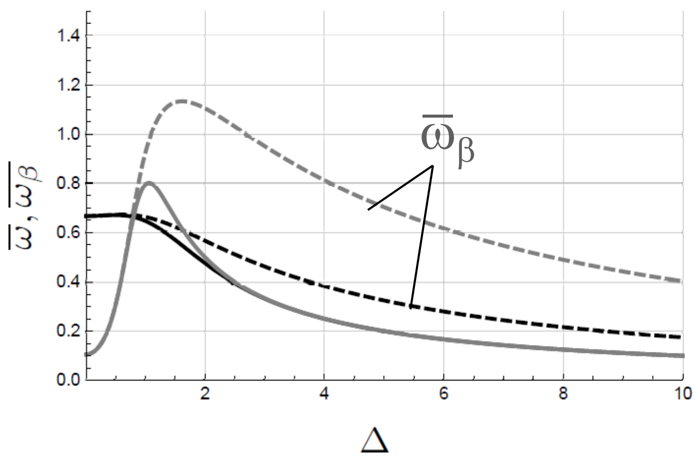
Comparison of filtered source term



Δ = 5 δ_{th}, $\bar{c}$ = 0.6

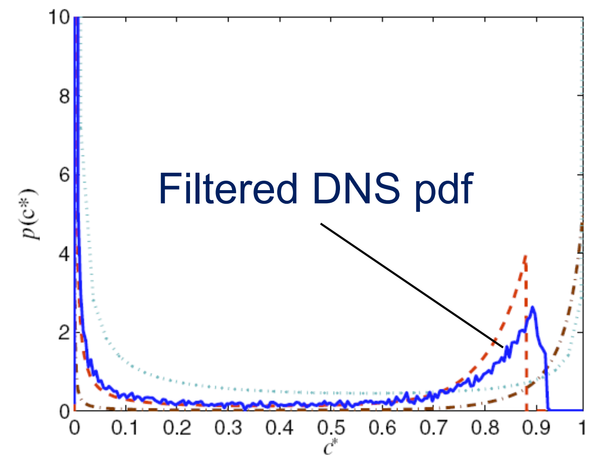


Δ = 3 δ_{th}, $\bar{c}$ = 0.2



black: m=4, gray: m=12

(δ_{th}~1.8)



Jin, Grout, Bushe, Flow Turbulence Combust (2008) 81:563–582

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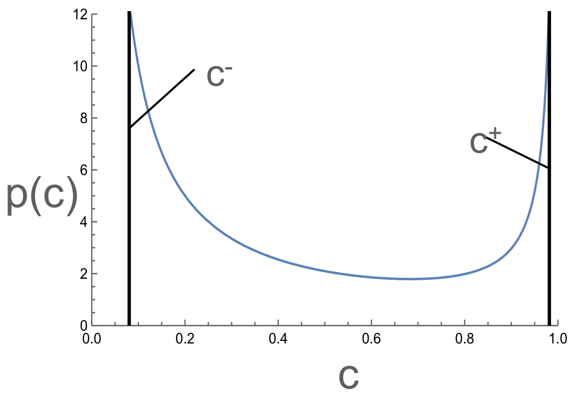
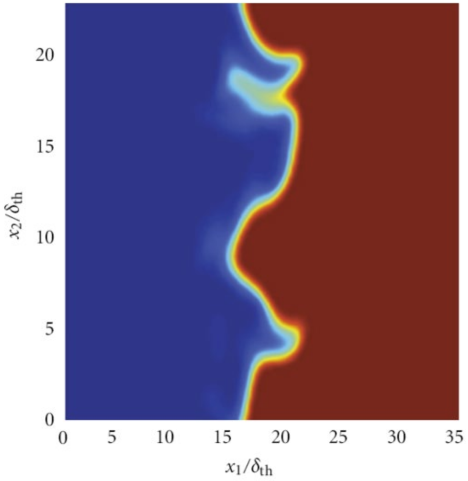
Relation between 1D and multi-D PDF



1D pdf: $p(c) = \frac{1}{\Delta}\left(\frac{dc}{dx}\right)^{-1} H(c - c^{-})\, H(c^{+} - c)$

Multi-D pdf: $p(c) = \frac{\Sigma(c) I(c) (dc/dx)_{1D}^{-1}}{\Omega}$

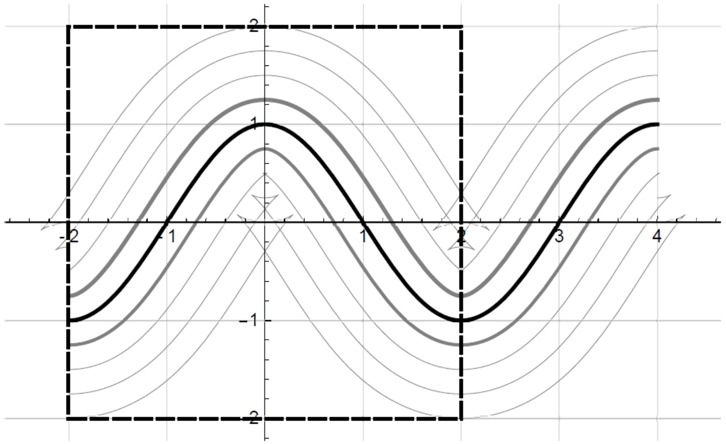


$\Sigma(c)$: Isosurface area

Ω: Filter volume, cube: $\Omega = \Delta^3$

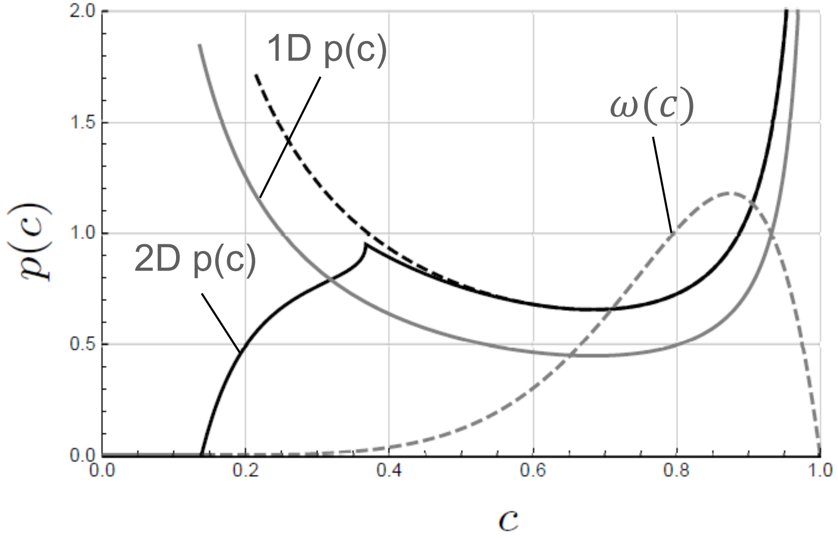
$I(c)$: $|\nabla c|_{3D} \,/\, |dc/dx|_{1D}$

PDF of 2D sinusoidal flame

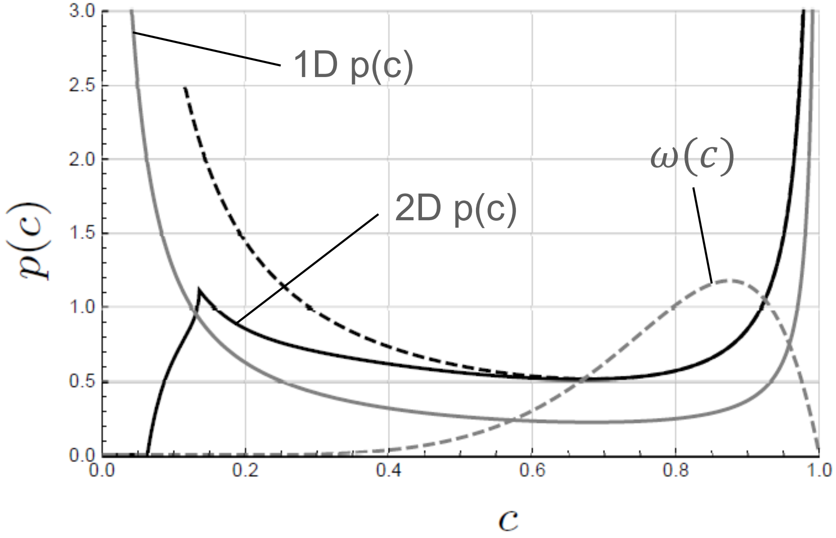


Assumptions:

- no change in inner flame structure
- no crossing of isolines



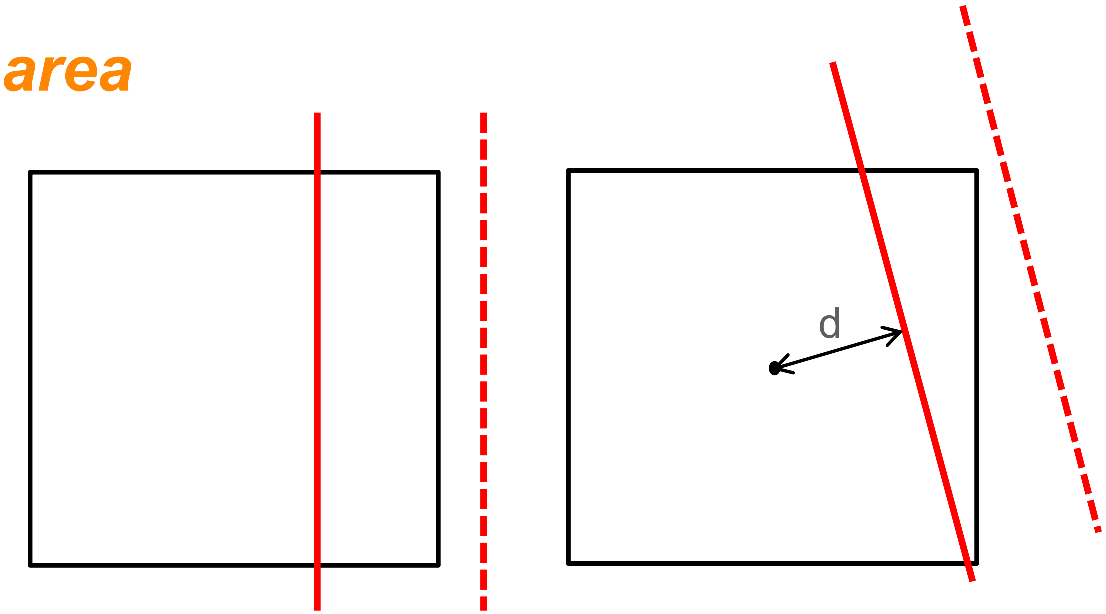
Δ = 2.2*δ_f,weak wrinkling



Δ = 5*δ_f, strong wrinkling

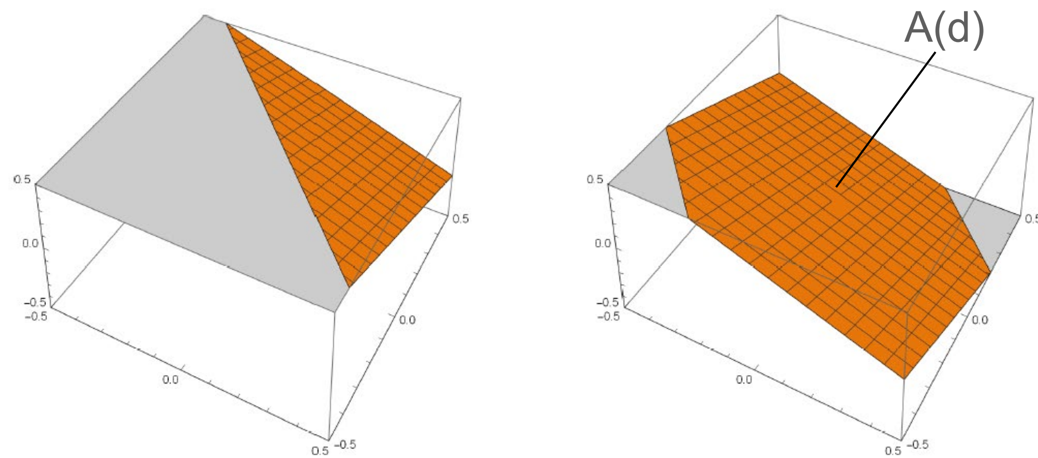
Multidimensional flame area

Planar flame front in 2D cell

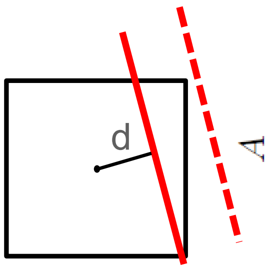


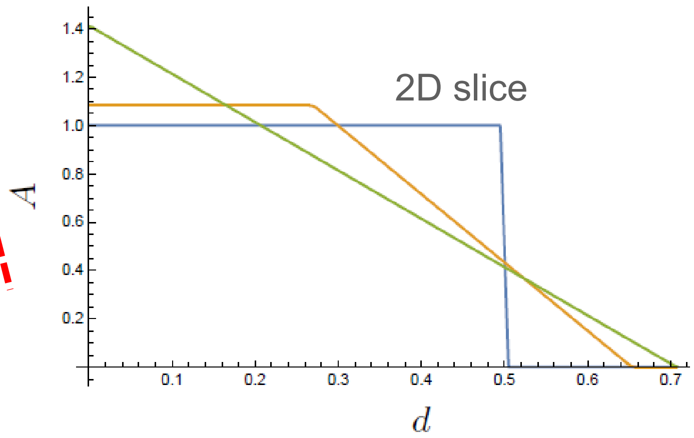
d: normal distance between flame front and cube centre

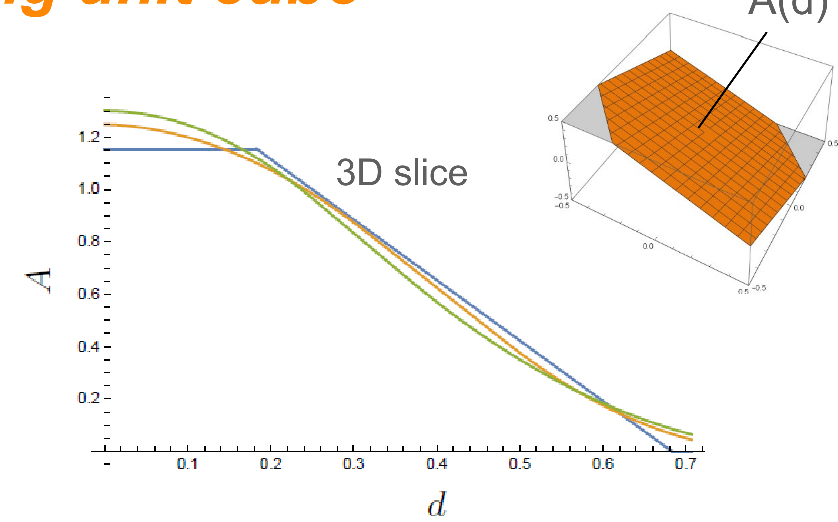
Planar flame front in 3D cell



Area distributions of plane cutting unit cube



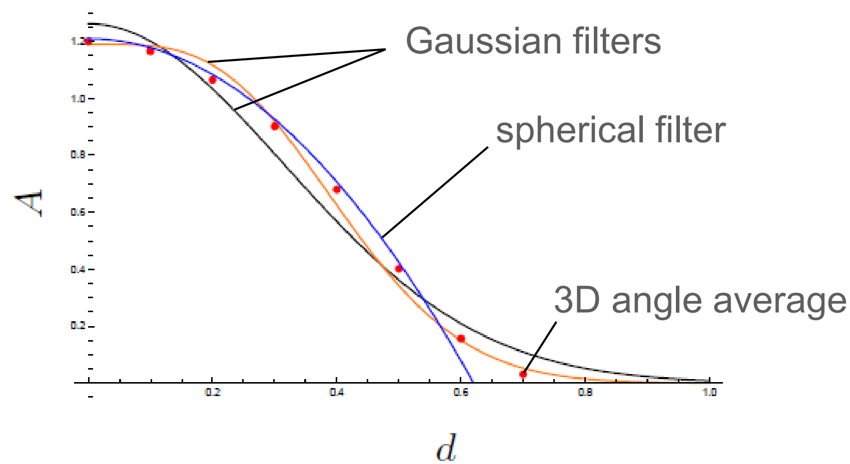




d: distance from unit cube center

A(d): cutting area in Ω

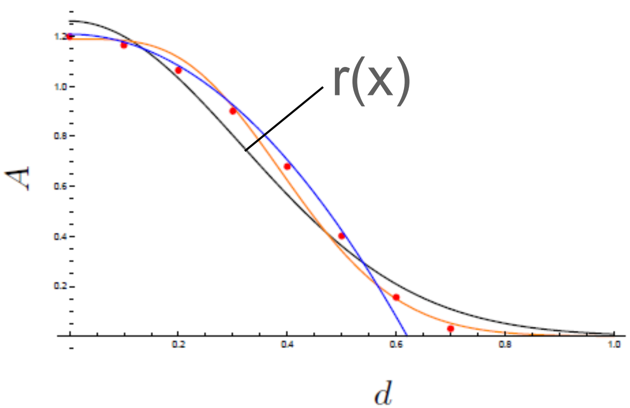
Piecewise constant/linear/parabolic for cube / sphere

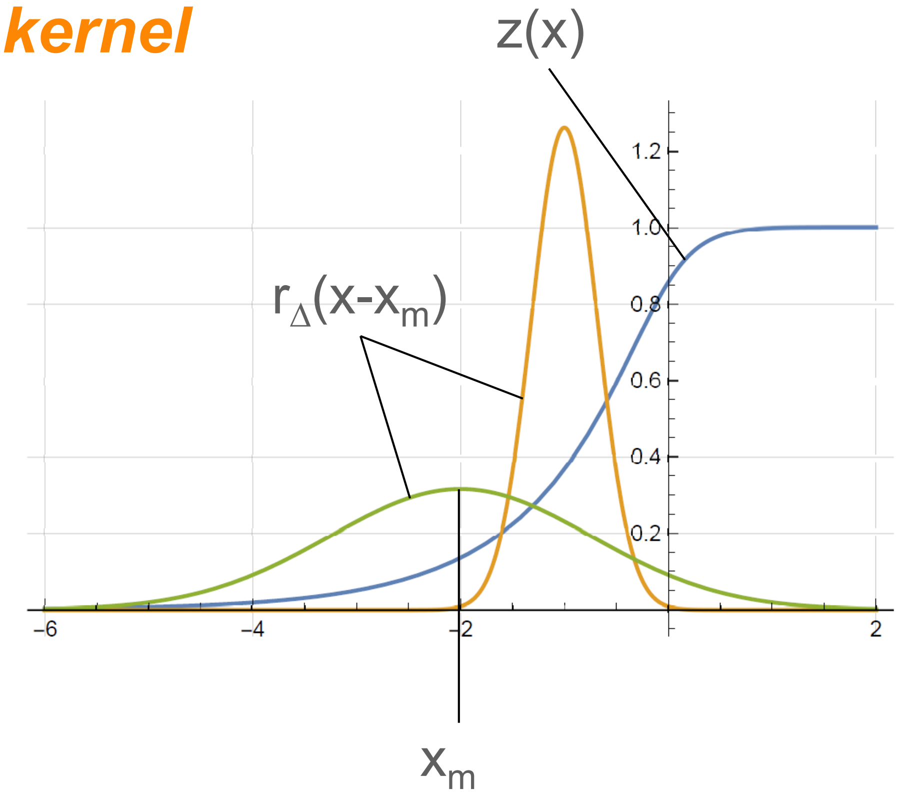


Filtering 1D profiles with filter kernel

- Multidimensional slice area A(d)

- Represented by filter kernel r(x)

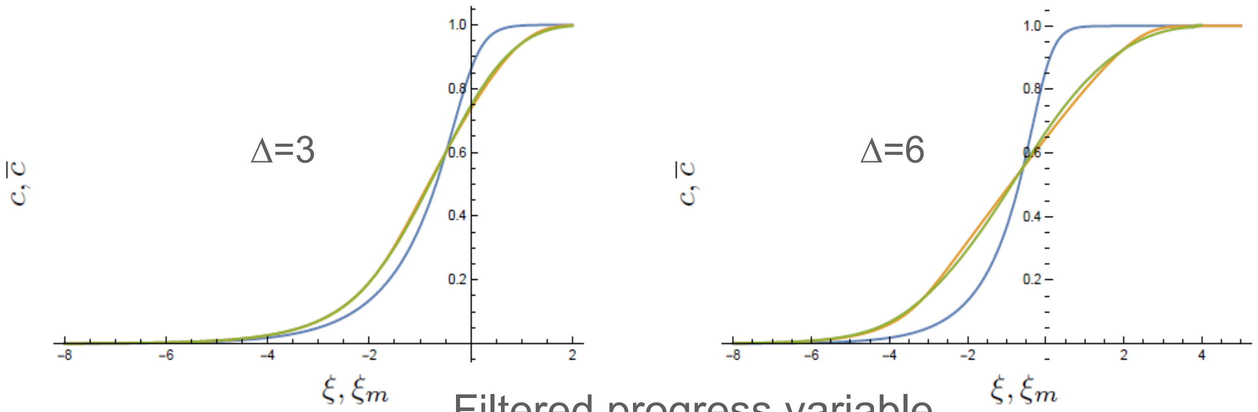




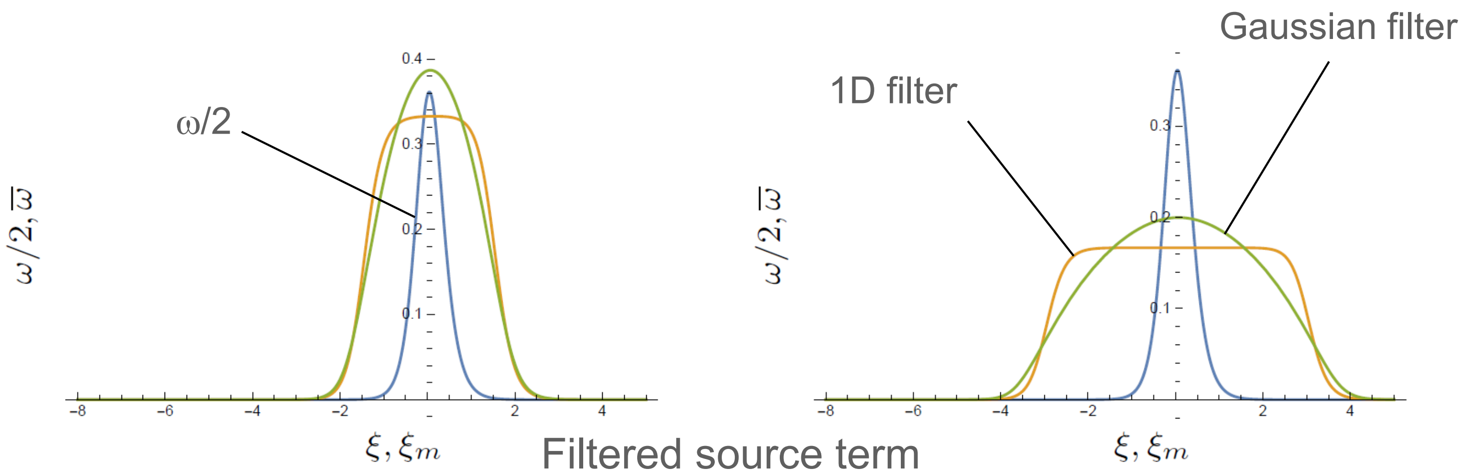
- Filtered value of z(x) with filter size Δ centered at $x=x_m$:

$$\bar{z}_\Delta(x_m) = \frac{1}{\Delta}\int_{-\infty}^{\infty} r\left(\frac{x-x_m}{\Delta}\right) z(x)dx$$

Effect of filter kernel

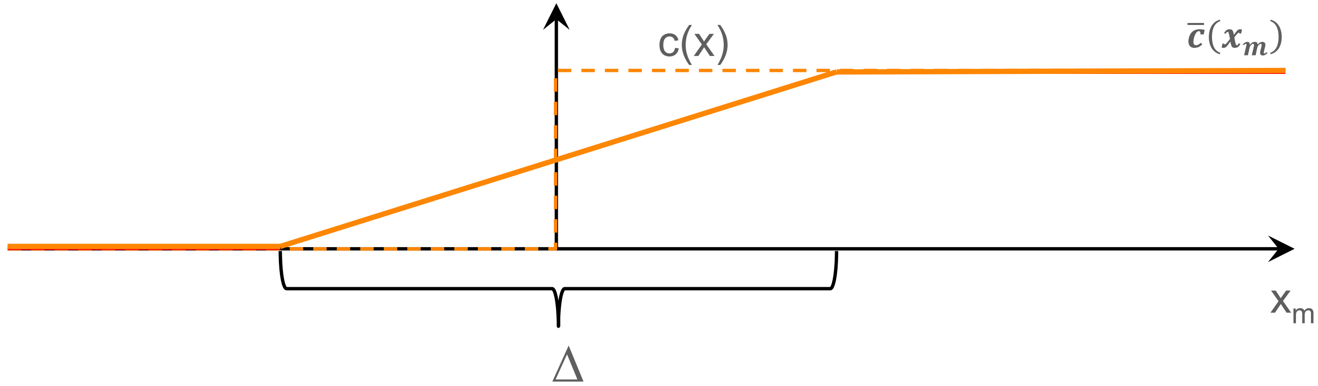


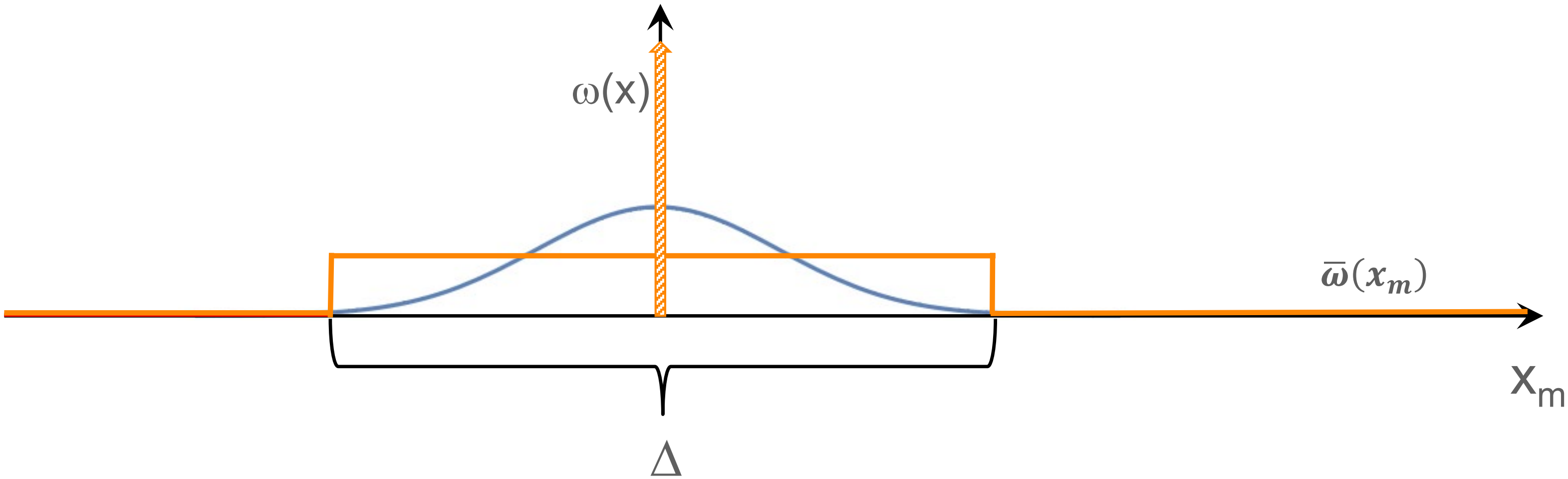
Filtered progress variable



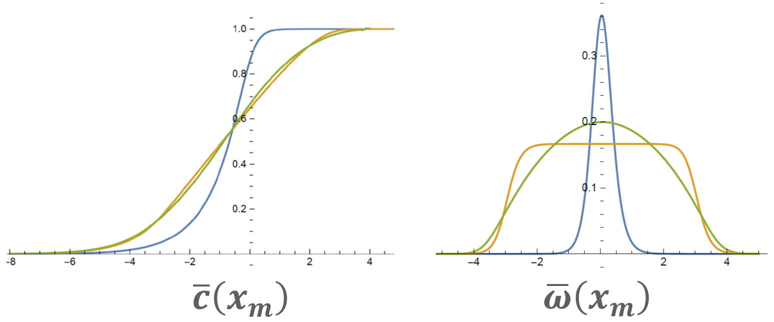
Filtered source term

Limit of filtered $\bar{c}(x_m)$, $\bar{\omega}(x_m)$ at large Δ

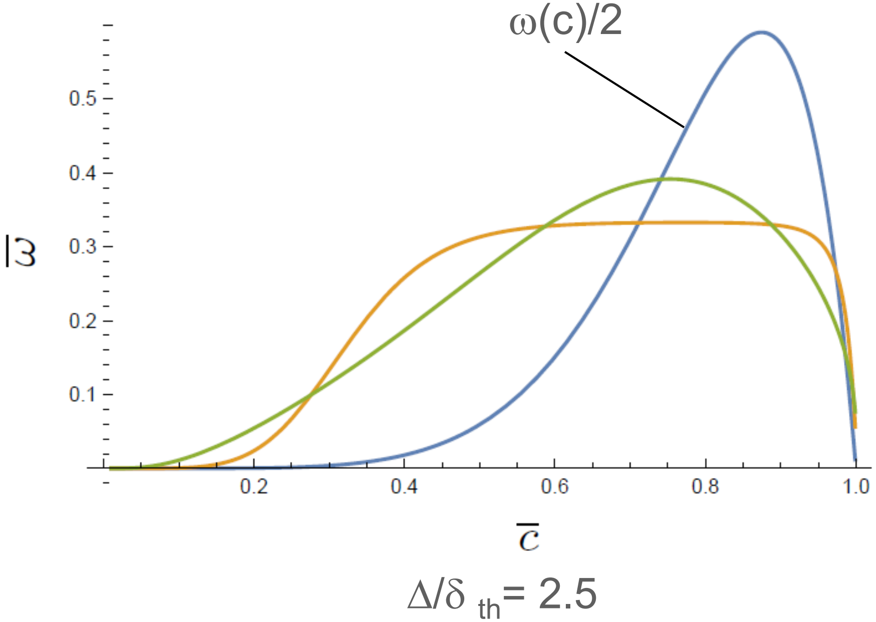


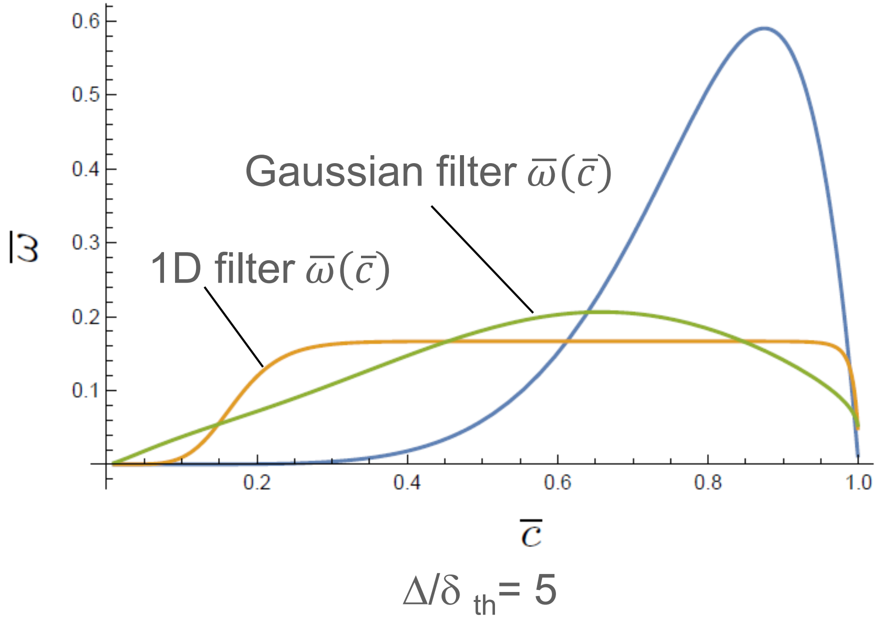


1D filtered $\overline{\omega}$ vs. $\overline{c}$

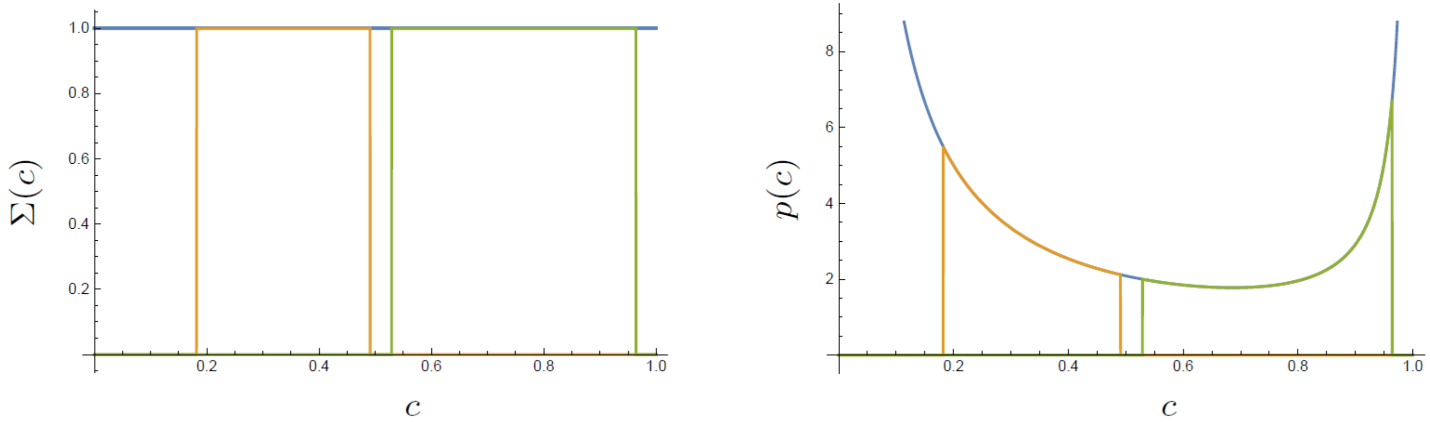


Parameterical plots: $\overline{\omega}(x_m)$ vs. $\overline{c}(x_m)$

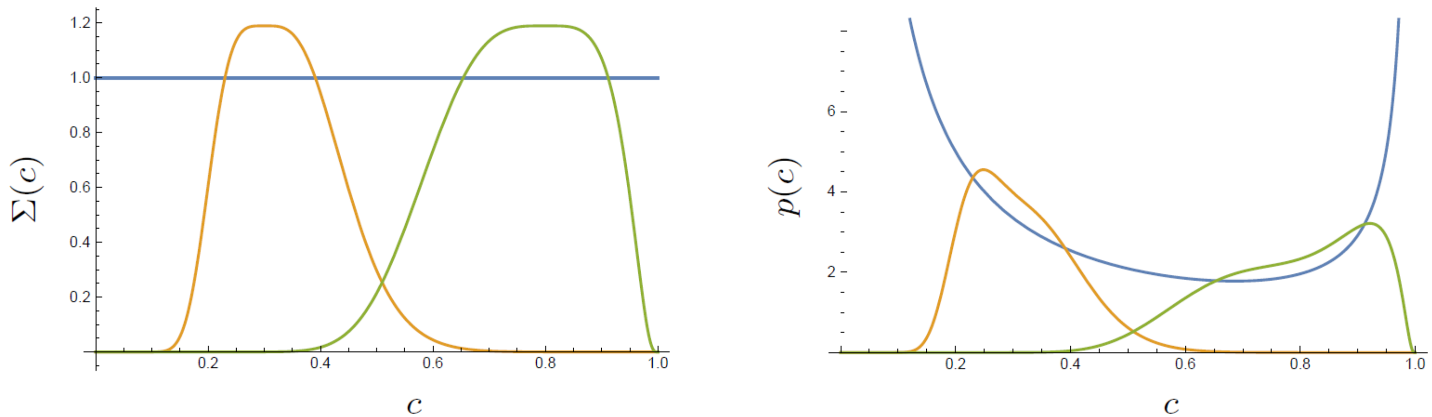




Area effect on pdf in c space

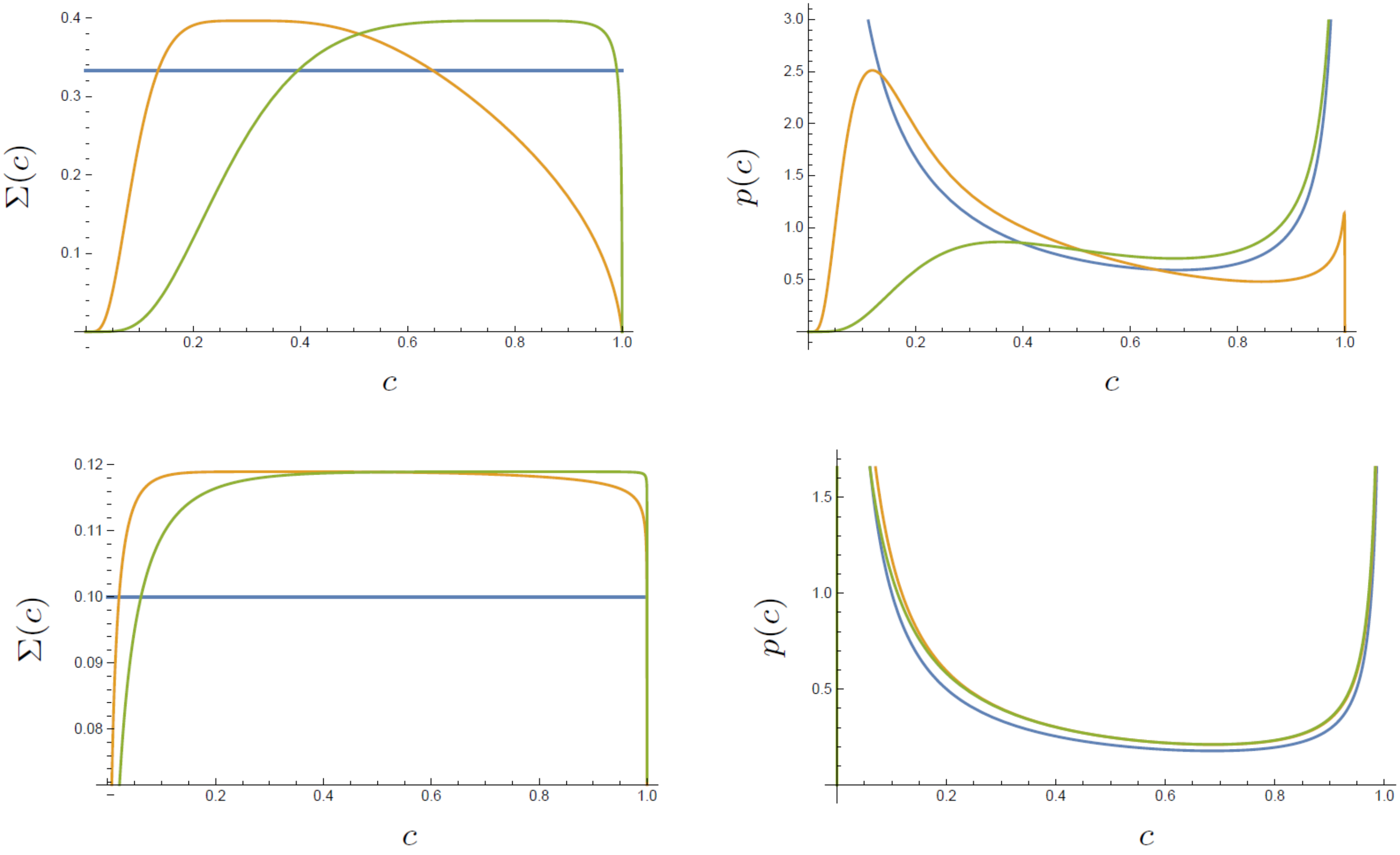


1D filter



3D filter

Area effect on pdf in c space



medium filter

large filter

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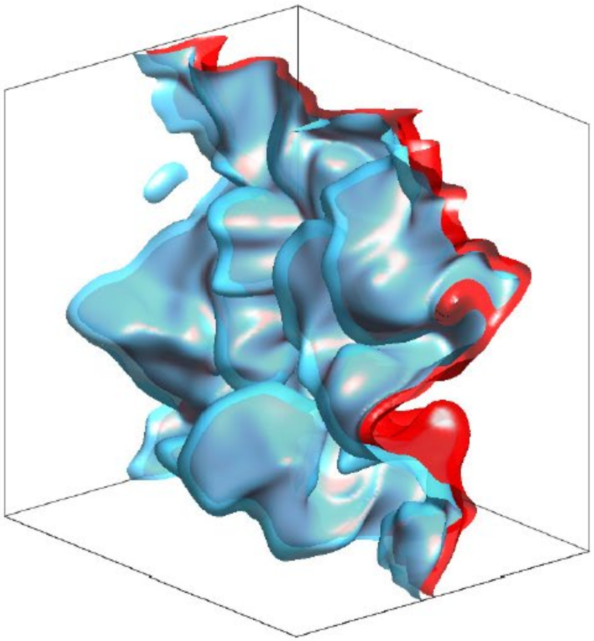
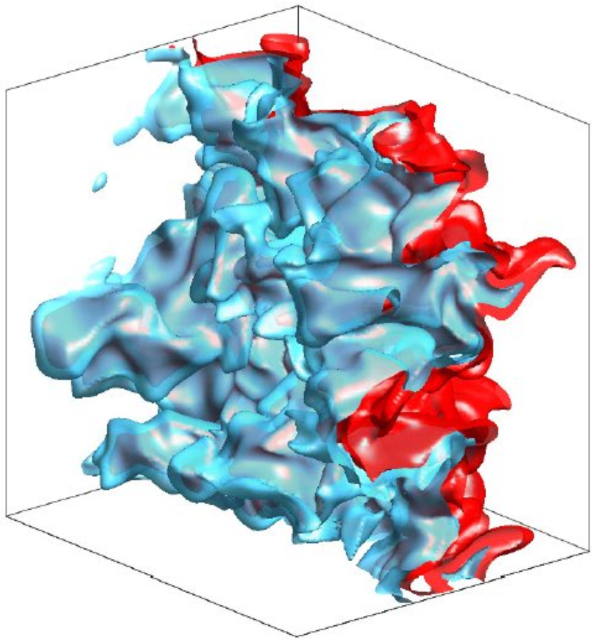
Statistically planar turbulent flame DNS

c isocontours 0.1, 0.9



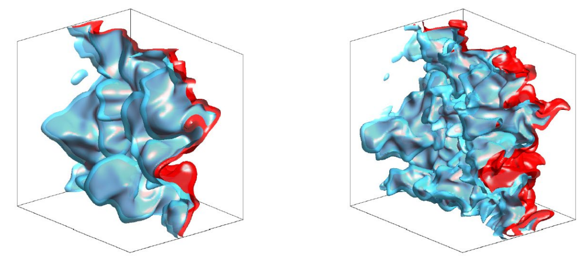
$u'/s_L = 5$

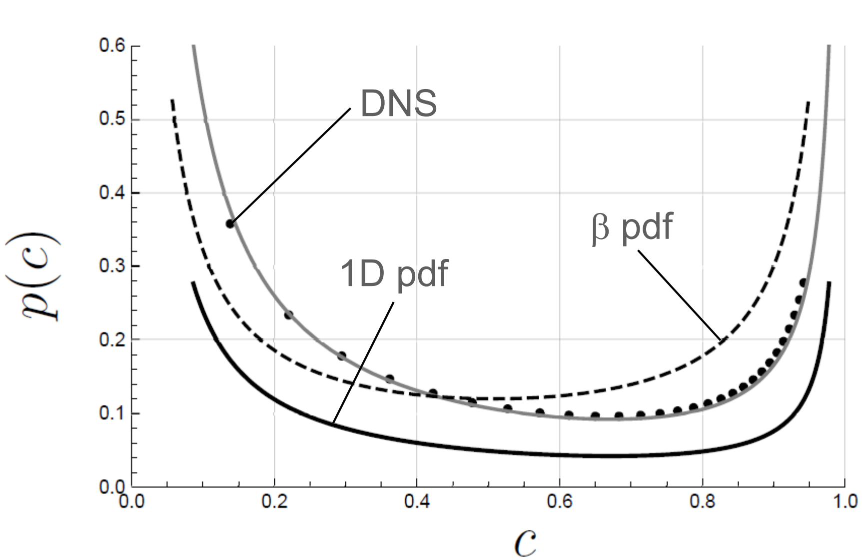


$u'/s_L = 15$

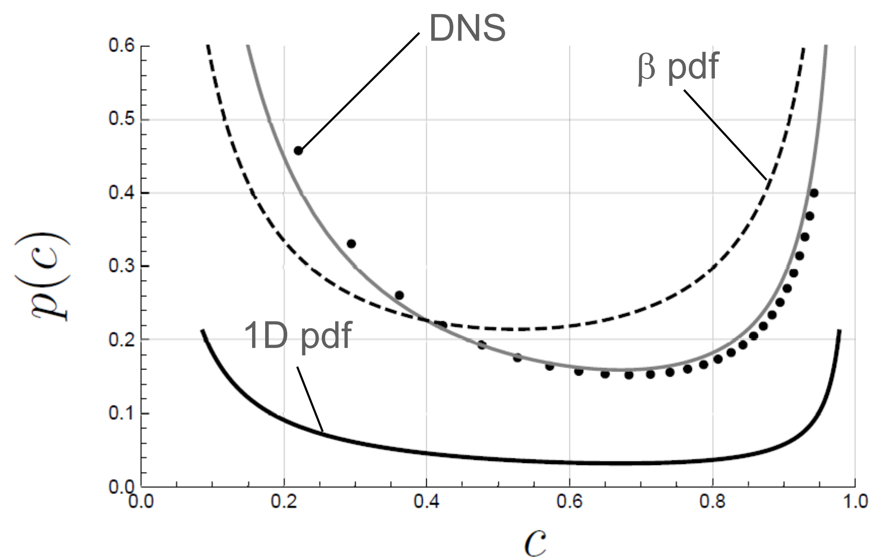
PDF for large (RANS-like) filter widths

$$p(c) = \frac{\Sigma(c) I(c) (dc/dx)_{1D}^{-1}}{\Omega}$$





u'/s_L = 5



u'/s_L = 15

Gray line: 1D pdf scaled with constant factor

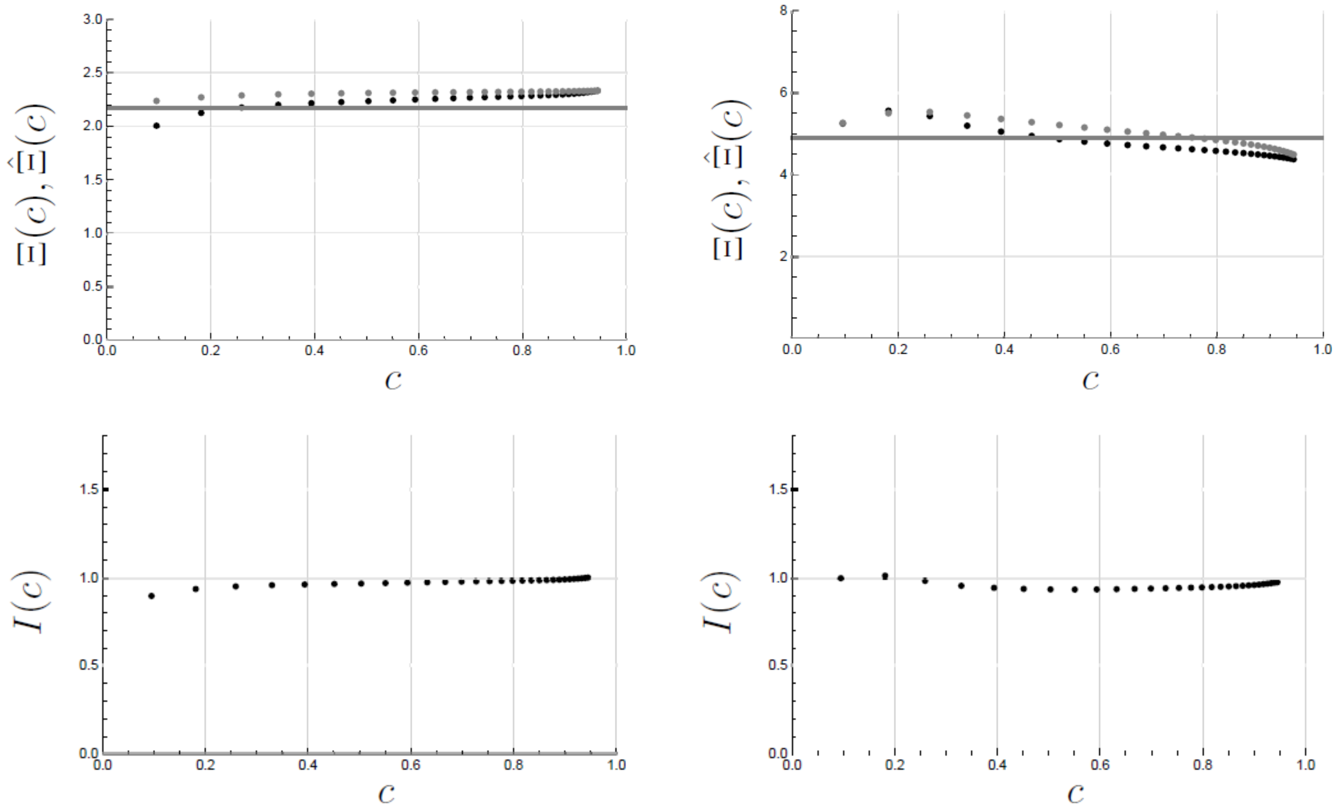
DNS analysis: change of inner flame structure

Wrinkling factor

$\Xi = \Sigma_T / \Sigma_L$

Inner flame structure

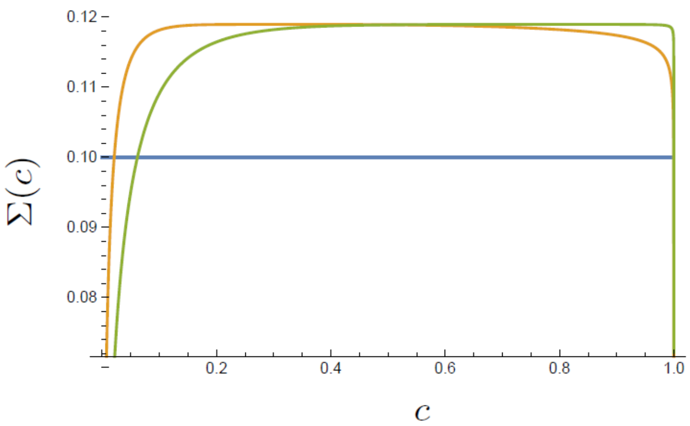
$I = |\nabla c|_{3D} \,/\, |dc/dx|_{1D}$

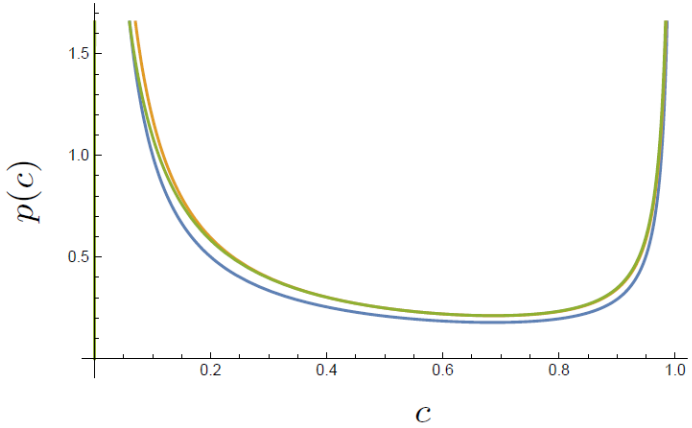


$u'/s_L = 5$ $u'/s_L = 15$

I(c) ~ 1: same c(x) gradients in laminar and turbulent flame

Area effect in c space - large filter width

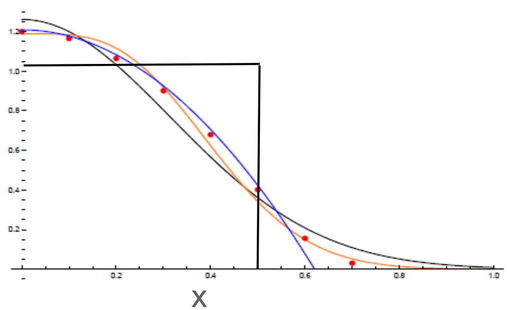


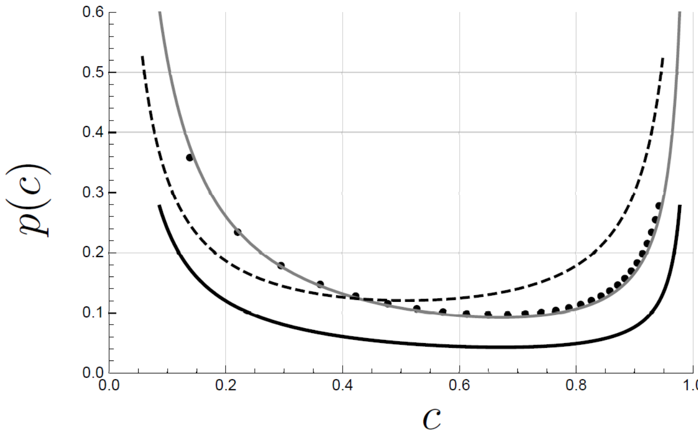


3D RANS filter

- RANS filter: $\Sigma(c)$ flat
- Σ level increased ($r(0)>1$)

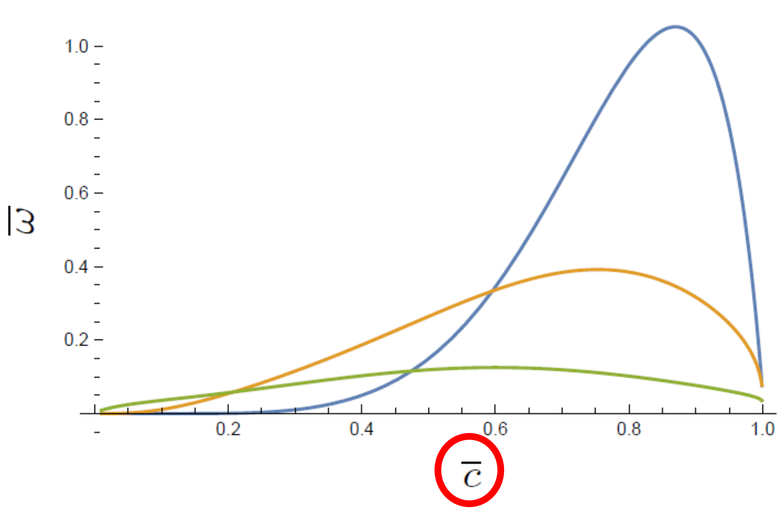
r(x)

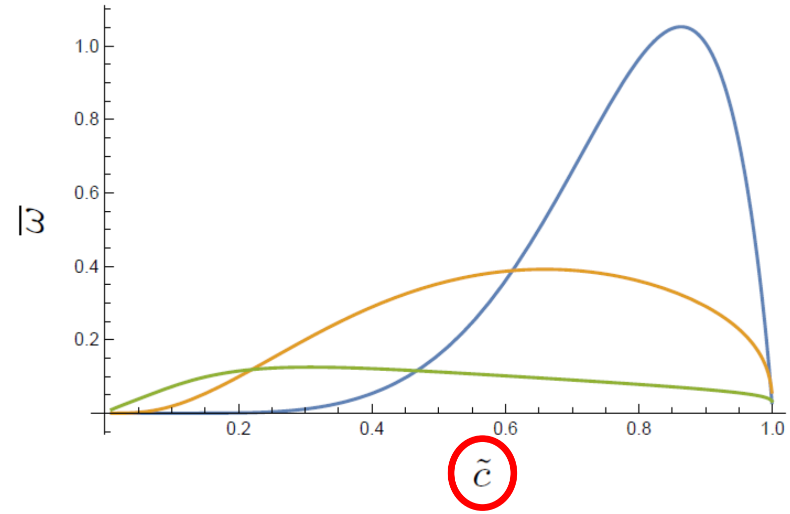




DNS (RANS filter)

LES model for $\overline{\omega}$ vs. $\tilde{c}$

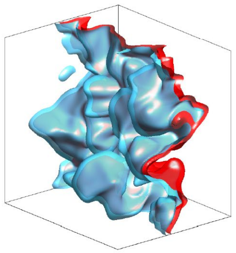
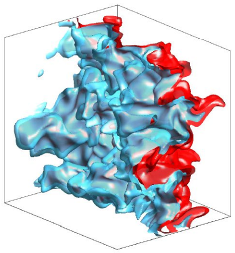




- Generate 1D $\tilde{c}(x_m)$ from 1D filtered $\overline{\rho c}$

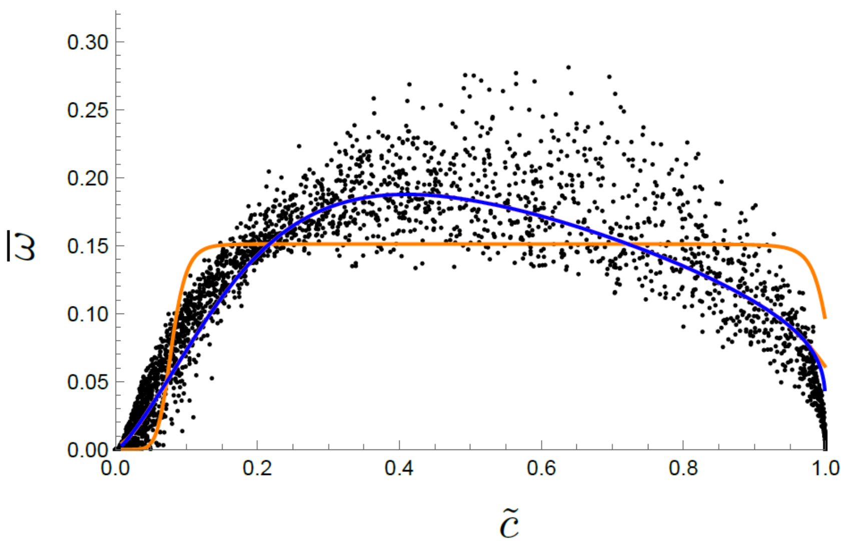
- Plot $\overline{\omega}(x_m)$ vs. $\tilde{c}(x_m)$

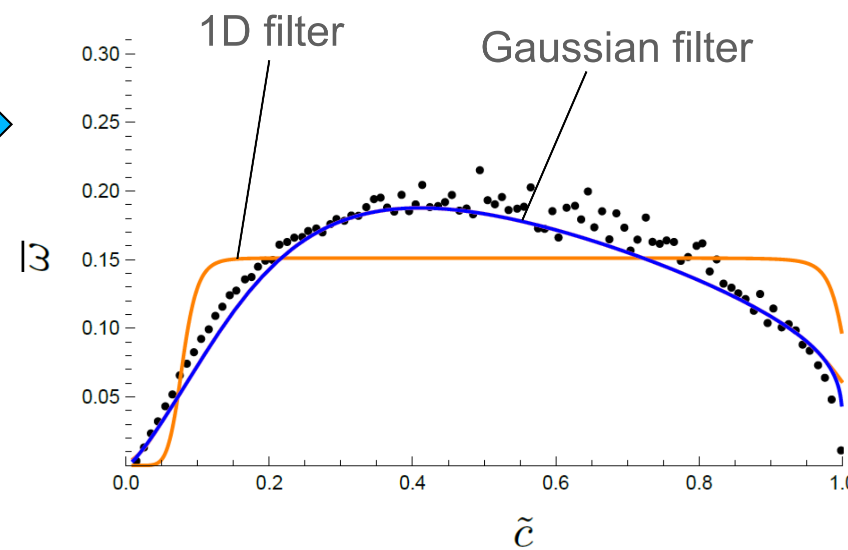
Filtering / binning of DNS data

– $\overline{\omega}$ box-filtered from DNS

- sort / average $\overline{\omega}$ in $\tilde{c}$ bins



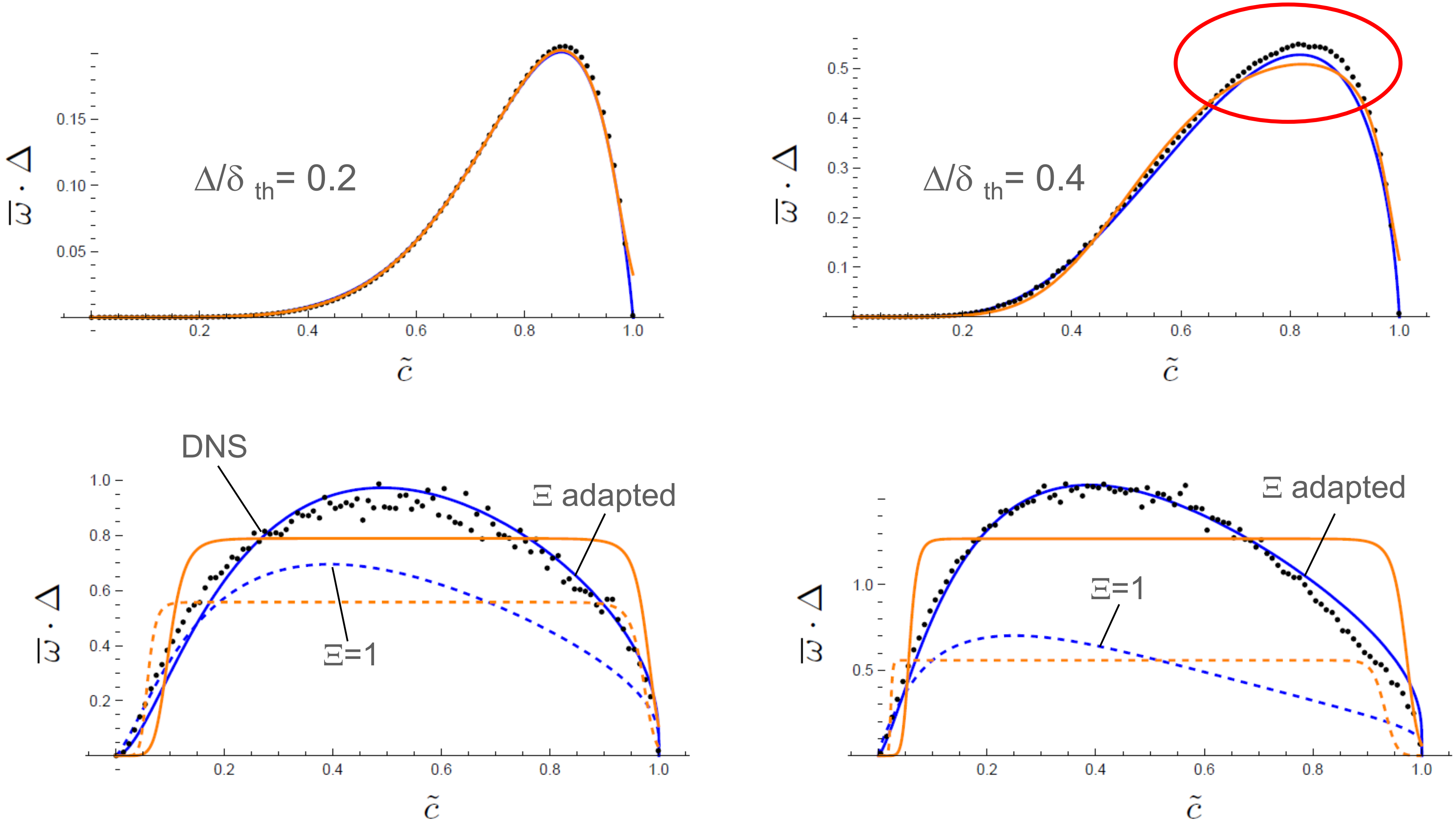


Raw filtered DNS ω

Filtered + binned DNS ω

DNS validation of model $\overline{\omega}$ vs. $\tilde{c}$

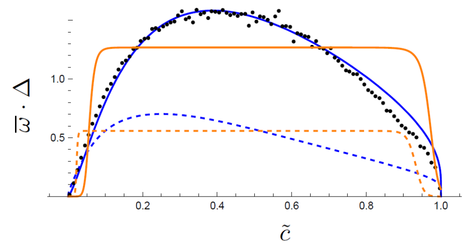
subgrid wrinkling effect



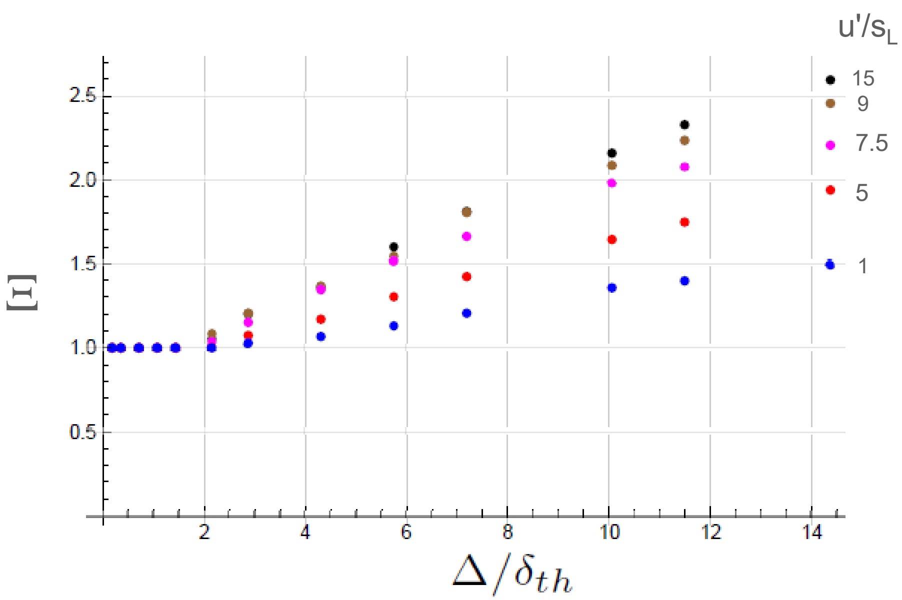
u'/s_L = 7.5, Δ/δ_{th} = 4.8

u'/s_L = 15, Δ/δ_{th} = 11.2

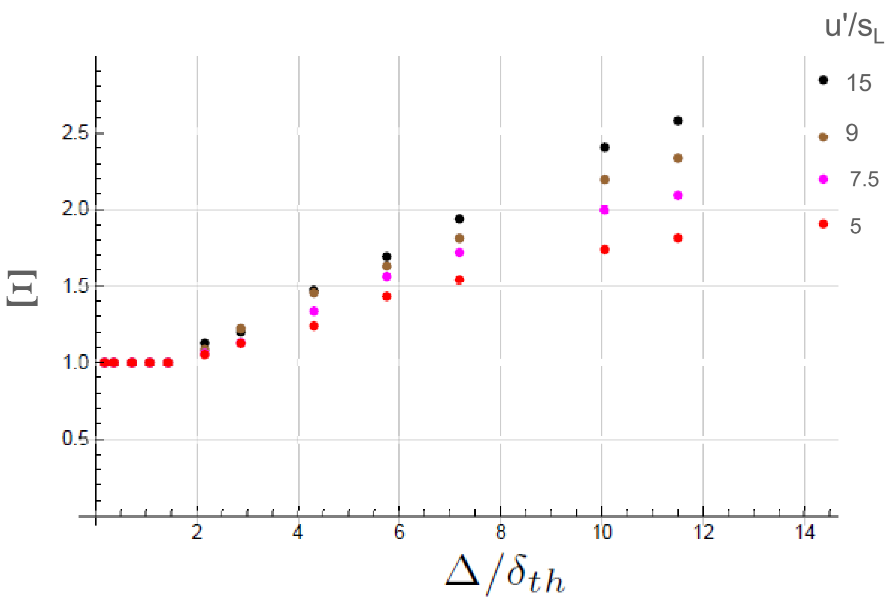
DNS-fitted wrinkling factors



Wrinkling factor Ξ derived from fit to DNS ω_{max}



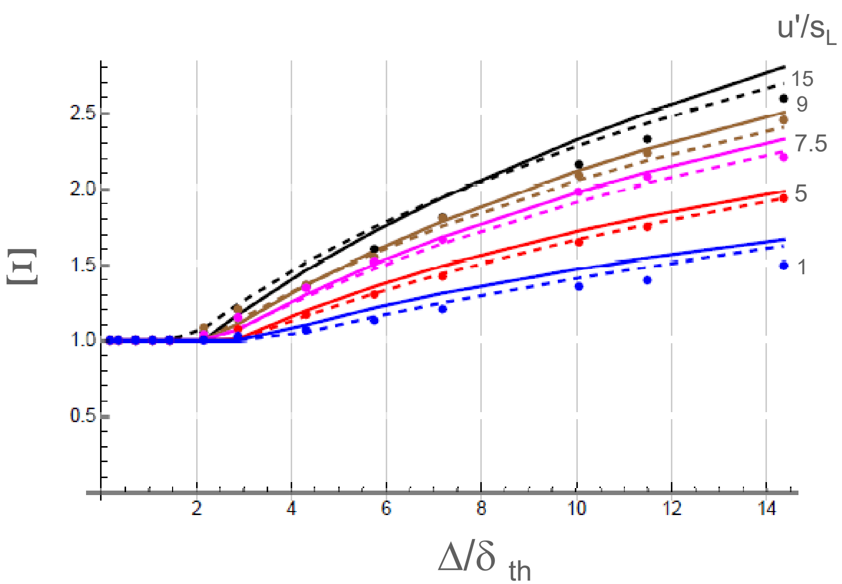
τ=4.5



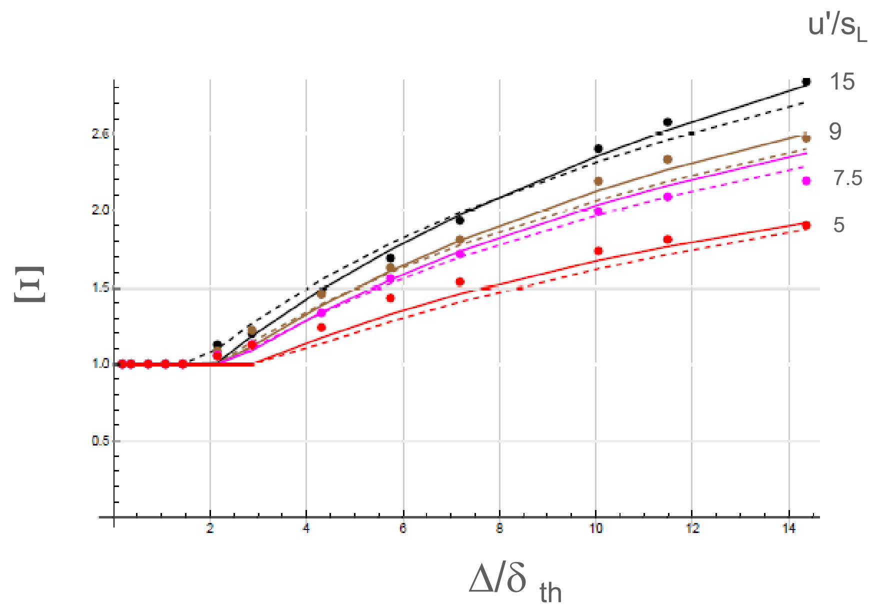
τ=3

Wrinkling factor models

solid lines: mod. Fureby model (u'_Δ/s_L), dashed: mod. Keppler model (Ka_Δ)



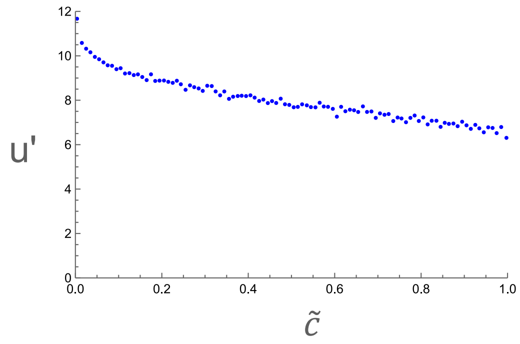
τ=4.5

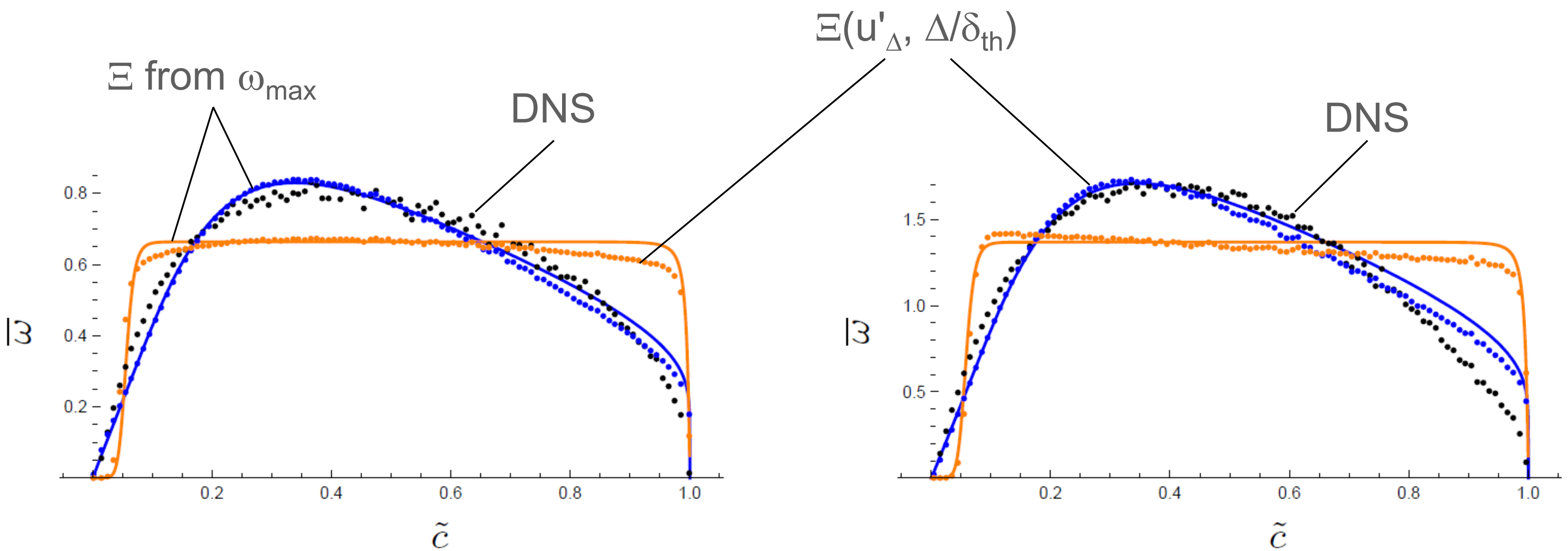


τ=3

Validation wrinkling factor models

- Filter at $\Delta' = \Delta/\Xi$
- $\Xi(u'_\Delta, \Delta/\delta_{th})$ from model with $\tilde{c}$-binned u'_Δ

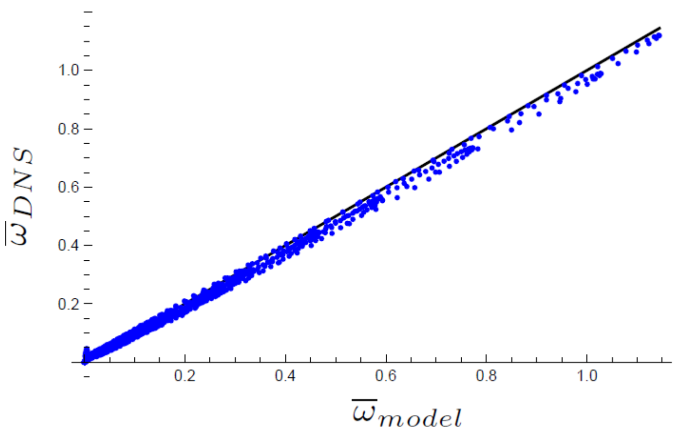




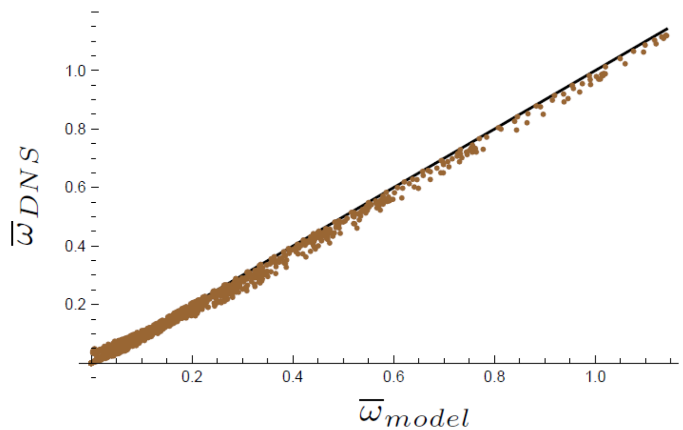
$u'/s_L = 1$, $\Delta/\delta_{th} = 6.4$

$u'/s_L = 15$, $\Delta/\delta_{th} = 12.5$

Validation of complete new model

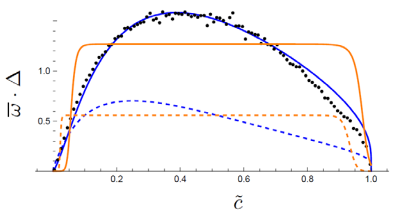


u'/s_L = 1, all Δ



u'/s_L = 9, all Δ

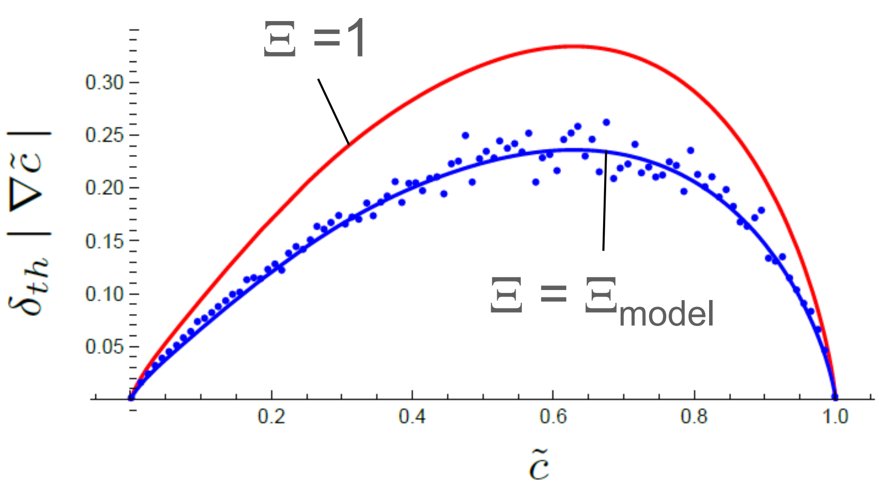
Filtered DNS ω vs. model ω



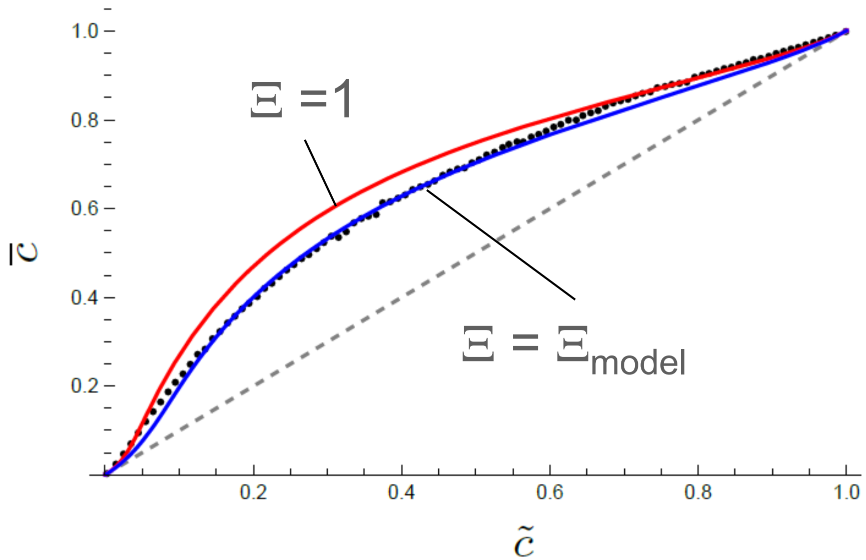
- Same results for modified Fureby / Keppeler wrinkling factors
- Agreement similar for all u'/s_L, Δ/δ_{th} and for τ=3, 4.5
- no model parameter fitted to particular case

Prediction of other variables

- Filter other 1D quantities at Δ/Ξ



LES gradient of $\tilde{c}$



Relation between $\bar{c}$ and $\tilde{c}$

Overview

Introduction – LES of turbulent premixed flames

Premixed laminar flame structure

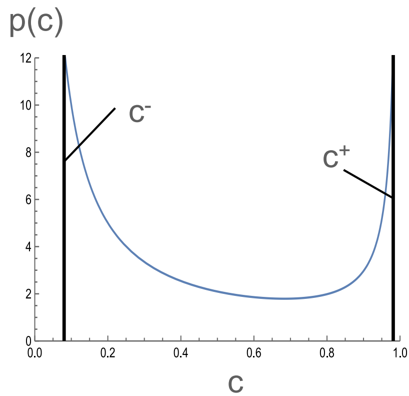
Laminar flame pdf

Multidimensional effects

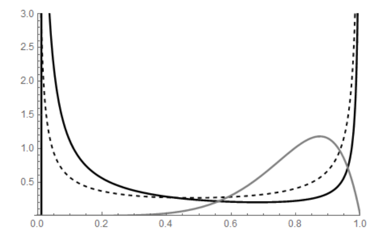
Valididation with DNS data

Conclusions and future work

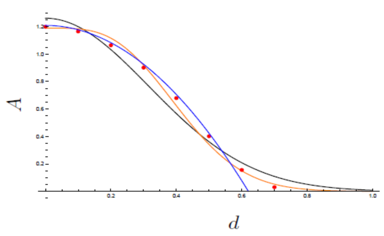
Conclusions

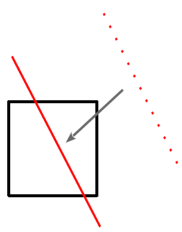


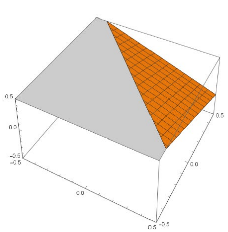
- Analytic c(ξ), source term ω(c) and pdf for premixed combustion
- Flamelet pdf not integrable for c→0,1
- $\bar{c}$ or $\tilde{c}$ and Δ/δ_{th} determine pdf limits c^-,c^+
- no δ functions at c=(0,1)
- Flamelet pdf more accurate than β pdf at large Δ/δ_{th}

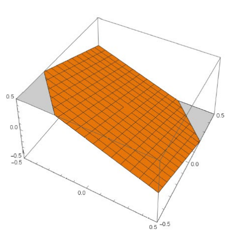


- Multidimensional effect: slicing area A(d)
- Generates filter kernel r(x)



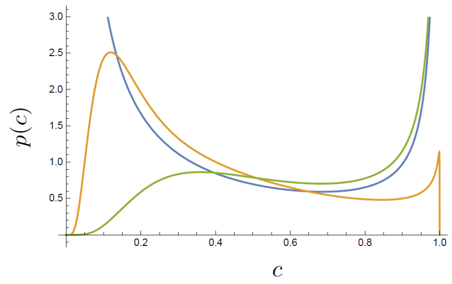


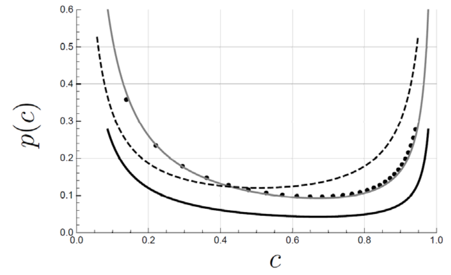


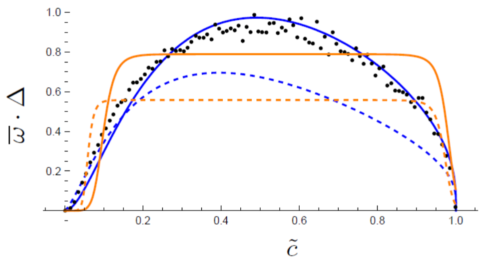


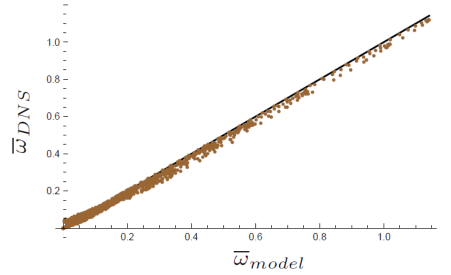
Conclusions (II)

- Complicated multi-D effects on flamelet pdf
- ~ 1D pdf with constant Ξ for large filters
- Analytic model for $\tilde{c}(x_m)$, $\overline{\omega}(x_m)$: 1D filter with kernel r(x)
- Wrinkling factor effect: filter 1D profiles at Δ'= Δ/Ξ
- Ξ models derived from DNS data
  (mod. Fureby, mod. Keppeler)
- Good agreement with ALL filtered/binned DNS data









Thank YOU for YOUR attention !

Backup

Simple analytic expressions for means

Cell averaged source term:

$$\boxed{\overline{\omega(c)}_m} = \int_0^1 \omega_m(c) p_m(c) dc = \frac{1}{\Delta} \int_{c^-}^{c^+} \frac{\omega_m(c)}{c(1-c^m)} dc = \boxed{\frac{(c^+)^{m+1} - (c^-)^{m+1}}{\Delta}}$$

Cell averaged flamelet source:

$$\boxed{\overline{\frac{\partial^2 c}{\partial \xi^2} + \omega(c)}} = \overline{\frac{\partial c}{\partial \xi}} = \frac{1}{\Delta} \int_{c^-}^{c^+} \frac{\frac{\partial c}{\partial \xi}}{dc/d\xi} dc = \frac{1}{\Delta} \int_{c^-}^{c^+} dc = \boxed{\frac{c^+ - c^-}{\Delta}}$$

True for ALL flamelet pdf's

Conclusions flamelet / beta pdf

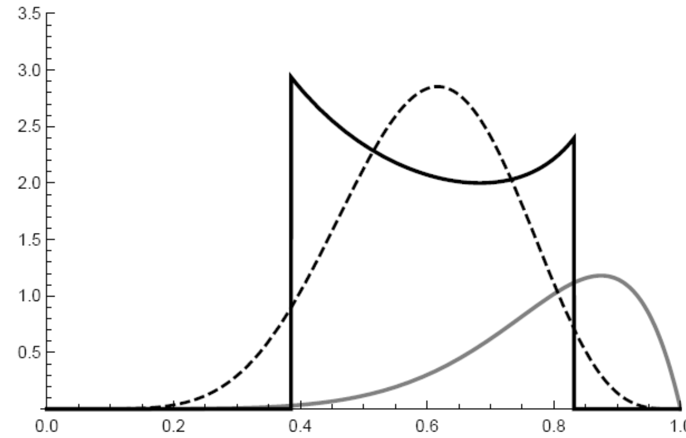
- Flamelet pdf: form independent of $\bar{c}, \Delta$

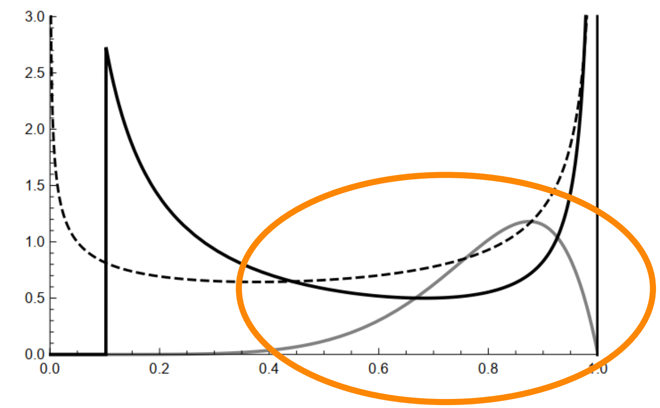
  c^-, c^+ depend on $\bar{c}, \Delta$

- Beta pdf: depends on $\bar{c}, \overline{c'^2}$

- Beta pdf overpredicts $\overline{\omega}$ for large Δ/δ_f

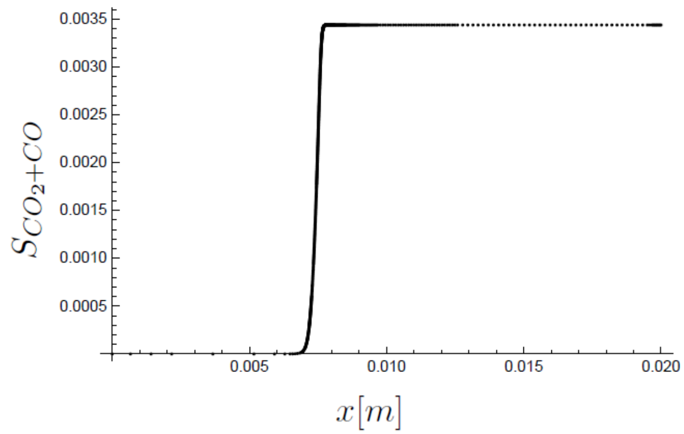
- $\overline{\omega}$ insensitive to pdf for small Δ



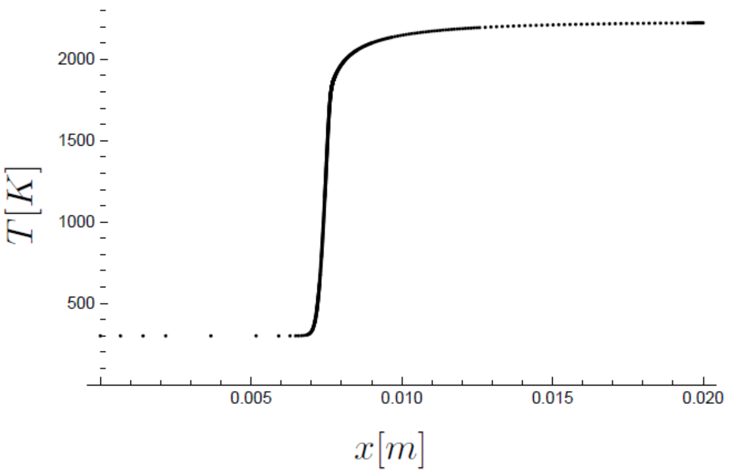


$\overline{\omega_\beta} \sim 2 * \overline{\omega}_{exact}$

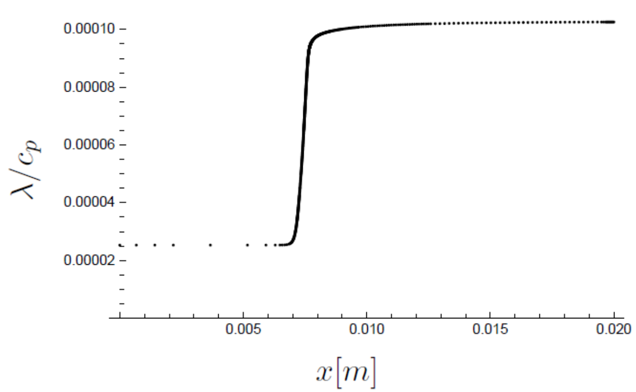
Analytic profile with GRI 3.0 chemistry

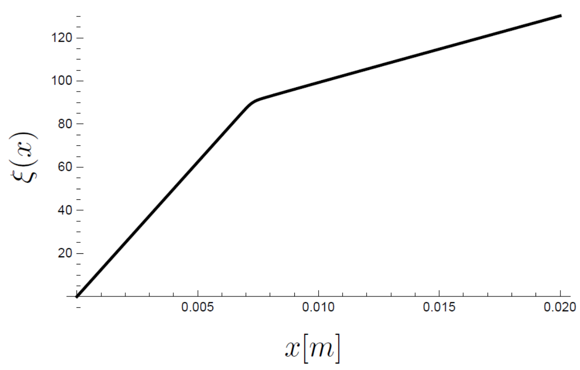


ϕ=1 profile of $y_{CO}/W_{CO}+y_{CO2}/W_{CO2}$



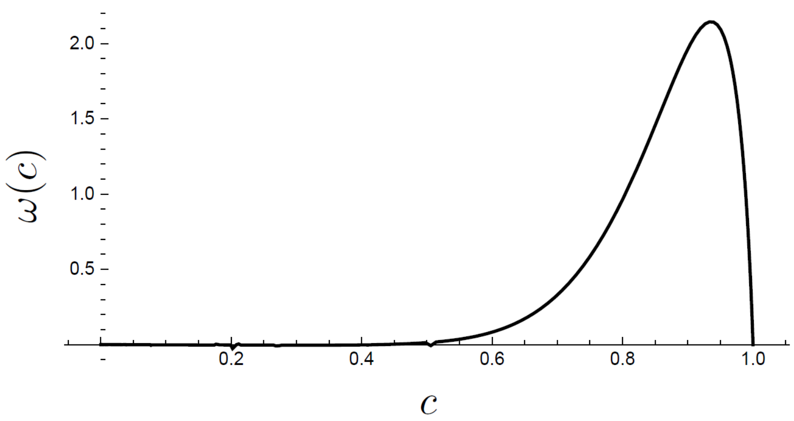
ϕ=1 profile of temperature



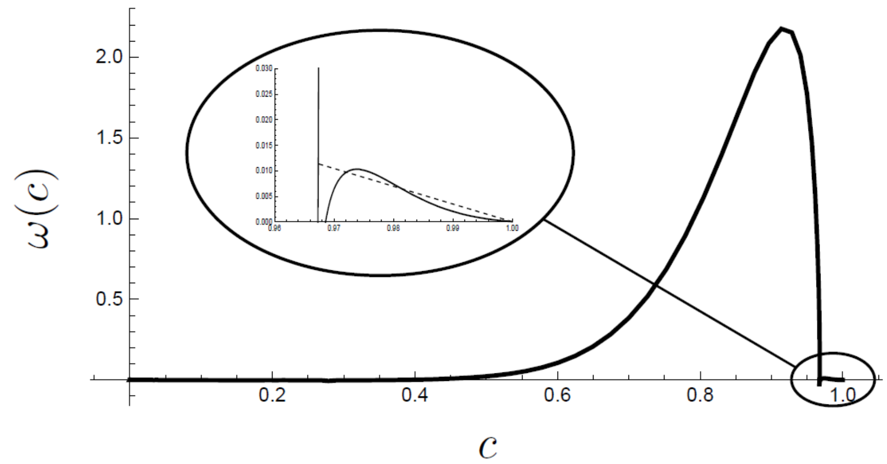


Transformation from x to canonical coordinate

Analytic profile with GRI 3.0 chemistry



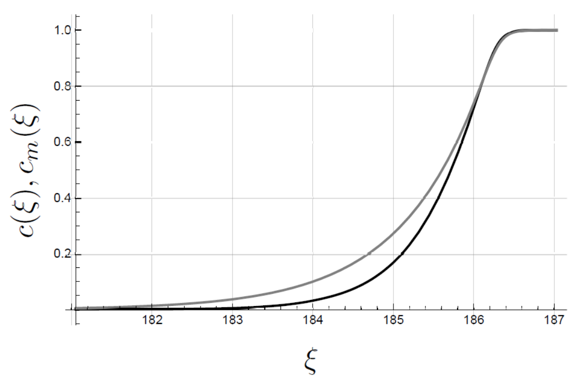
ϕ=1 source term of $y_{CO}/w_{CO}+y_{CO2}/W_{CO2}$



ϕ=1 source term of $y_{H2}/W_{H2}+y_{H2O}/W_{H2O}$

Effect of strain:

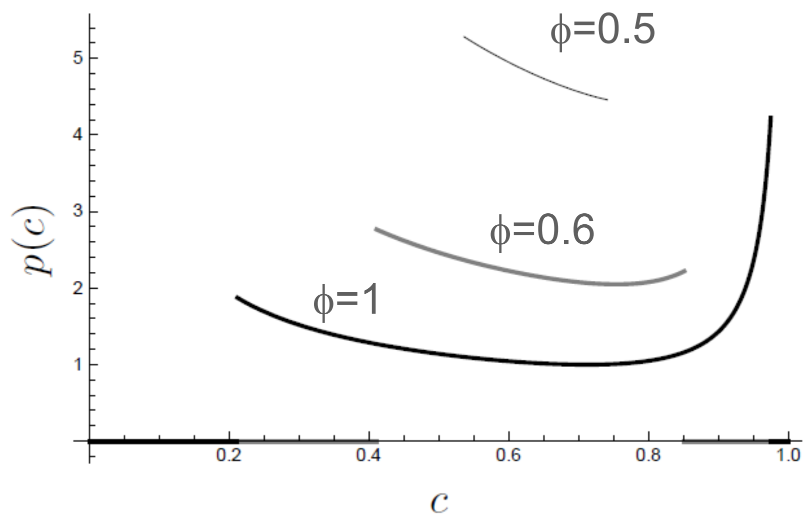
- drop of s_L
- thinner reaction zone



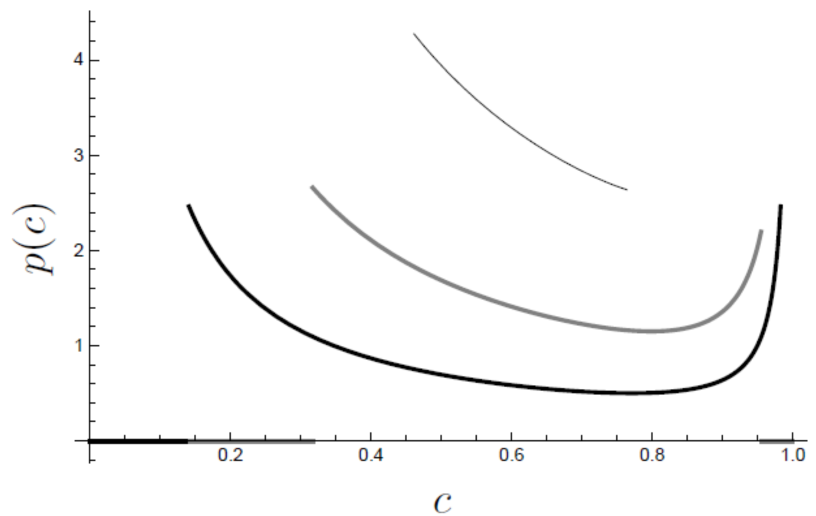
PDF for stratified flames

- leaner flame → thicker reaction zone

→ different scaling from x to ξ

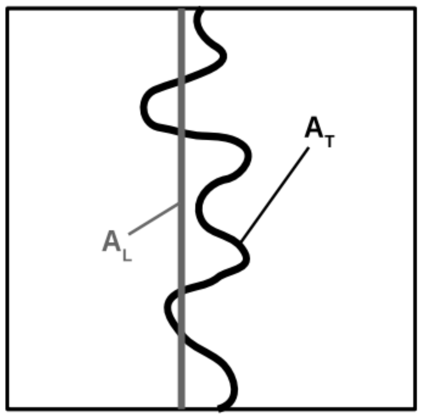


PDF with real c_p/λ



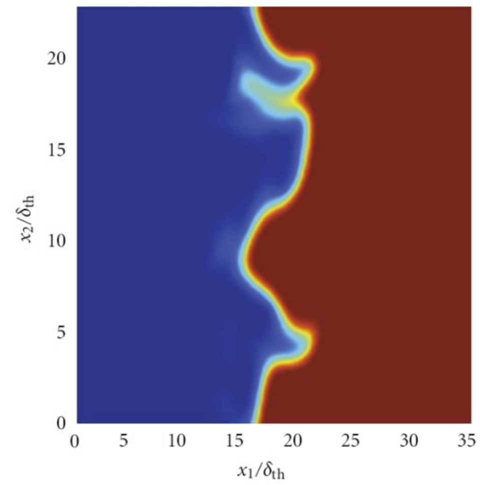
PDF with unburnt value of c_p/λ

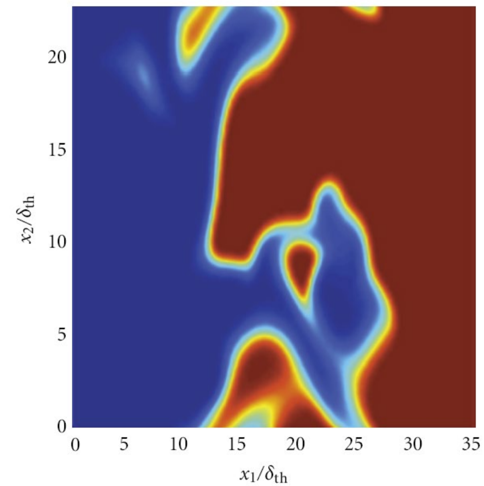
Effects of flame wrinkling



FSD type assumption:

$$\Sigma_{wrinkled} = \Xi\, \Sigma_{laminar}$$





Chakraborty, Klein, Cant, J. Combustion, 2011, doi:10.1155/2011/473679

Wrinkling factor models

$$u_F = 1.4 \cdot \left(\frac{u'_\Delta}{s_{L0}} \right)$$

$$D_F = \frac{2}{u_F + 1} + \frac{7/3}{1/u_F + 1}$$

$$\Gamma_F = 0.19 \cdot u_F \cdot \left(\frac{\Delta}{\delta_{th}} \right)^{1.15}$$

$$\Xi_F = Max \left[1, \Gamma_F^{D_F - 2} \right]$$

Modified Fureby model

$$Ka_\Delta = \left(\frac{u'_\Delta}{s_L} \right)^{3/2} \left(\frac{\Delta}{\delta_{th}} \right)^{-1/2}$$

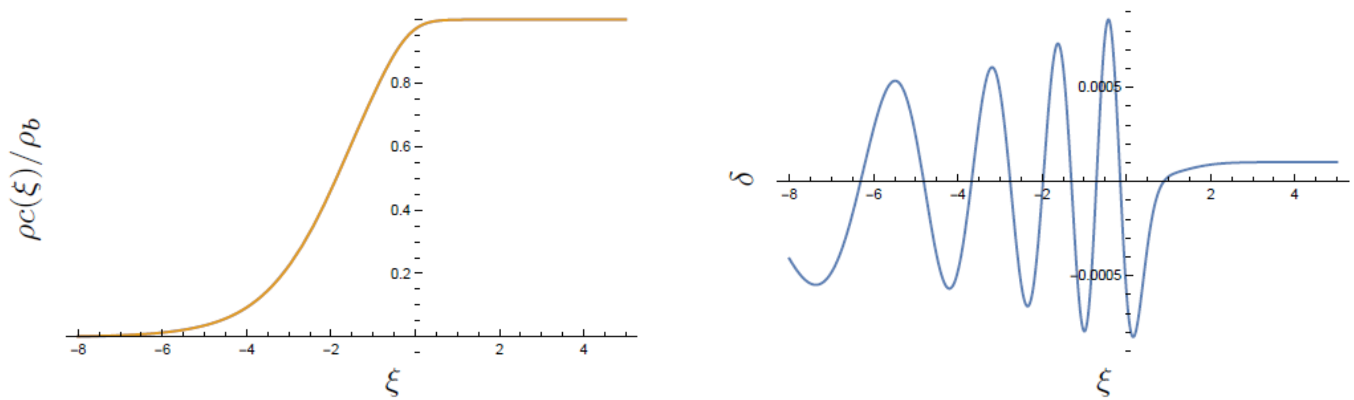
$$D_k = \frac{8/3 \cdot Ka_\Delta + 3.1}{Ka_\Delta + 1.4}$$

$$\Gamma_k = 0.69 \left(2 * \frac{\Delta/\delta_{th}}{max(Ka_\Delta^{-1/2}, 2))} \right)$$

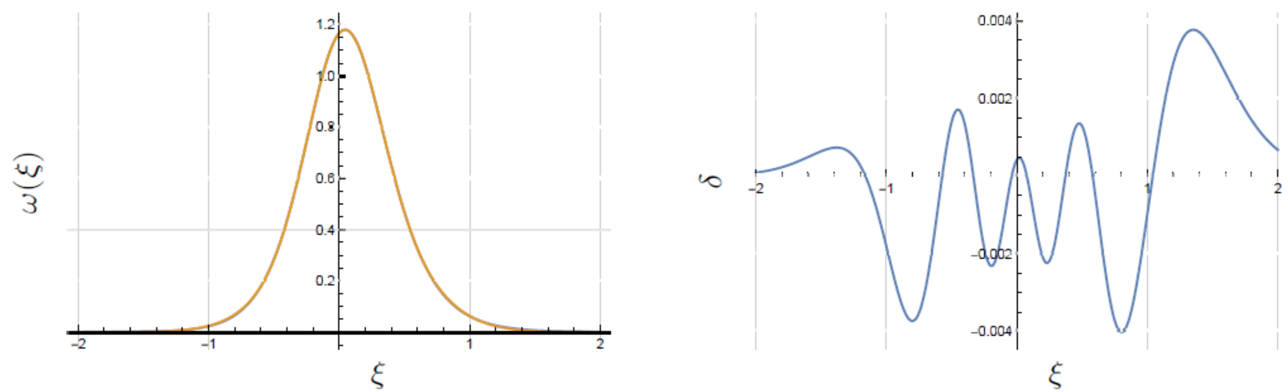
$$\Xi_k = Max \left[1, \Gamma_k^{D_k - 2} \right]$$

Modified Keppeler model

Representation of ρ(x)c(x), ω(x)



Approximation of ρ(x)c(x) by 4 erf functions



Approximation of ω(x) by 3 Gaussians