Imperial College London

# Numerical Modelling of Deflagration to Detonation Transition

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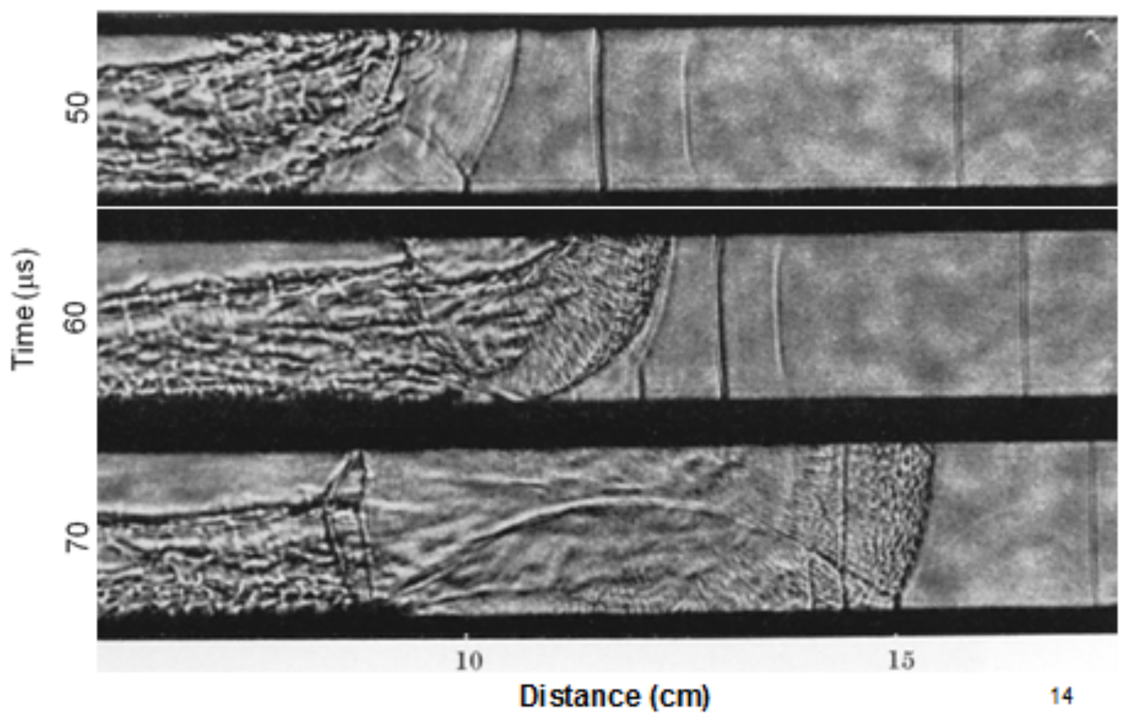
54th UKELG Discussion Meeting "Advances In Explosion Modelling"

University of Warwick, 30th October 2015

# Deflagration to Detonation Transition (DDT)




- Transition distance
- DDT times
- Overpressures


*Can we predict DDT in realistic geometries with reasonable cost?*

# Motivation

- *Can anything be modelled sufficiently accurately?*
- Modelling Deflagrations, Premixed Flames ?

  B-
- Modelling  Detonation Waves ?

  B
- Modelling DDT  ….?

# What affects DDT?

Fluid Instabilities

Chemistry (ignition)

Turbulence

Pressure

Transport Properties

Non-ideal gas

# Challenges of Modelling DDT

Wide Range Scales

Premixed flame

Chemistry

Turbulence

Shock/Detonation Front

# Approaches….

- Adaptive Mesh Refinement (AMR)
    - Numerical technique

DNS

- Turbulent Premixed Models +
    - Premixed model + ad-hoc  DDT criteria

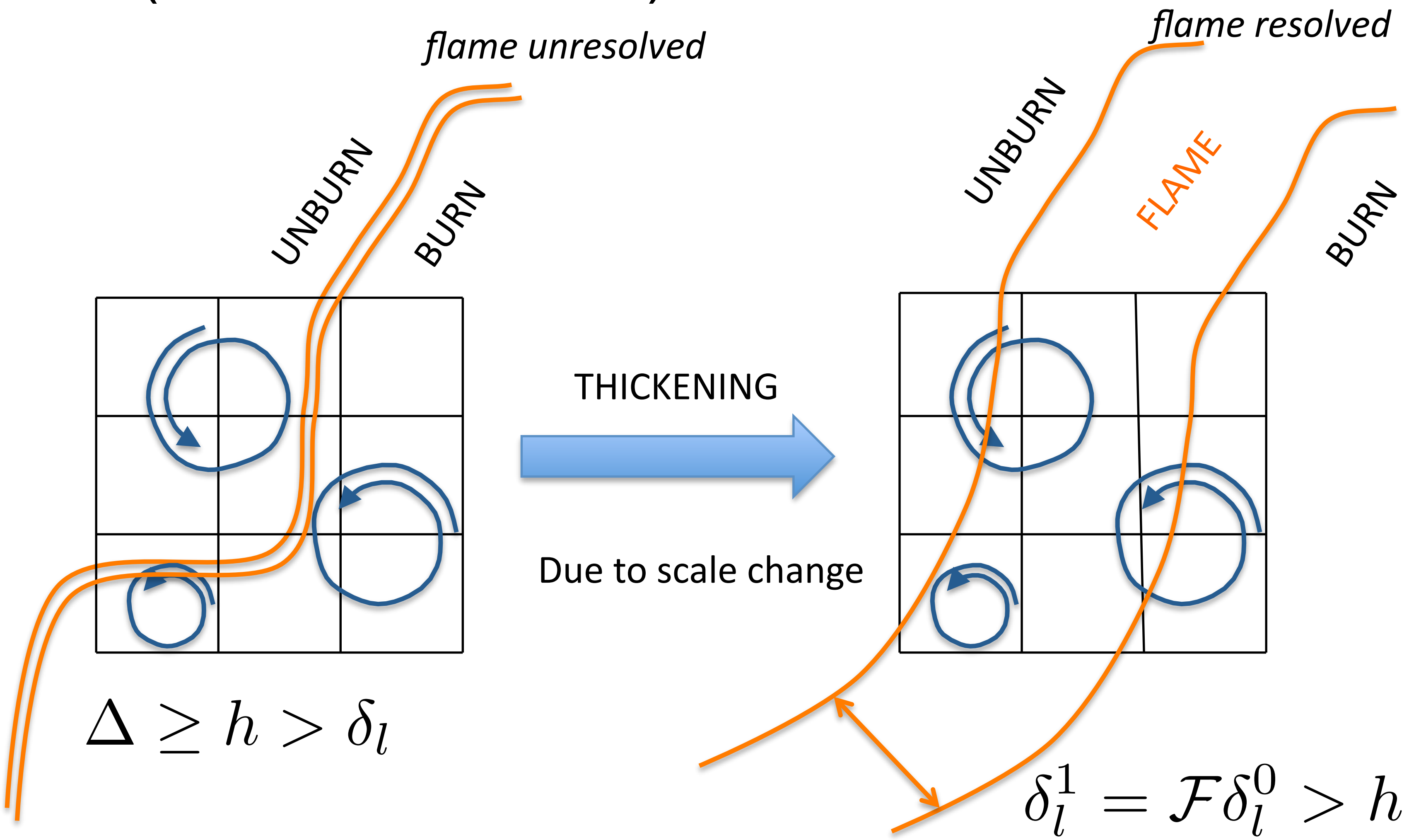
LES/URANS?

- Artificial Thickening
    - Modelling approach

LES

# Artificial Thickening

- ATF (or TFLES or TFM)




Flame Structure??

# ATF-Transformation

- Transformation of *time* and *length* scales

$$d\xi = \mathcal{F} dx \qquad d\tau = \mathcal{F} dt$$

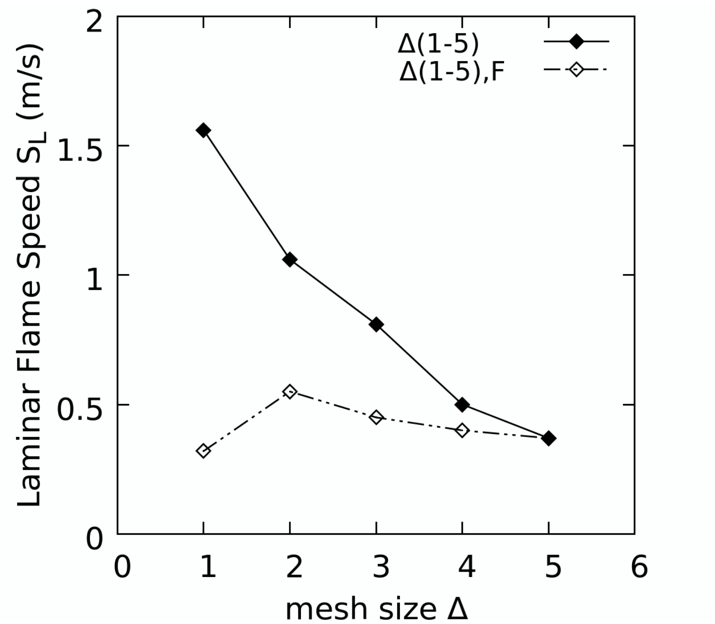
- Laminar flame speed "preserved"

$$\frac{d\xi}{d\tau} = \frac{dx}{dt} \qquad s_l \equiv s_l^1 = s_l^0$$

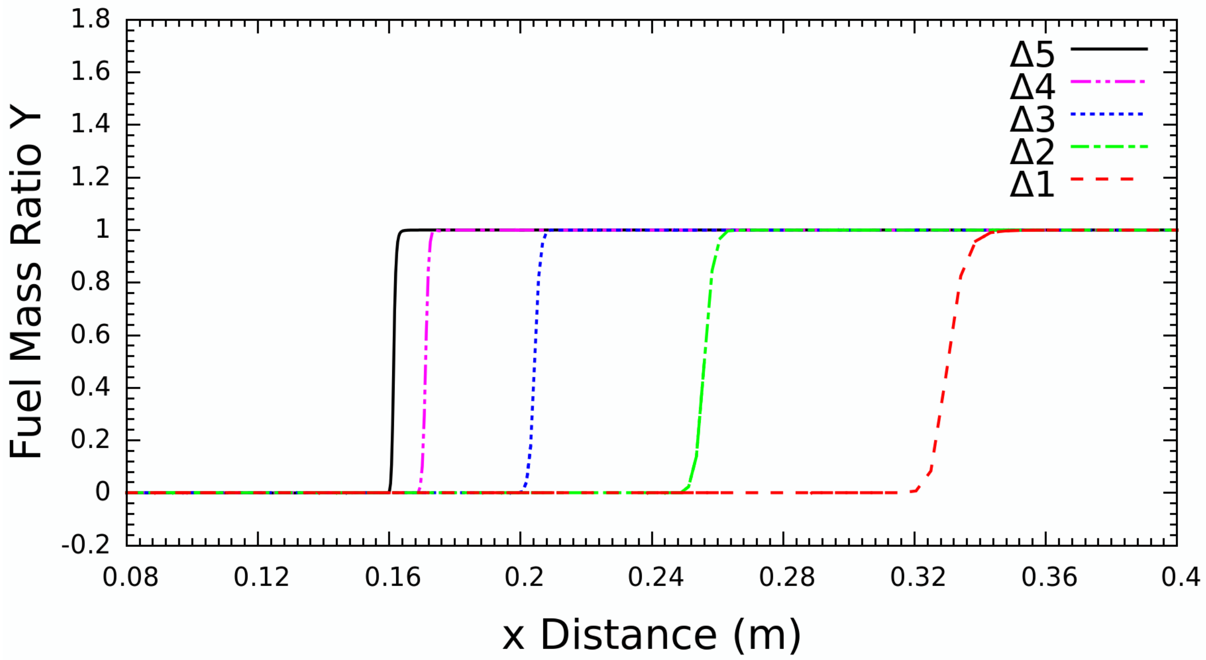
- New flame thickness (resolved ??)

$$\delta_l^1 \sim \mathcal{F} \delta_l^0$$

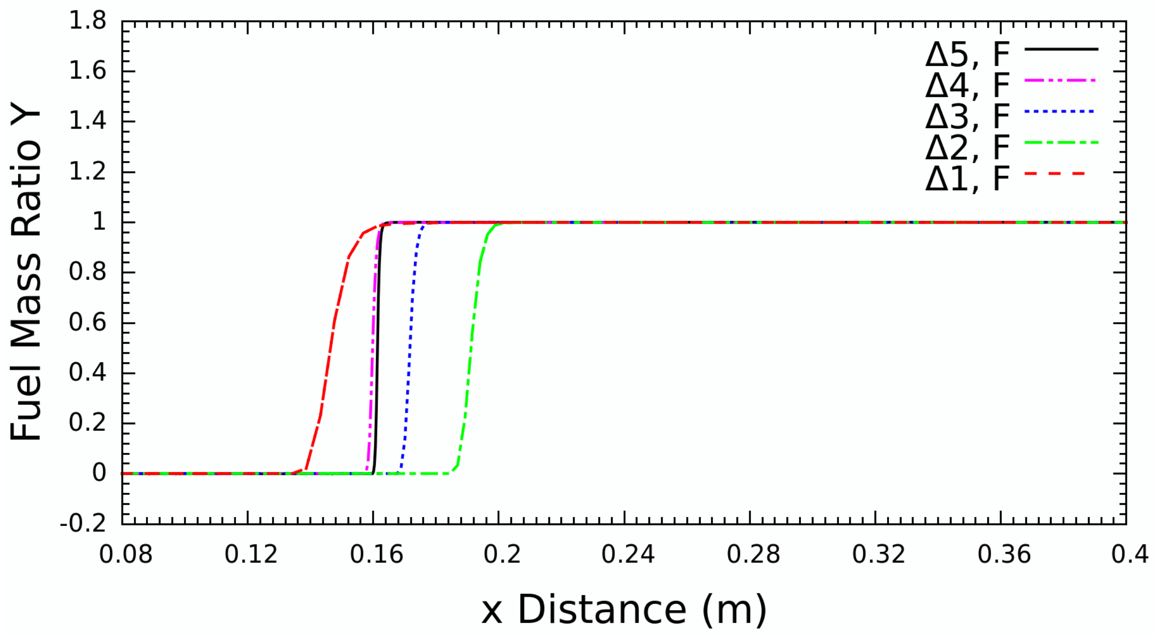
# Premixed Laminar Flame




$$\Delta_k = \Delta_1 2^{-k}$$




no-model




model

# ATF-Transformation

- "New" Species transport

$$\frac{\partial \rho Y}{\partial \tau} + \frac{\partial \rho u_j Y}{\partial \xi_j} = \frac{\partial}{\partial \xi_j}\left(\mathcal{F}\rho D \frac{\partial Y}{\partial \xi_j}\right) + \frac{\dot{\omega}}{\mathcal{F}}$$

- Turbulence-Chemistry Interaction

$$\mathrm{Da}^1 = \frac{\tau_I}{\tau_c} = \frac{l_t/u'}{\delta_l^1/s_l} = \frac{l_t/u'}{\mathcal{F}\delta_l^0/s_l} = \frac{\mathrm{Da}^0}{\mathcal{F}}$$

- *Thickening increases turbulence/chemistry interaction !!*

# Restoring Interaction

- Efficiency Function

$$\frac{\partial \rho Y}{\partial \tau} + \frac{\partial \rho u_j Y}{\partial \xi_j} = \frac{\partial}{\partial \xi_j}\left(\mathcal{E}\mathcal{F}\rho D \frac{\partial Y}{\partial \xi_j}\right) + \frac{\mathcal{E}\dot{\omega}}{\mathcal{F}}$$

$$s_l^* = \mathcal{E} s_l \qquad \mathrm{Da}^* = \mathcal{E}\frac{\mathrm{Da}^0}{\mathcal{F}}$$

- Efficiency due to unresolved wrinkling

$$\mathcal{E} = \frac{\Xi_{\delta_l^0}}{\Xi_{\delta_l^1}} \geq 1$$

*very complex models?*
*in DDT context?*

$$\Xi_\delta = 1 + \alpha(\mathrm{Re})\Gamma\left(\frac{\Delta_e}{\delta}, \frac{u_{sgs}}{s_l}\right)\frac{u_{sgs}}{s_l}$$

# Alternative

- Can we thicken turbulence?

$$\mathrm{Da}^1 = \frac{l_t^1/u'}{\delta^1/s_l} = \frac{\mathcal{F} l_t/u'}{\mathcal{F}\delta^0/s_l} = \mathrm{Da}$$

- No efficiency function needed

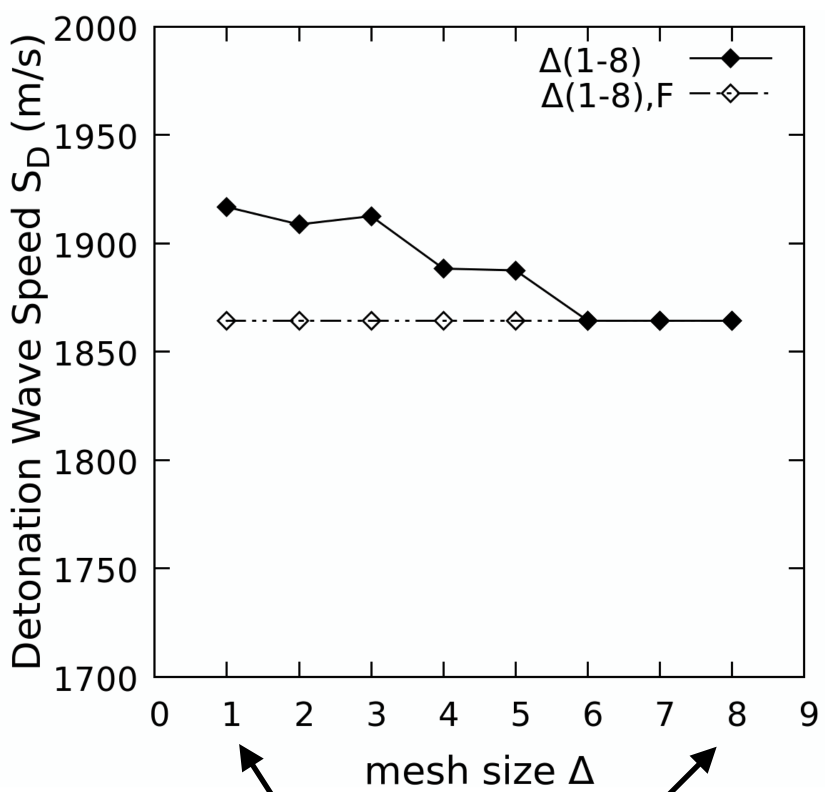
- Need variable thickening (otherwise domain bigger !!)

$$\mathcal{F}(x) \qquad\qquad \mathcal{F} = 1 + (\mathcal{F}_{max} - 1)\,\Omega$$

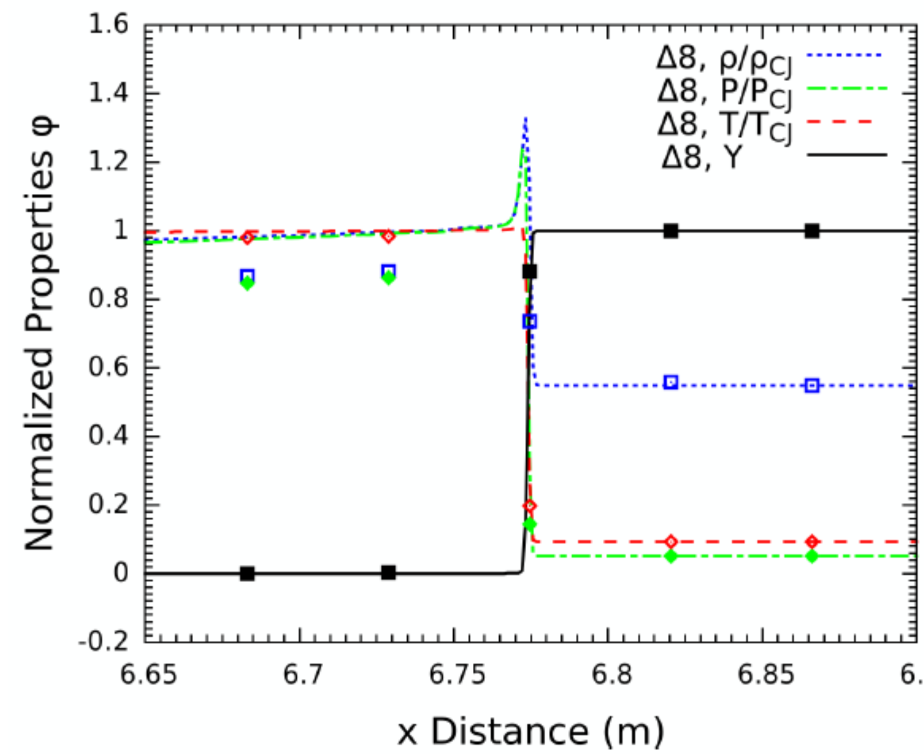
- Thickened region sensor

$$\Omega = 16 Y^2 (1 - Y)^2$$

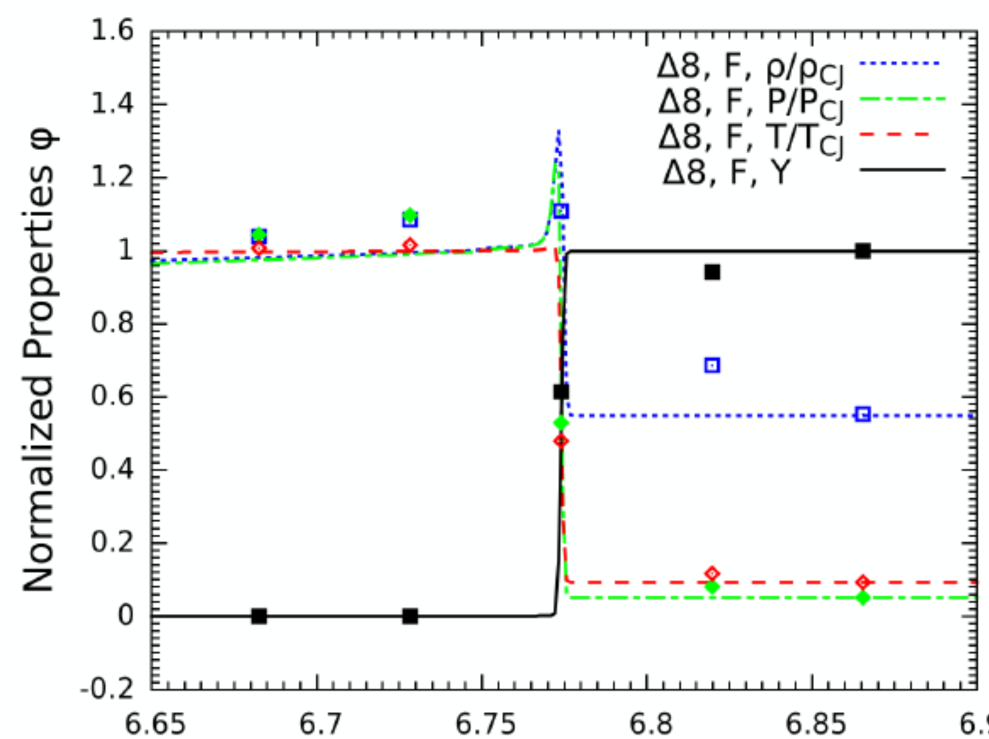
# Detonation Wave




cost ratio
1:16380



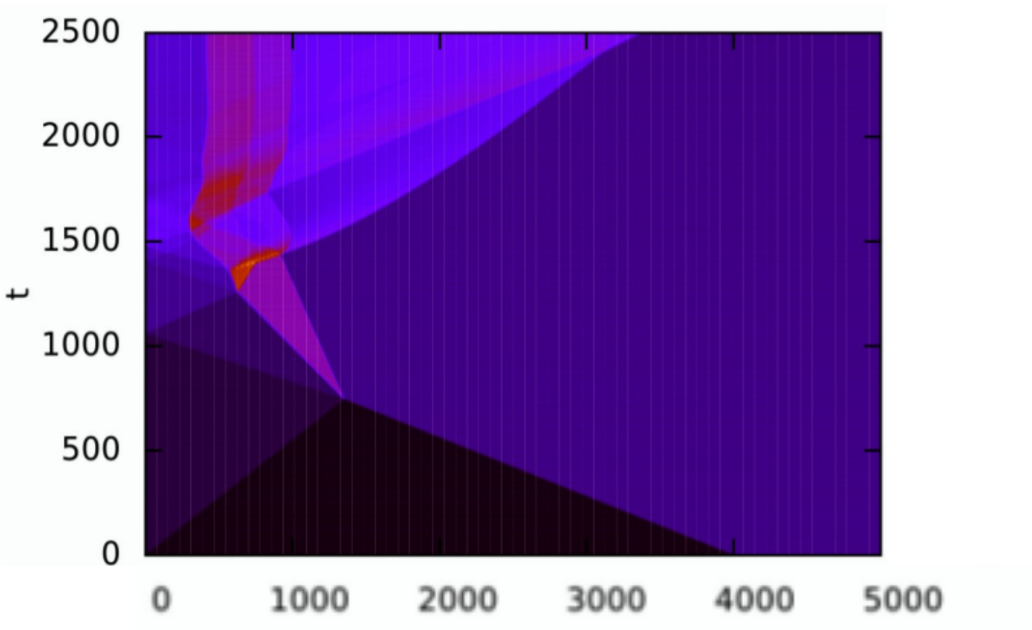

no-model




model

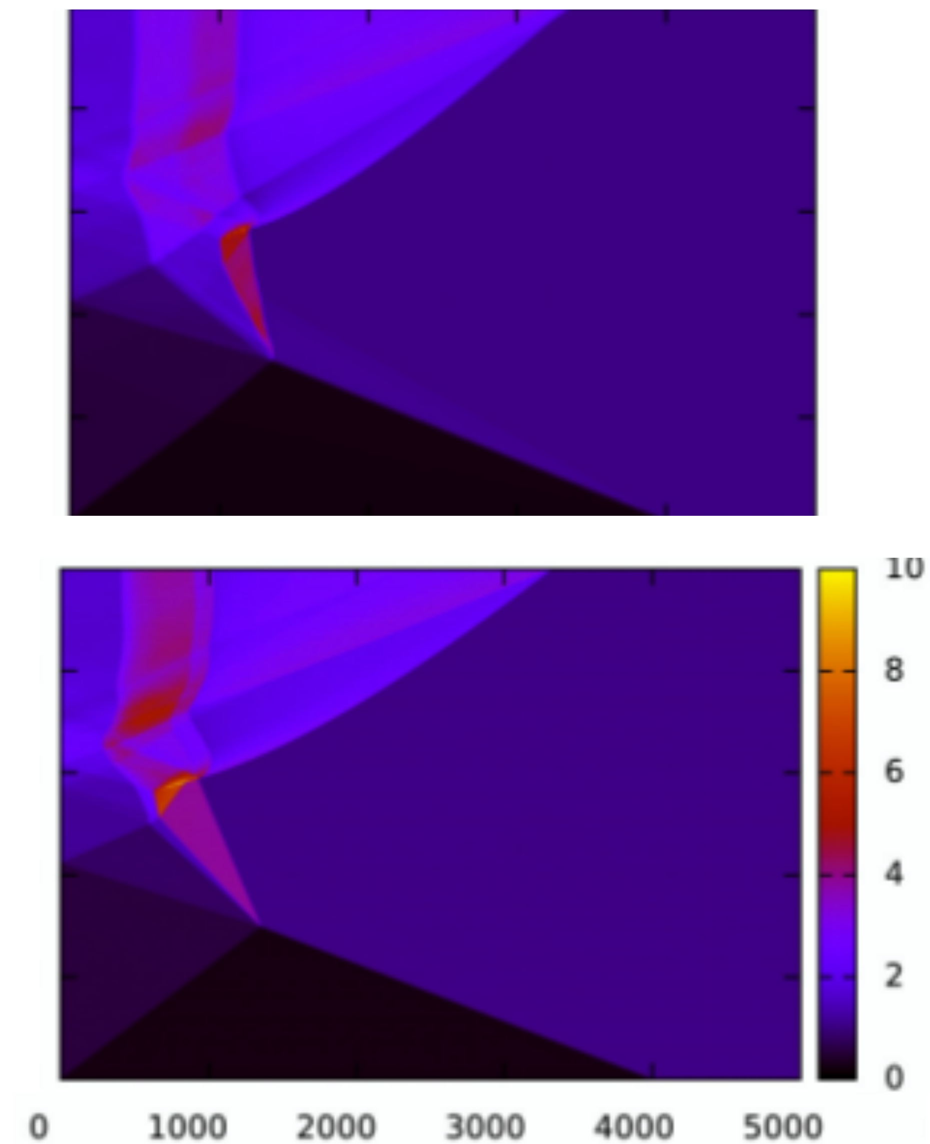
# Detonation Initiation

"DNS" $\Delta = \delta/64$




$x/\delta$ ⟵

$M_s$=2.2




no-model

model

$x/\delta$

$\Delta = \delta$

Shock-Flame Interaction Test,
Maxwell et al (2015)

# LES -ATF

F inside

SGS contribution
(outside thickened region)

$$\frac{\partial \overline{\rho}}{\partial \tau} + \frac{\partial \overline{\rho}\,\widetilde{u}_i}{\partial \xi_i} = 0,$$

$$\frac{\partial \overline{\rho}\,\widetilde{u}_i}{\partial \tau} + \frac{\partial \widetilde{\rho}\,\widetilde{u}_i\,\widetilde{u}_j}{\partial \xi_j} + \frac{\partial \overline{p}}{\partial \xi_i} = \frac{\partial \check{\sigma}_{ij}}{\partial \xi_j} - (1-\Omega)\frac{\partial \tau_{ij}}{\partial \xi_j},$$

$$\frac{\partial \overline{\rho}\,\widetilde{e}}{\partial \tau} + \frac{\partial (\overline{\rho}\,\widetilde{e} + \overline{p})\widetilde{u}_j}{\partial \xi_j} = \frac{\partial (\check{\sigma}_{ij}\,\widetilde{u}_i - \mathcal{F}\check{q}_j)}{\partial \xi_j} + (1-\Omega)\frac{\partial \mathcal{Q}_{H1j}}{\partial \xi_j} + \frac{\dot{\mathcal{S}}_r}{\mathcal{F}},$$

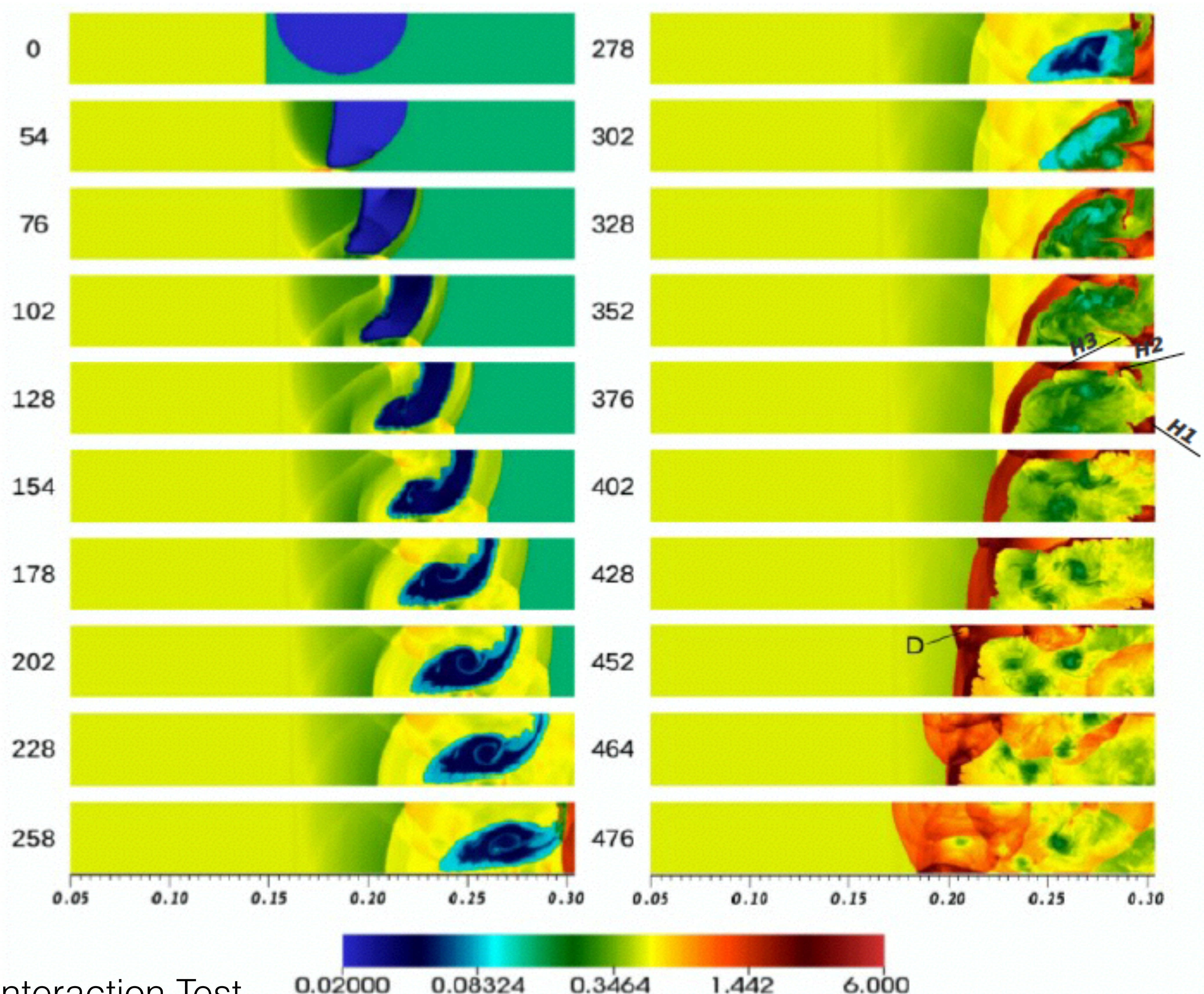
$$\frac{\partial \overline{\rho}\,\widetilde{Y}_k}{\partial \tau} + \frac{\partial \overline{\rho}\,\widetilde{u}_j\,\widetilde{Y}_k}{\partial \xi_j} = \frac{\partial}{\partial \xi_j}\left(\overline{\rho}\,\overline{\mathcal{D}}_k \mathcal{F}\frac{\partial \widetilde{Y}_k}{\partial \xi_j}\right) - (1-\Omega)\frac{\partial \mathcal{R}_{\mathcal{D}1kj}}{\partial \xi_j} + \frac{\overline{\rho}\,\check{\dot{\omega}}_k}{\mathcal{F}}.$$

chemistry

# Numerics

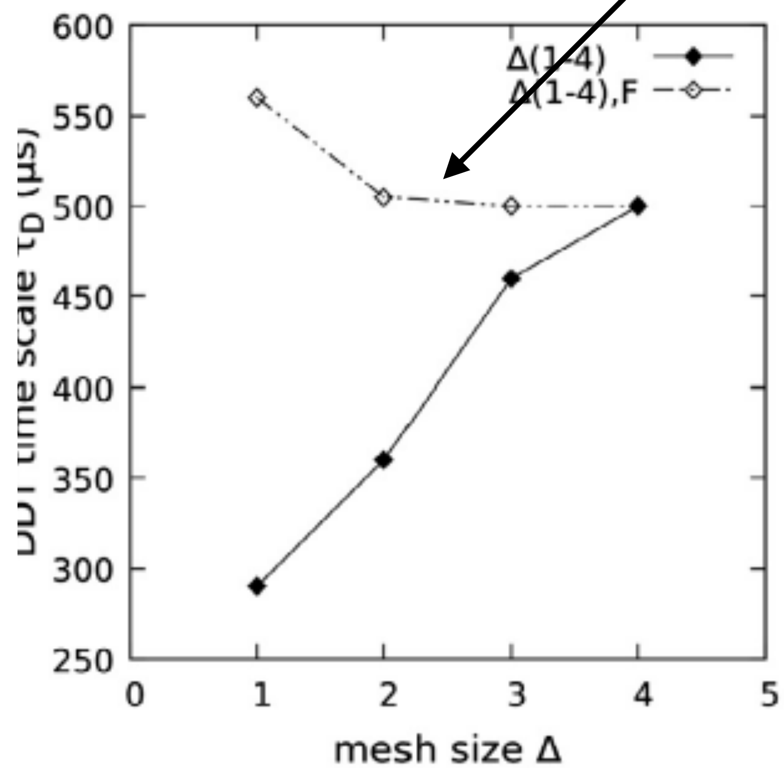
- In house code WENO5-HLLC
- Runge Kutta 3
- Shock Detector
- Smagorinsky model
- one-step kinetics
- *Other Capabilities (not used)*
    - *Detailed Transport, kinetics, no-ideal EOS*
    - *AMR*

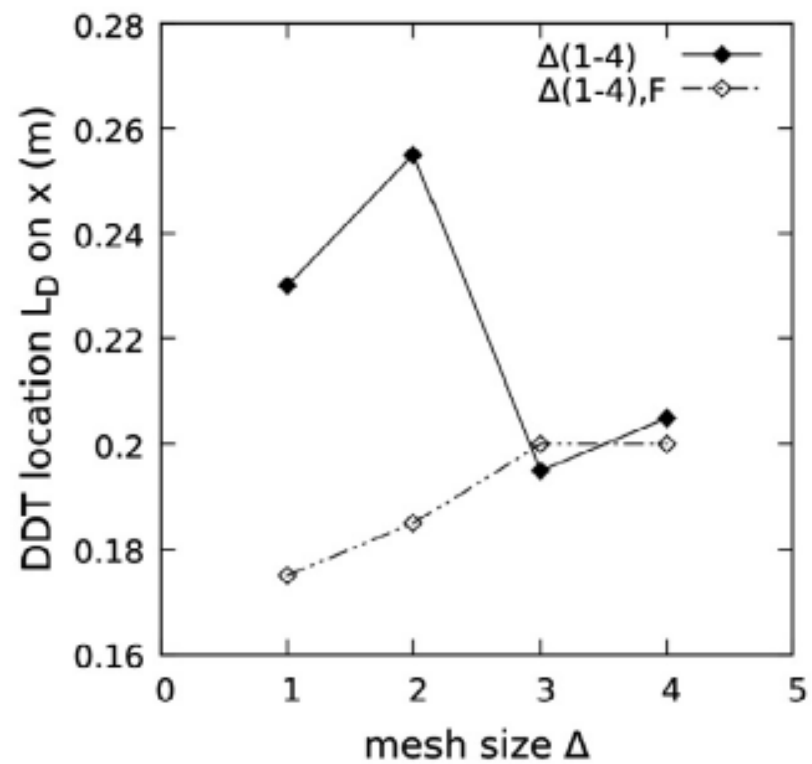
# The solution on density (kg/m³) is:



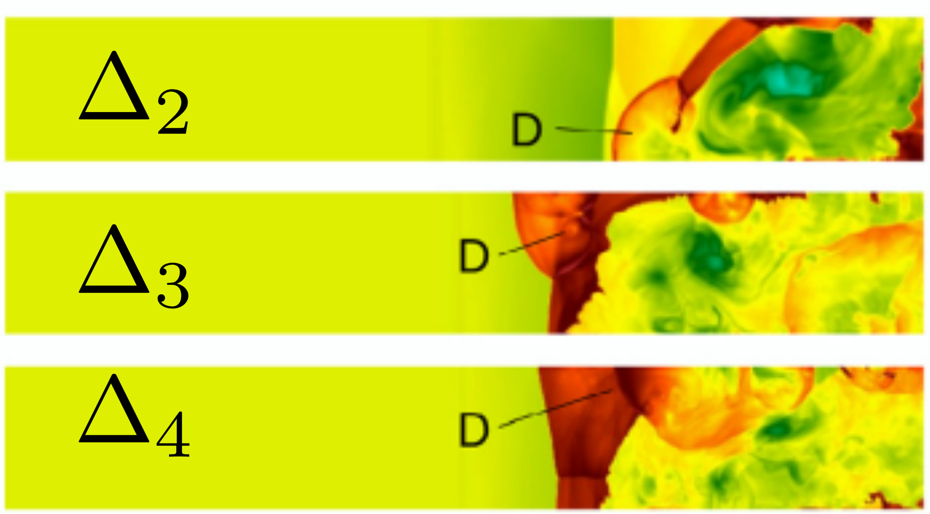

Shock-Flame Interaction Test
Gamezo (2001)

# Quasi-Mesh Independence DDT



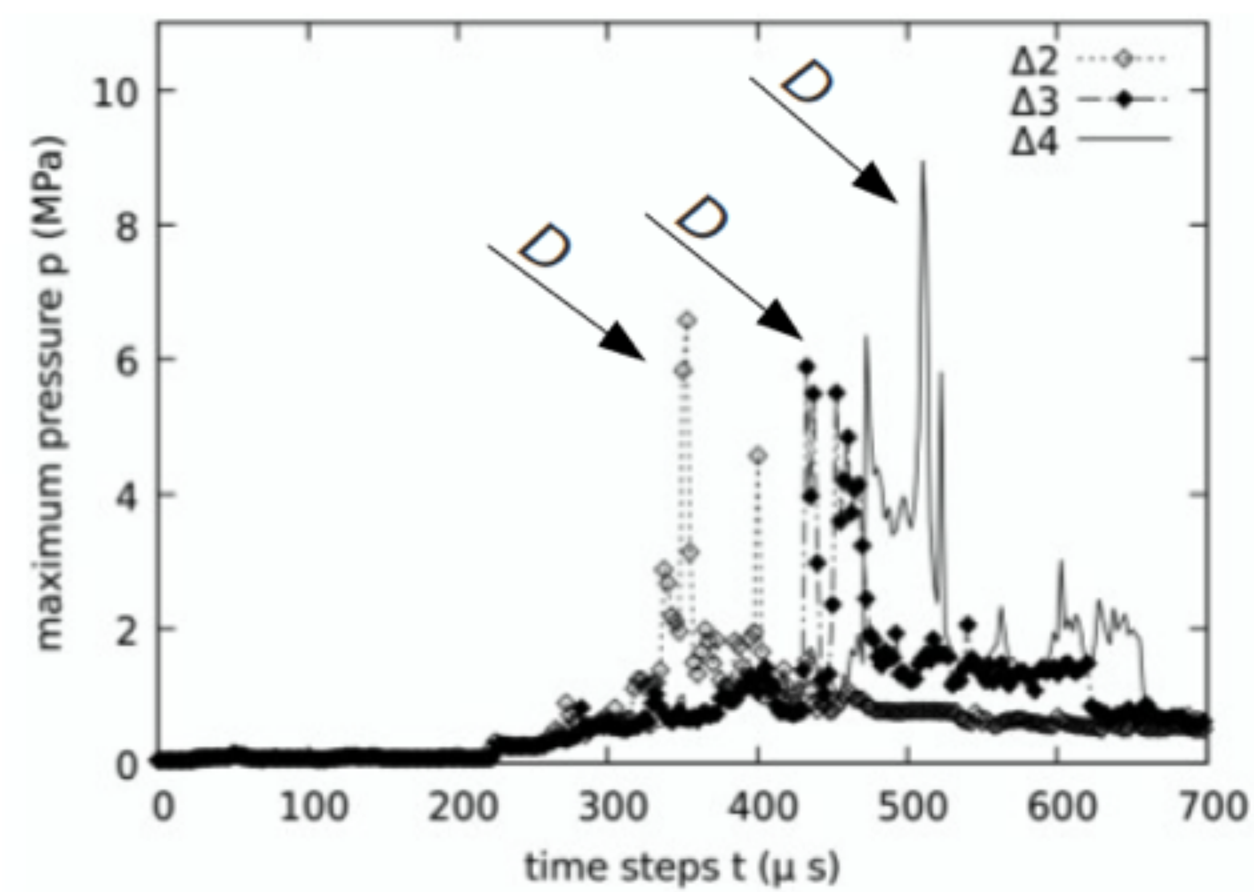

no-model



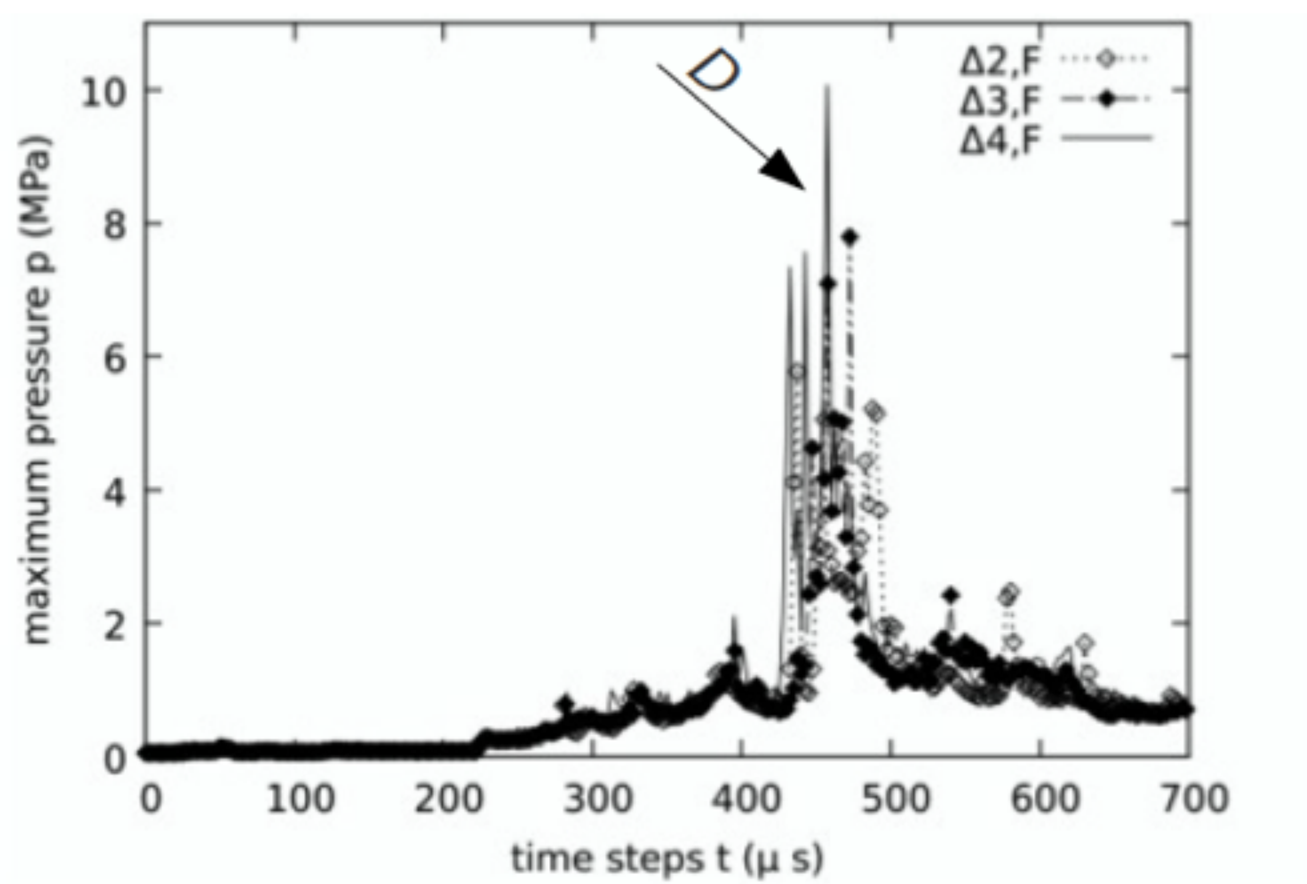

model

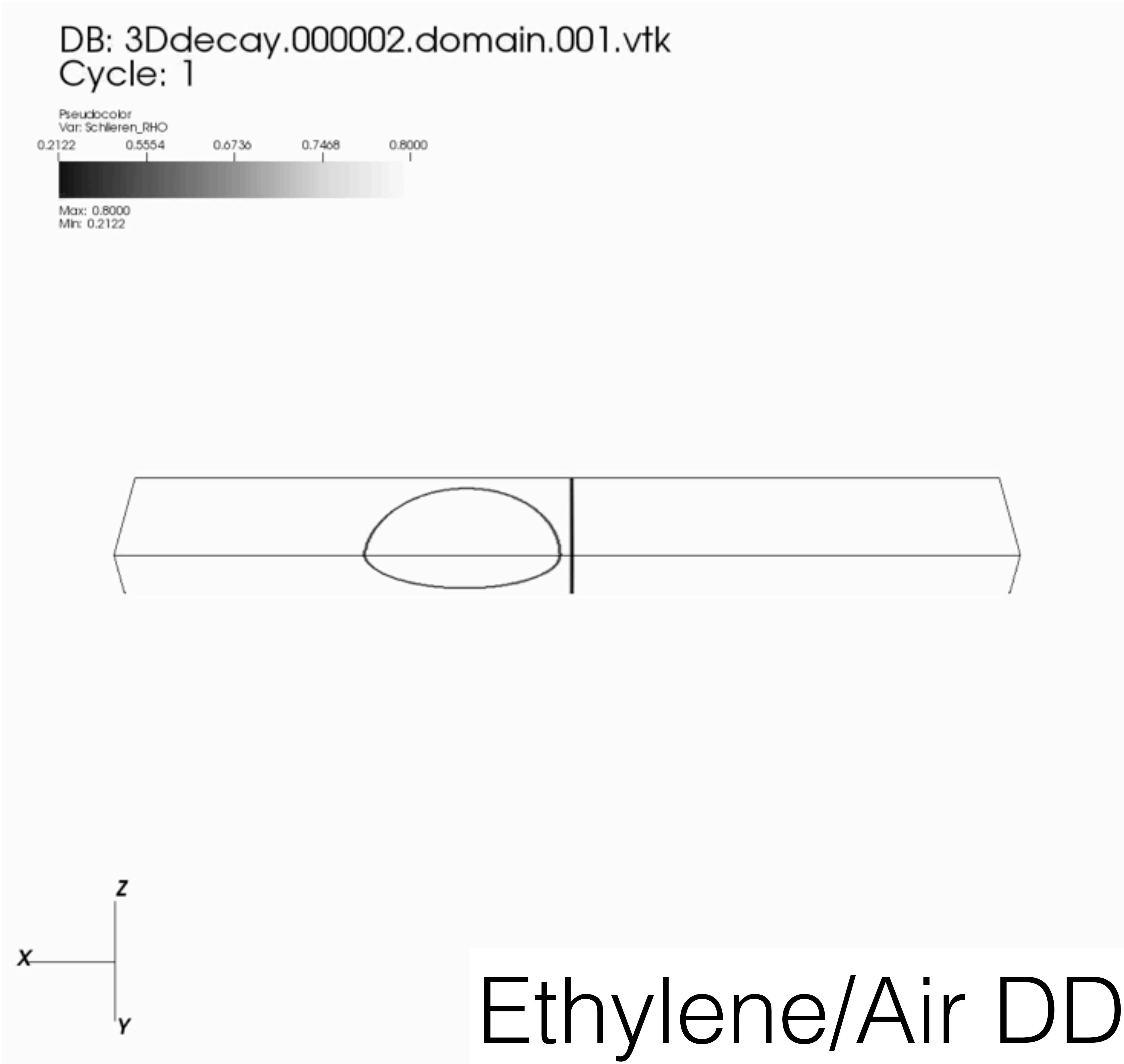
# Maximum Pressure

no-model




model






# Ethylene/Air DDT

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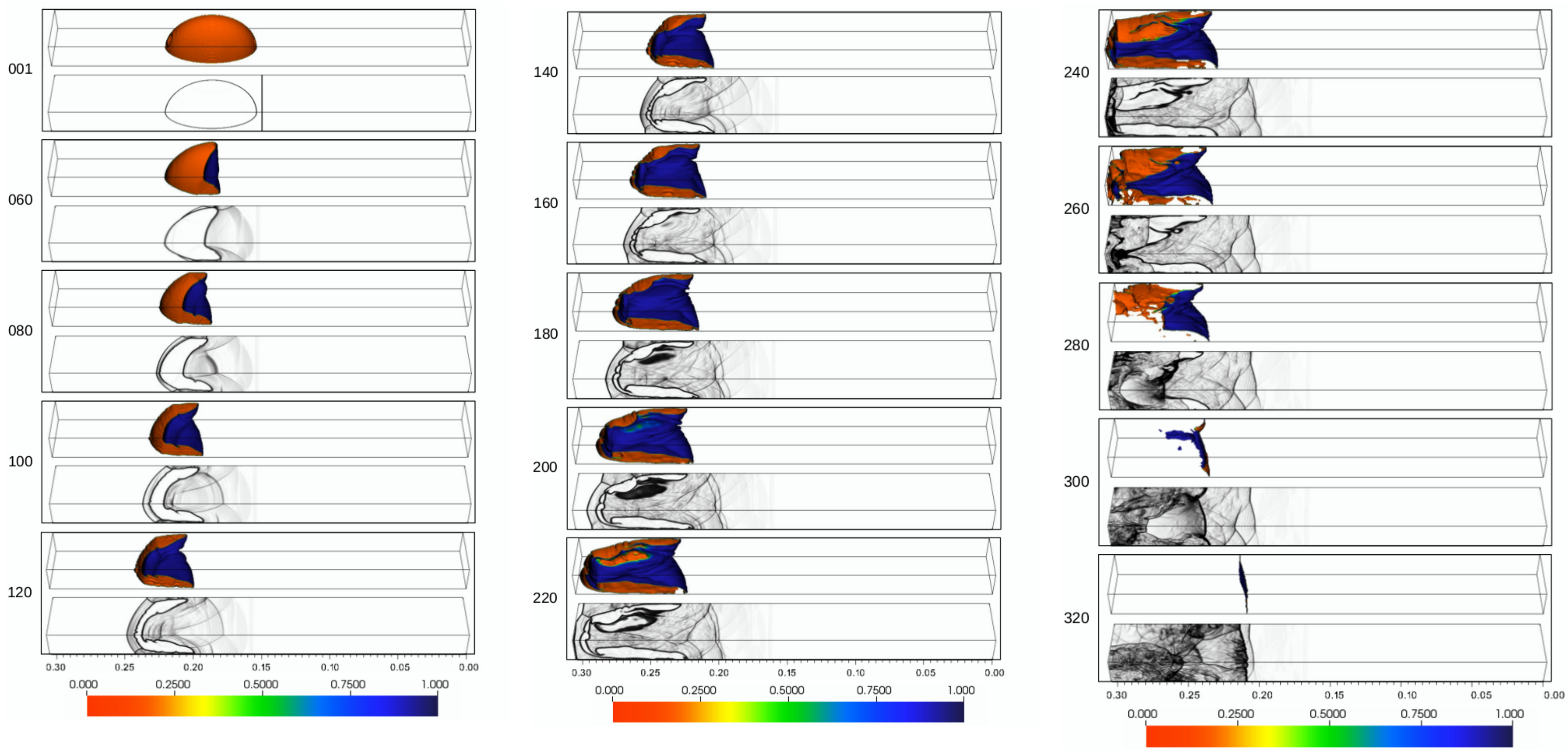
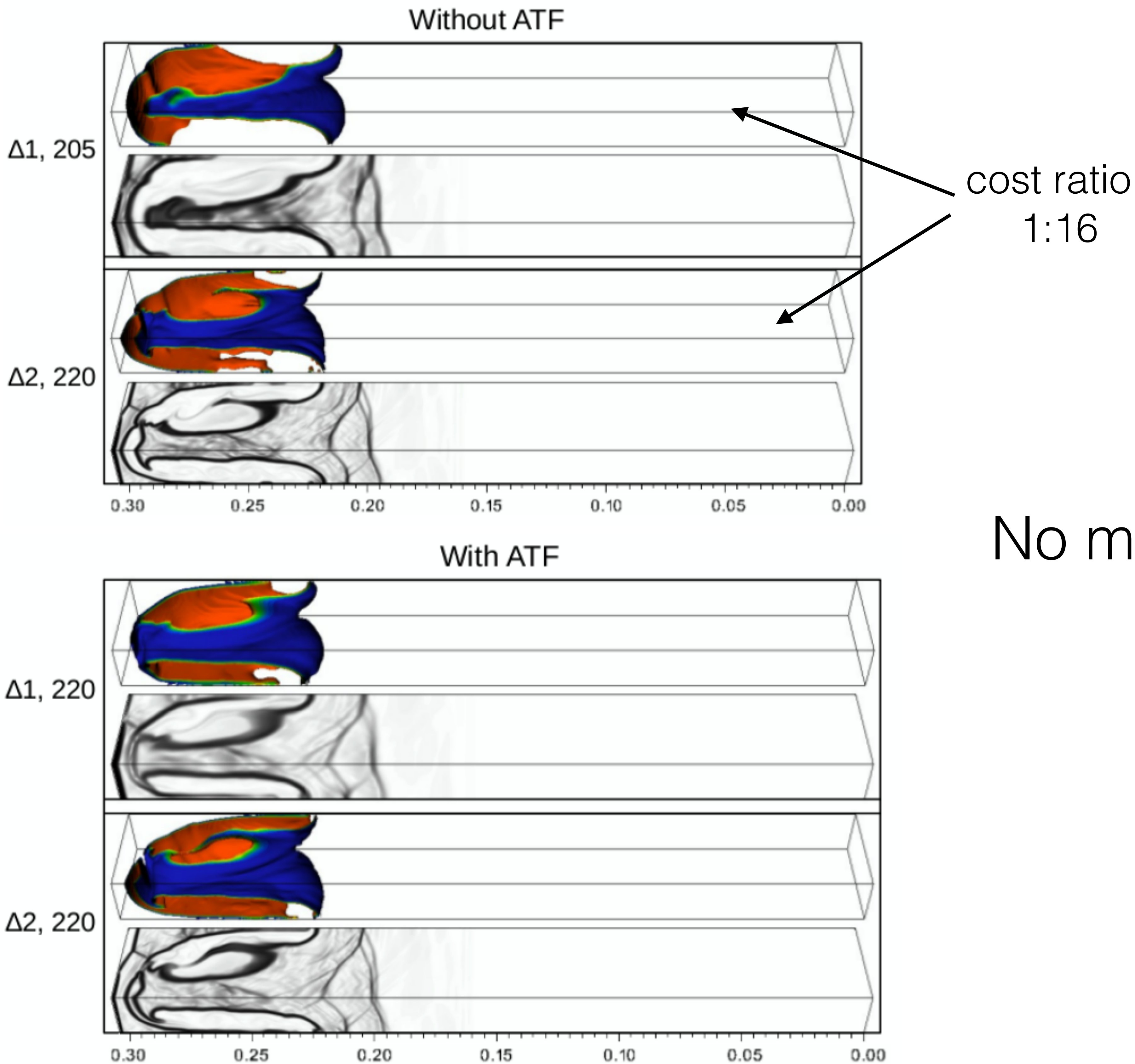
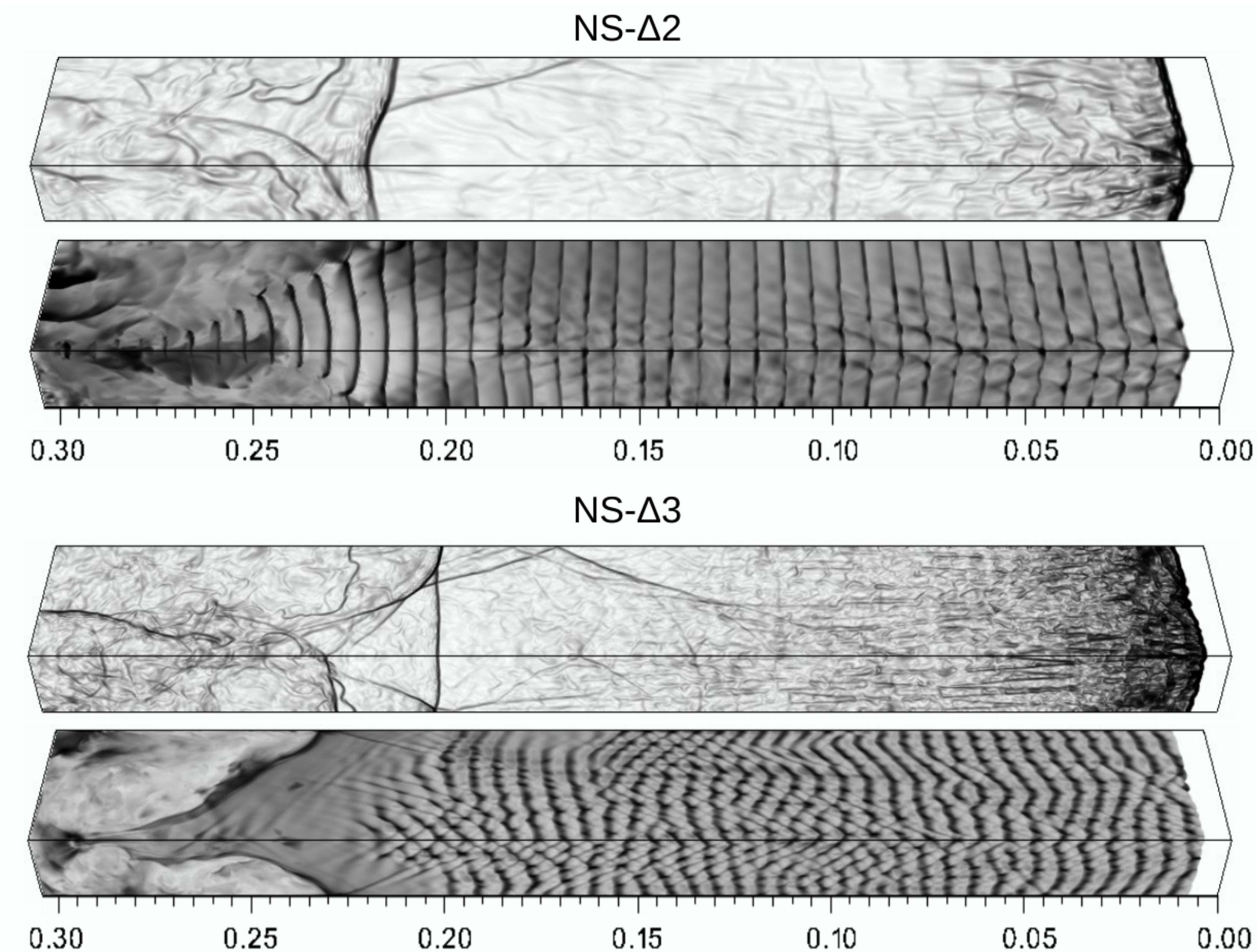





# No model early DDT

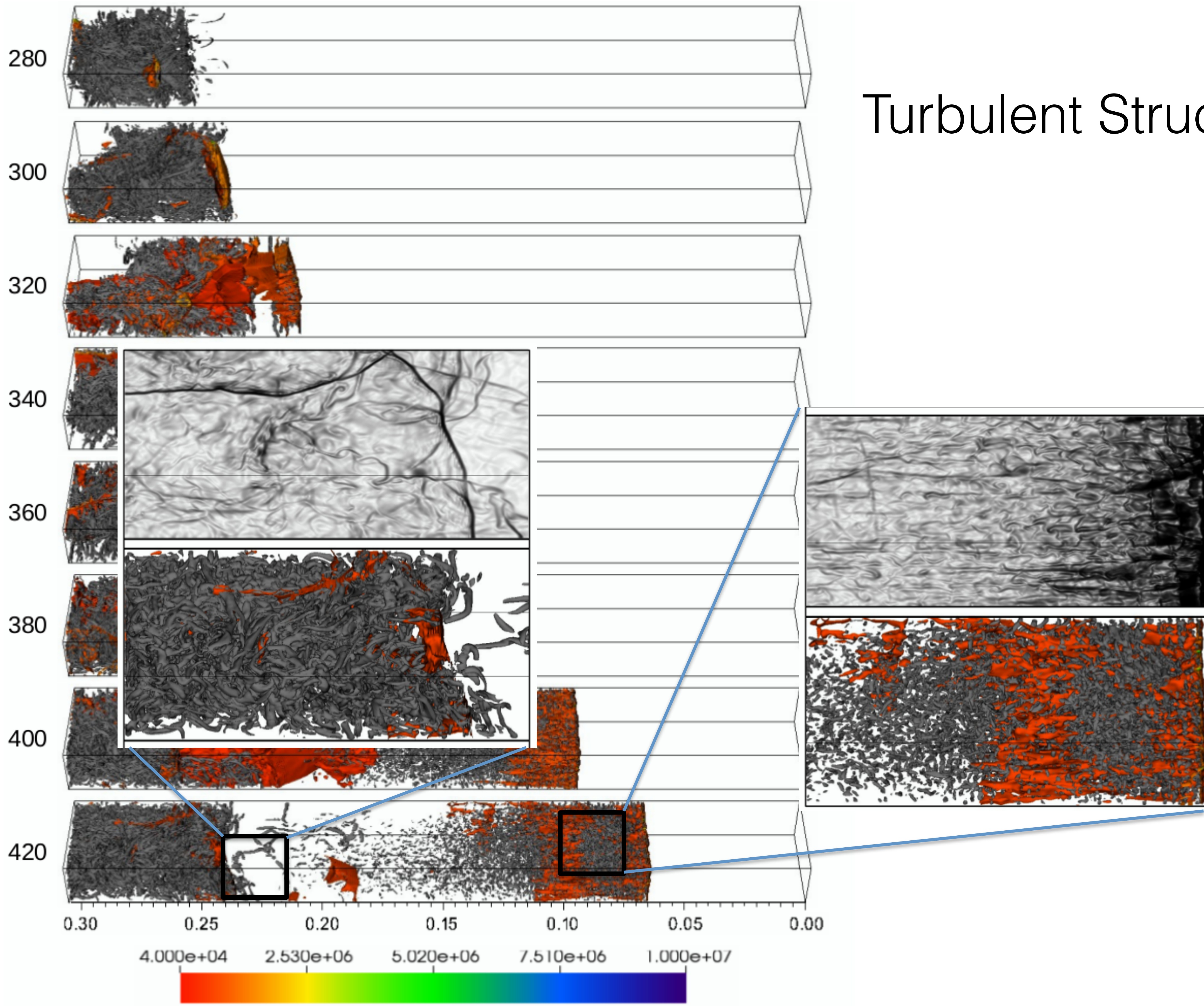
# Mesh Refinement

Computational Schlieren




Pressure History

# Turbulent Structures

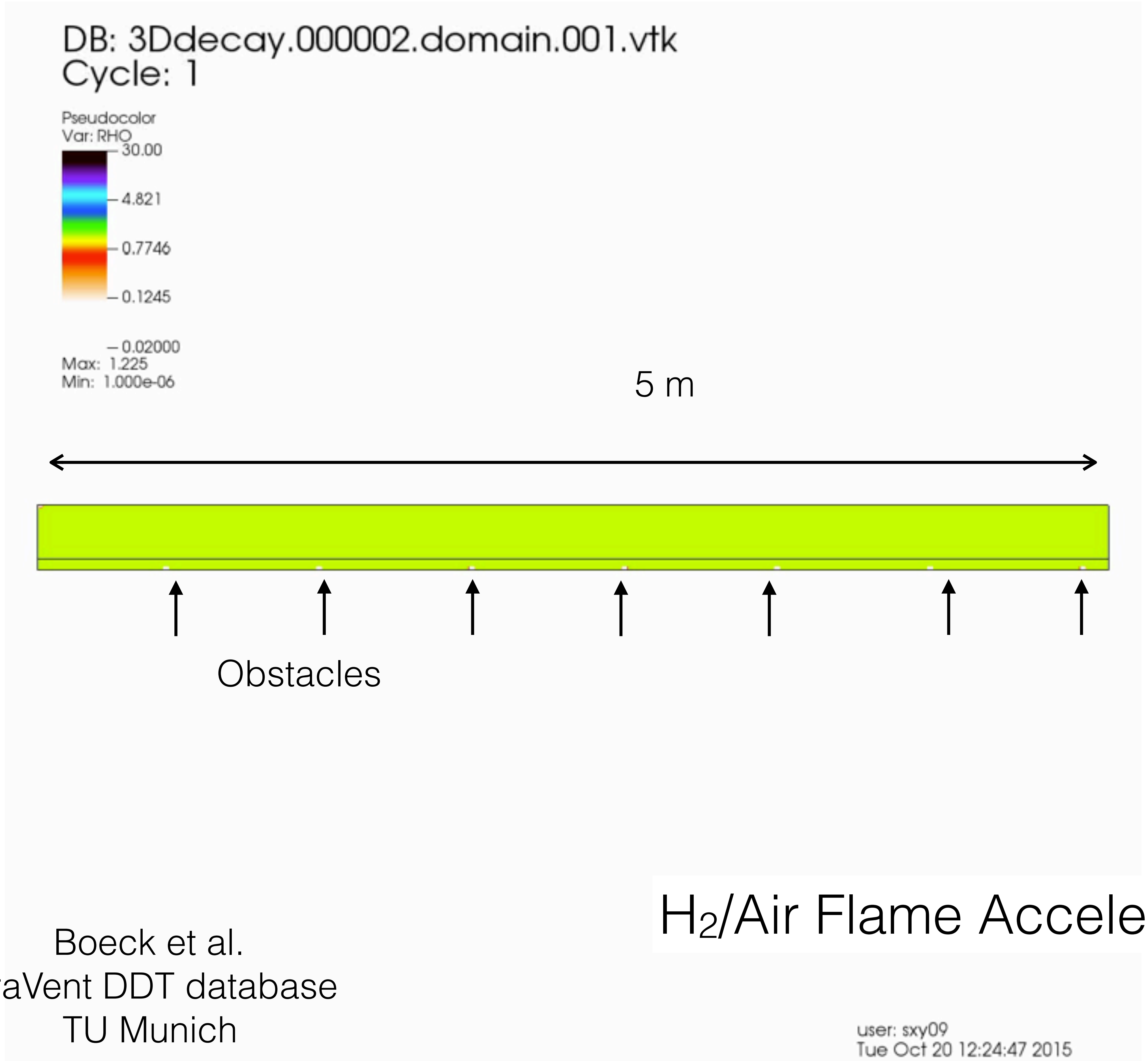


# Conclusions

*Can we predict DDT in realistic geometries with reasonable cost?*

… getting there

- Common assumptions not valid
- LES full ATF "cheap" and consistent (one free parameter)
- Complex chemistry/transport/dense gases
  - Need probably ATF/AMR combination




# $H_2$/Air Flame Acceleration DDT

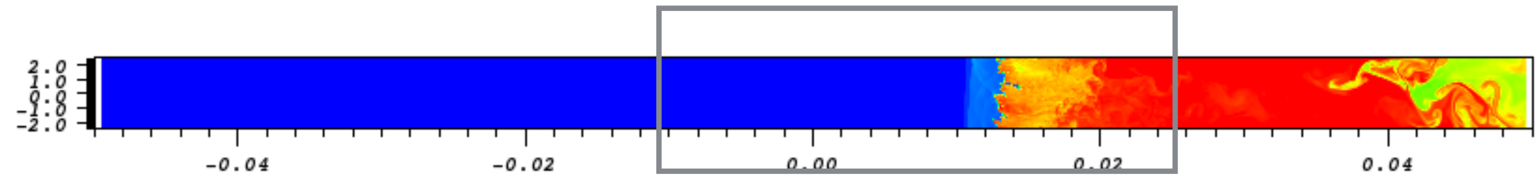
Boeck et al.
GraVent DDT database
TU Munich

# Questions?

“All models are wrong, but some are useful.”

-George Box (1979)

# Differential Diffusion

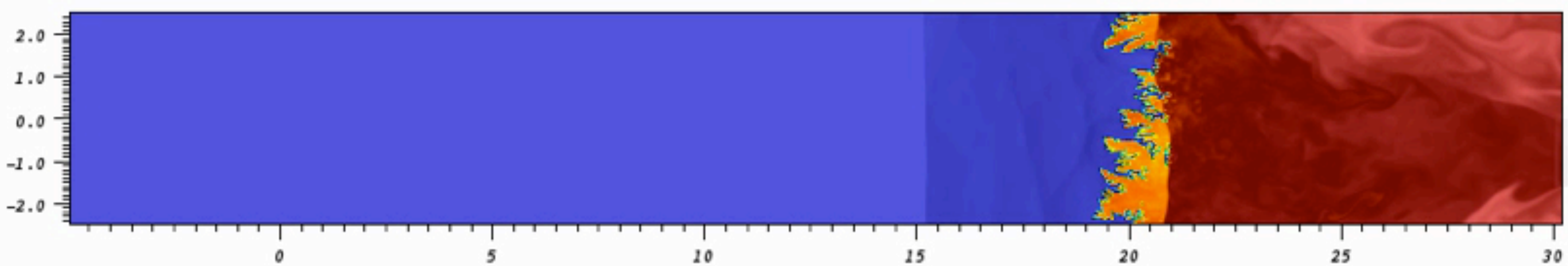



DB: solution.020200.domain.000.vtk
Cycle: 0

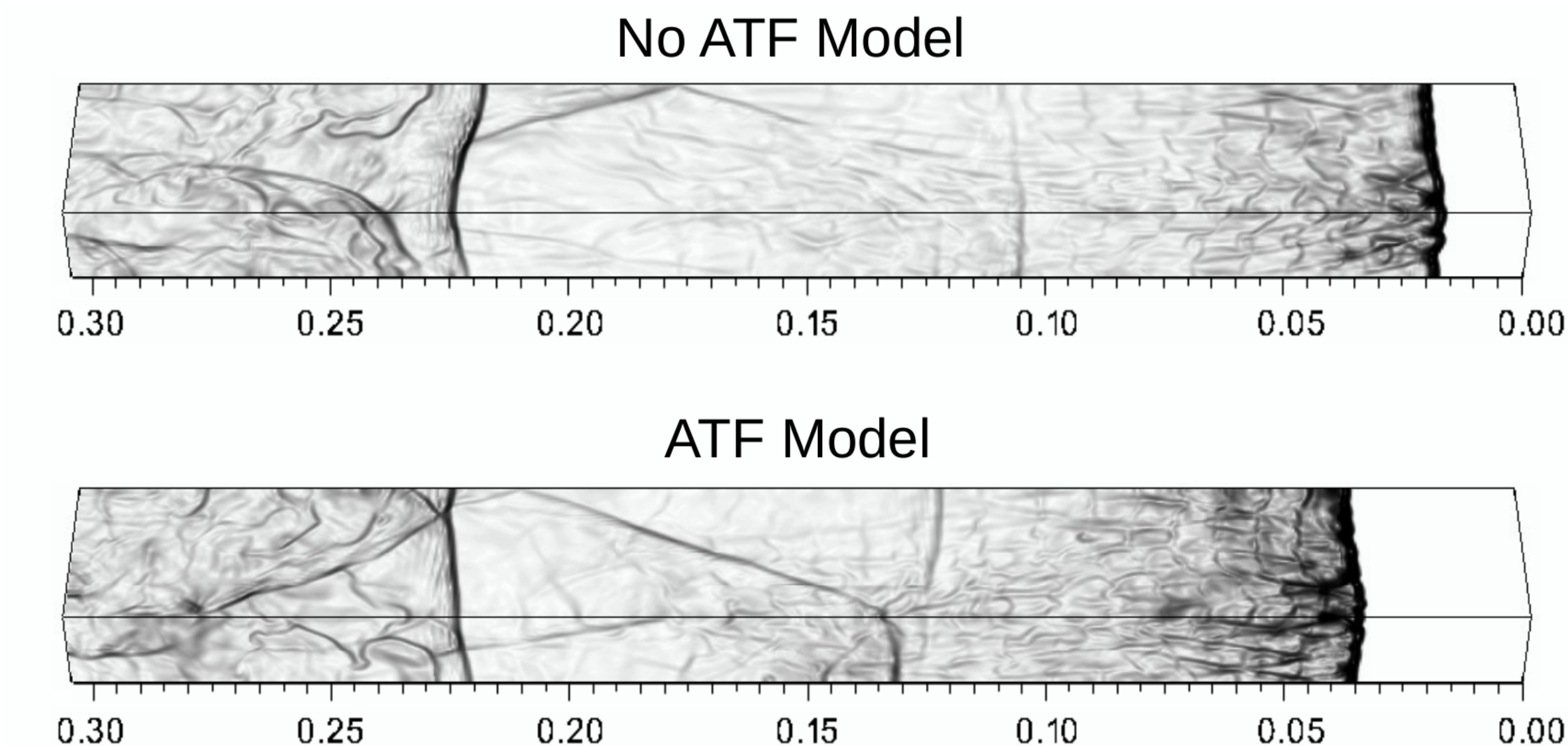
$$D_k = D$$


DB: solution.020200.domain.000.vtk
Cycle: 0

$$D_k \neq D$$

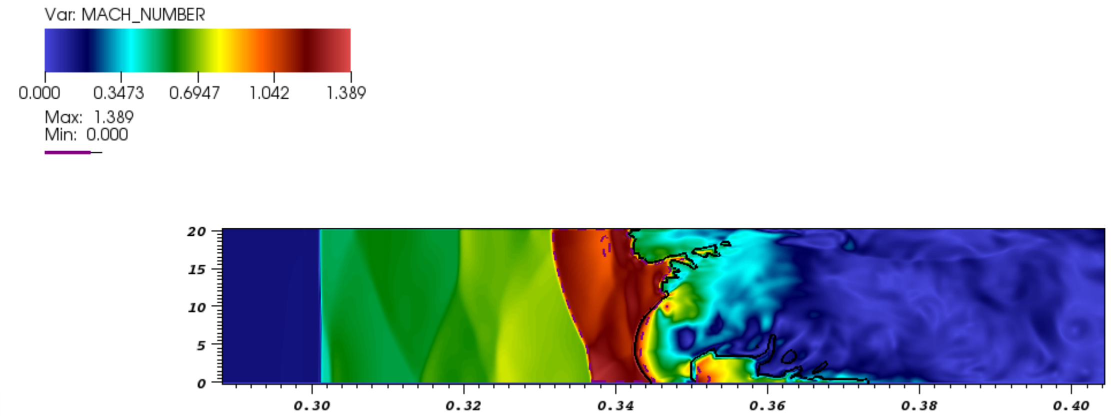



$H_2/O_2$ DDT




No model early DDT

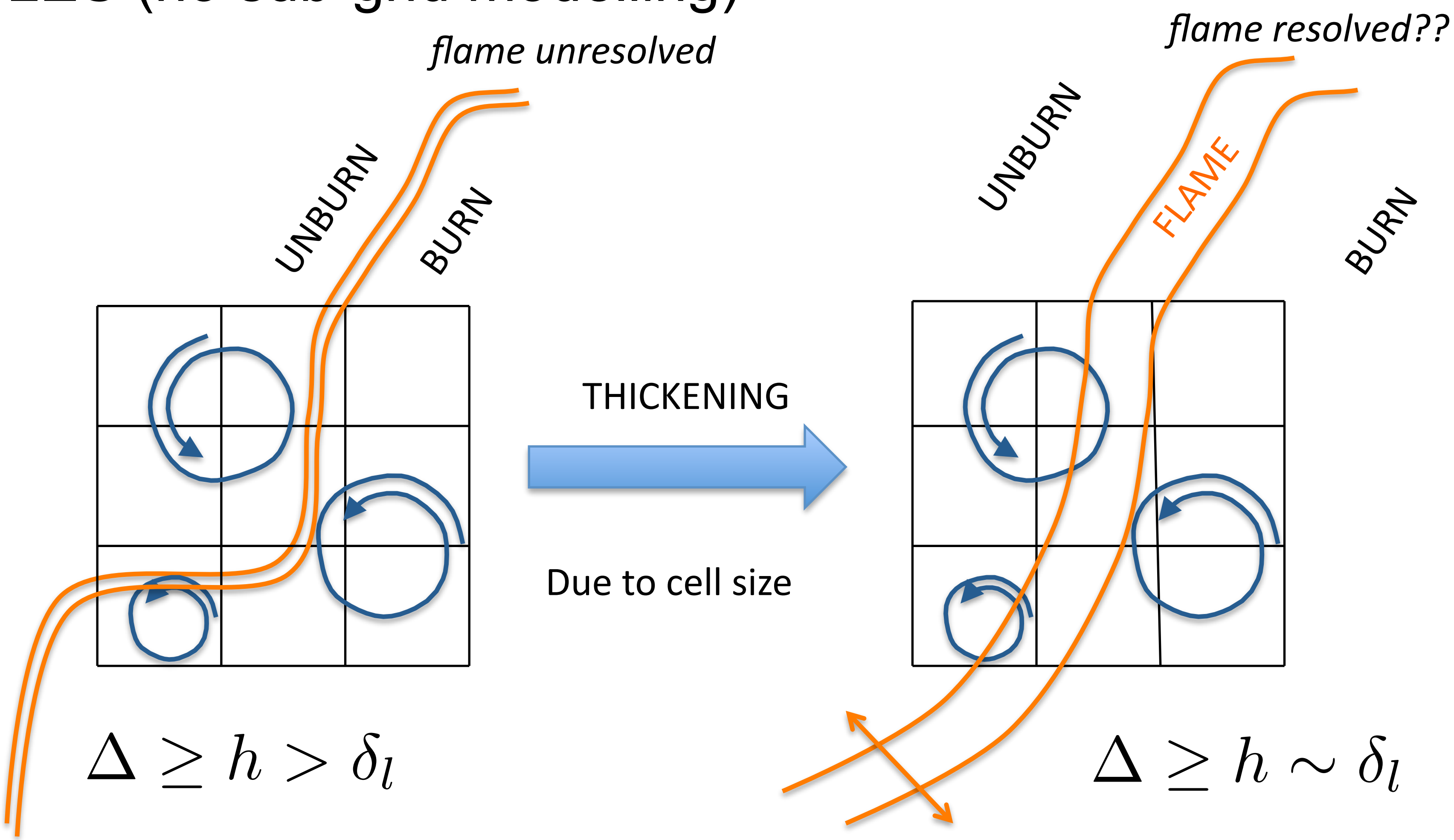
# Detail Kinetics





# Thickening

- LES (no sub-grid modelling)




$$\Delta \geq h > \delta_l$$

$$\Delta \geq h \sim \delta_l$$

"Implicit thickening"