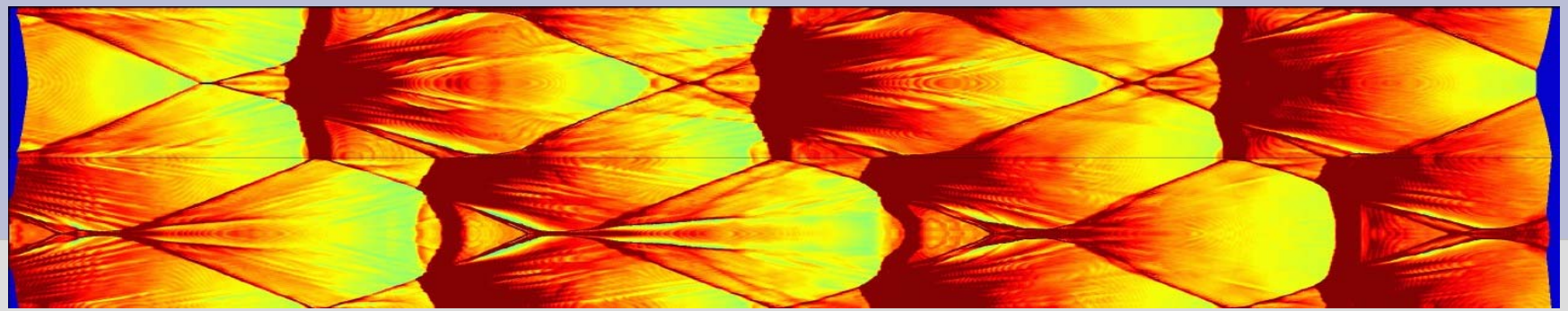

Detonations, Cellular Structure, Detonative Ignition and Deflagration to Detonation Transition: Lessons from 25 Years of Numerical Simulations

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First European Summer School on Hydrogen Safety

Belfast, August 2006

Thanks

- To Vladimir Molkov for the invitation
- To Elaine Oran for her considerable help (movies, pictures, papers, advice)
- To Koichi Hayashi & N. Tsuboi for their pictures

Overview

- Motivation
- History and early work
- Algorithms, frame of reference, BCs
- 1-D results: are they meaningful?
- 2 and 3-D cells; size; stability
- Chemistry: single, reduced schemes, full
- Failure, ignition, DDT, transmission

Motivation

- Hydrogen: detonates over wide range of concentrations
- Detonations: quite violent and destructive
- Ignition: still unpredictable
- Deflagration-to-detonation: poorly understood
- Major safety issue (see other talk)

History: Early Work
(the eighties)

- Taki & Fujiwara 1978; NRL: Oran, Boris, Kailasanath & collaborators, 1978, 1981, 1985 etc.
  - Both originally used FCT (Boris & Book)
  - Simple kinetics
  - Computation: cells!
  - Unburnt pockets

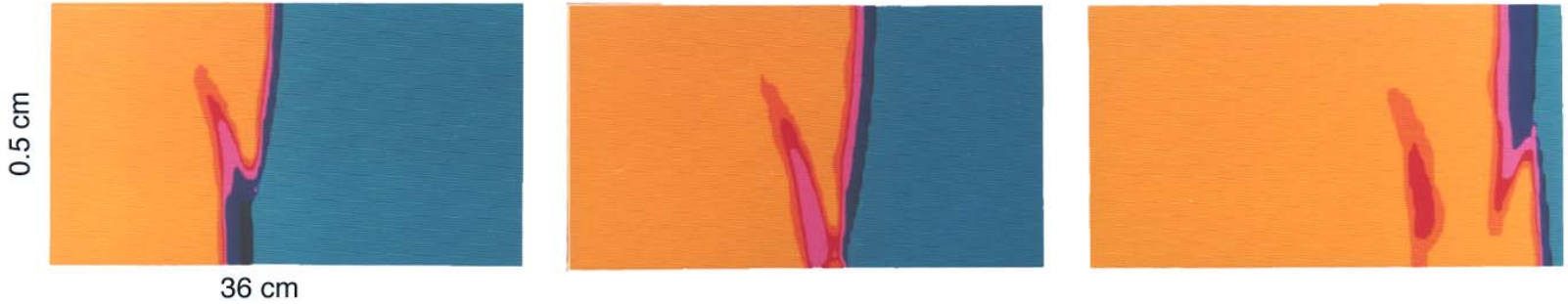
Formation of Unreacted Gas Pockets

Detonation moves into cold, unreacted gas

Shock reflects from the bottom wall

An unburned gas pocket is left behind the front

Extent of reaction



Temperature

Oran et al., 1980, 1982

Coming of age: the nineties

- Well-resolved cells (Bourlioux & Majda 1991, Quirk 1993; Williams, Bauwens & Oran, 1996a, b; Pankow & Fisher...; Matsuo,...)
  - Polemics about schemes, Godunov vs. FCT... (B&M)
  - Careful look at resolution (Quirk)
  - Detailed structure, 2D, 3D (Williams et al.)
- More complex chemistry & stiffness (Oran et al, Hayashi,...)

State-of-the-Art

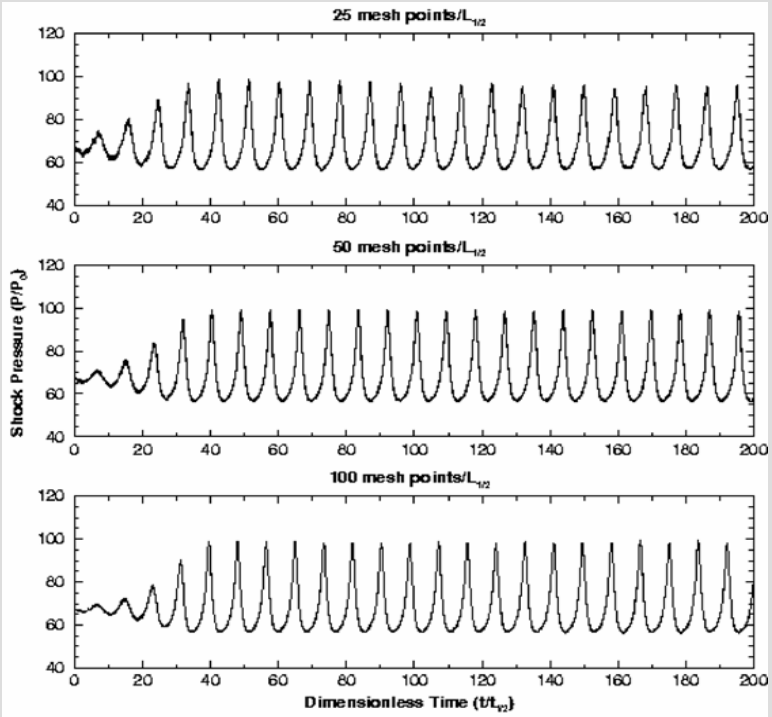
- “Anybody can get cells”
- Very large simulations (Oran; Tsuboi & Hayashi)
- Flame acceleration & DDT
- Complex kinetics (Hayashi)
- Look at chain-branching
- Where does the length scale come from?

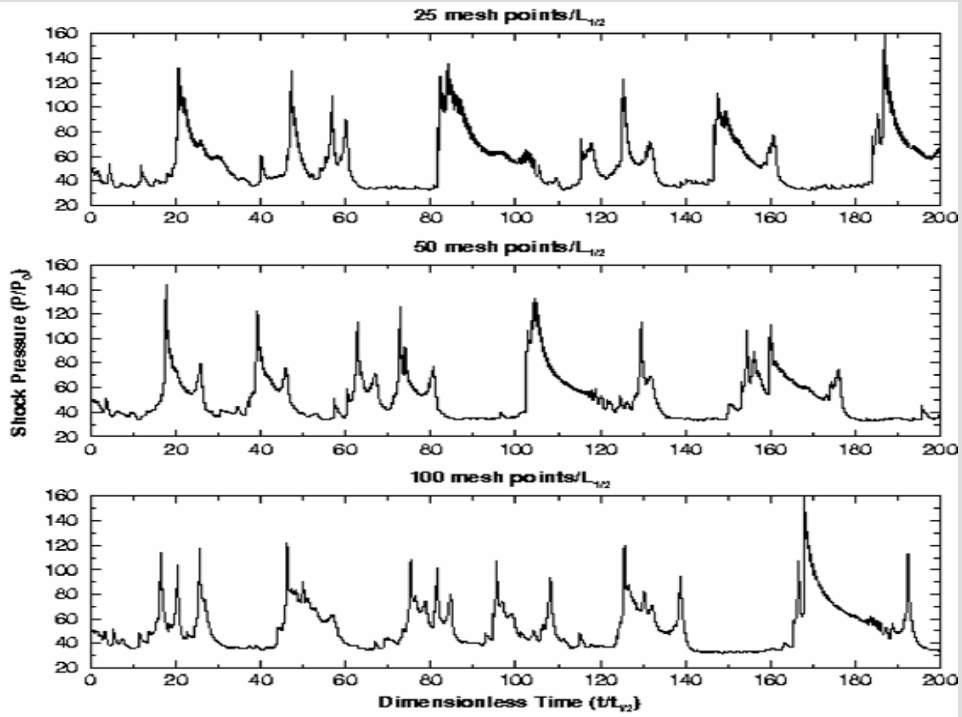
Frame of Reference, BCs, etc.

- Holy grail: free propagating waves
- Either long domain or moving window?
- How long?
- What subsonic BCs?
- Planar wave: overdrive is well-posed. But with cells?
- But does all of this matter?

1-D Results
(Ours, Matsuo, Karagozian, Short, Lee, etc.)

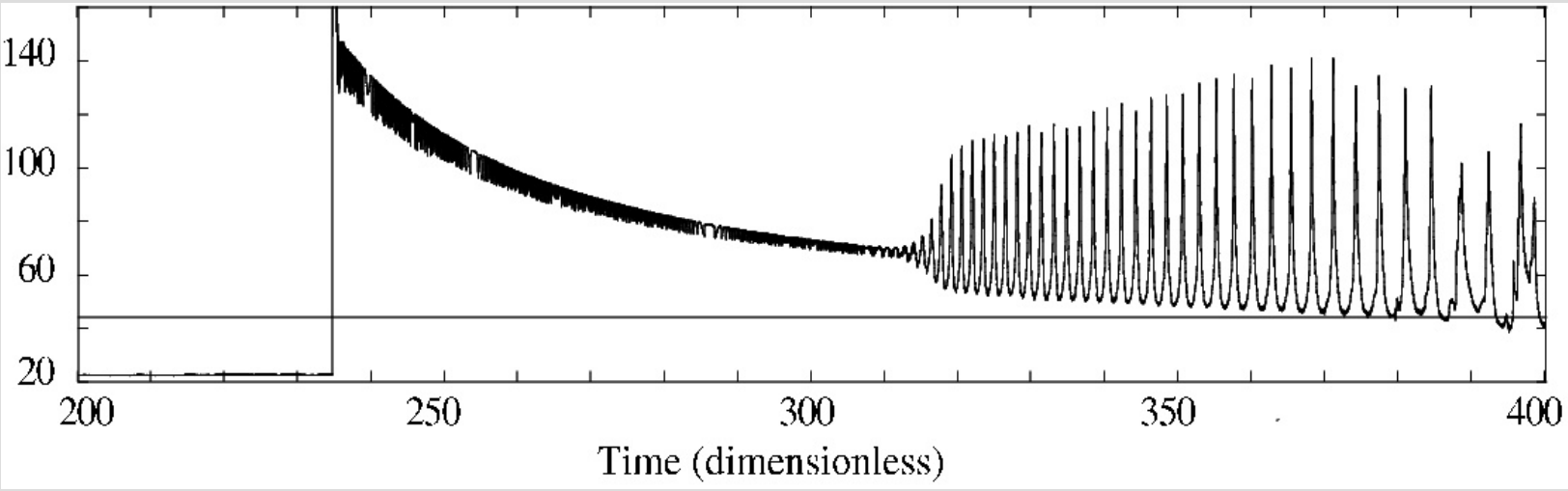
- Close to stability limit: nice and periodic; pick low frequency (Short)?





1-D Results (continued)

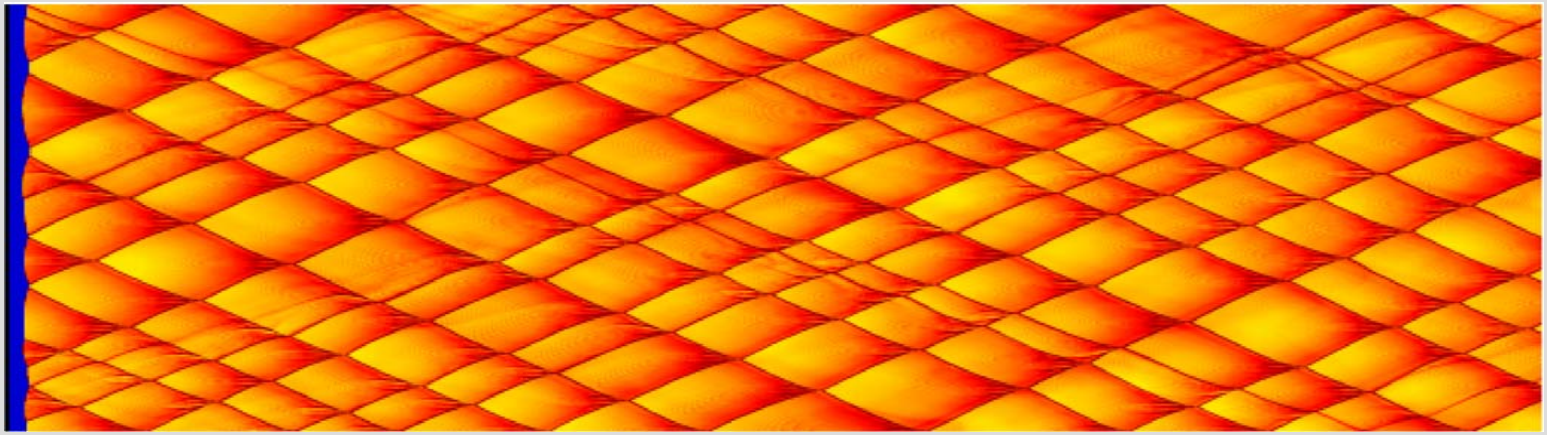
- Near-CJ: quite chaotic; big spikes
  - Related to DDT (Bauwens 2000, 2002)?
  - Do these really converge?



1-D Results (continued)

- On fixed domains: dominated by downstream BC and length (Karagozian)
- But: transverse modes always more unstable/ unstable first
- In practice, detonations always cellular
- So, not clear if 1-D truly meaningful?

2-D Cells (1)

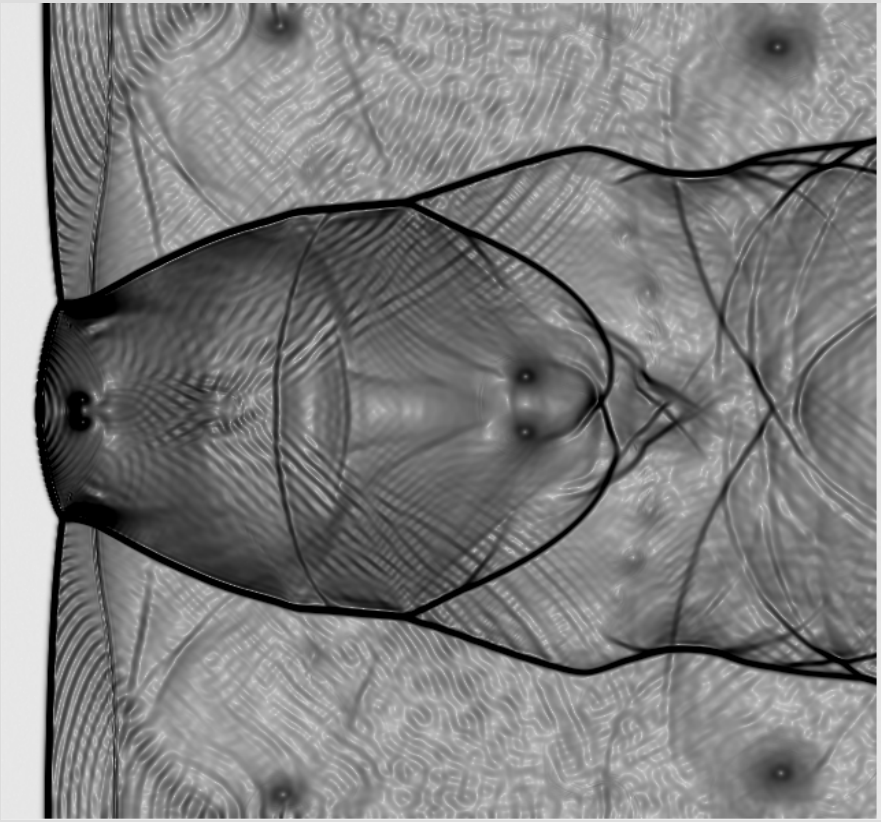


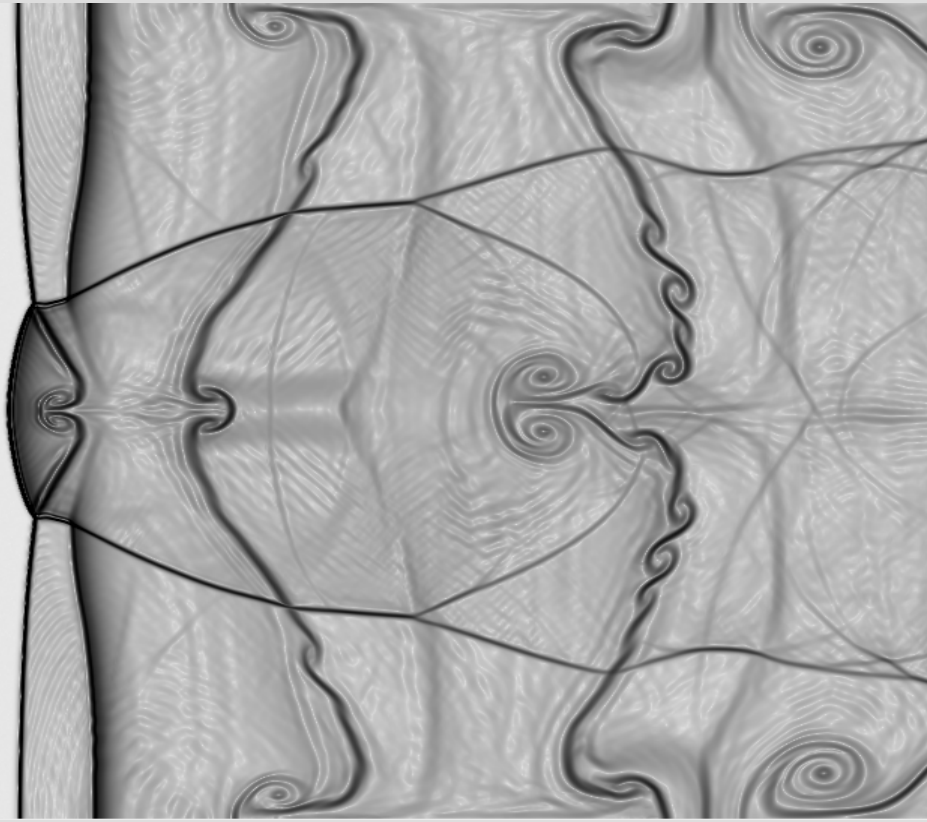
- Smoke foils (how?), cell regularity
- Cell size?
- Resolution (hot spots; Quirk)?

2-D Cells (2)

- Early results (Oran,Kailas et al.): unburnt pockets
- Bourlioux & Majda: relate to stability + look at resolution using $L_{1/2}$
- Complex shock structure (triple points)
- Confirming Strehlow's cell construction
- Slip lines: vortices, K-H unstable
- Reaction fronts: R-T unstable

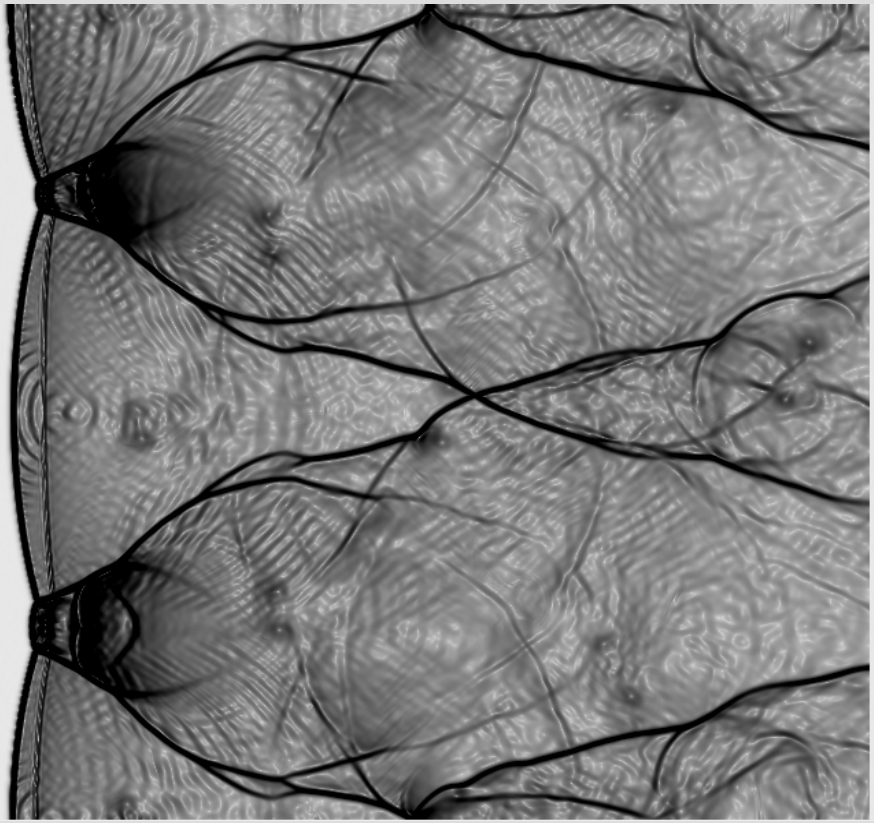
2-D Cells (3)
(Liang & Bauwens, 3 step chain-branching)

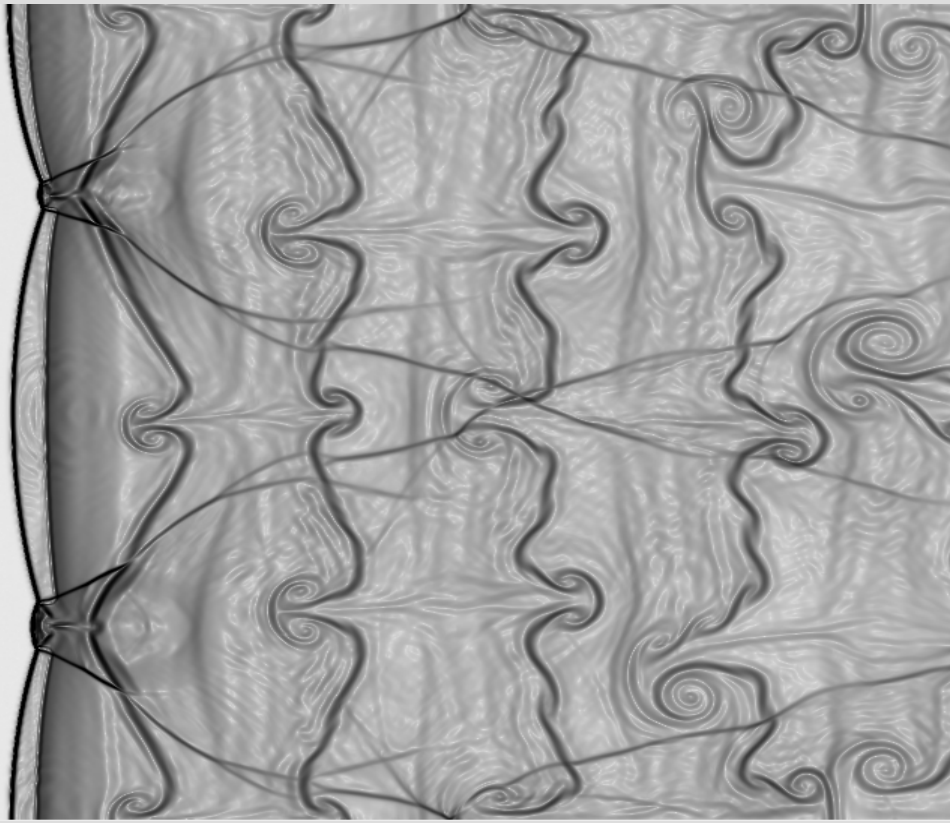




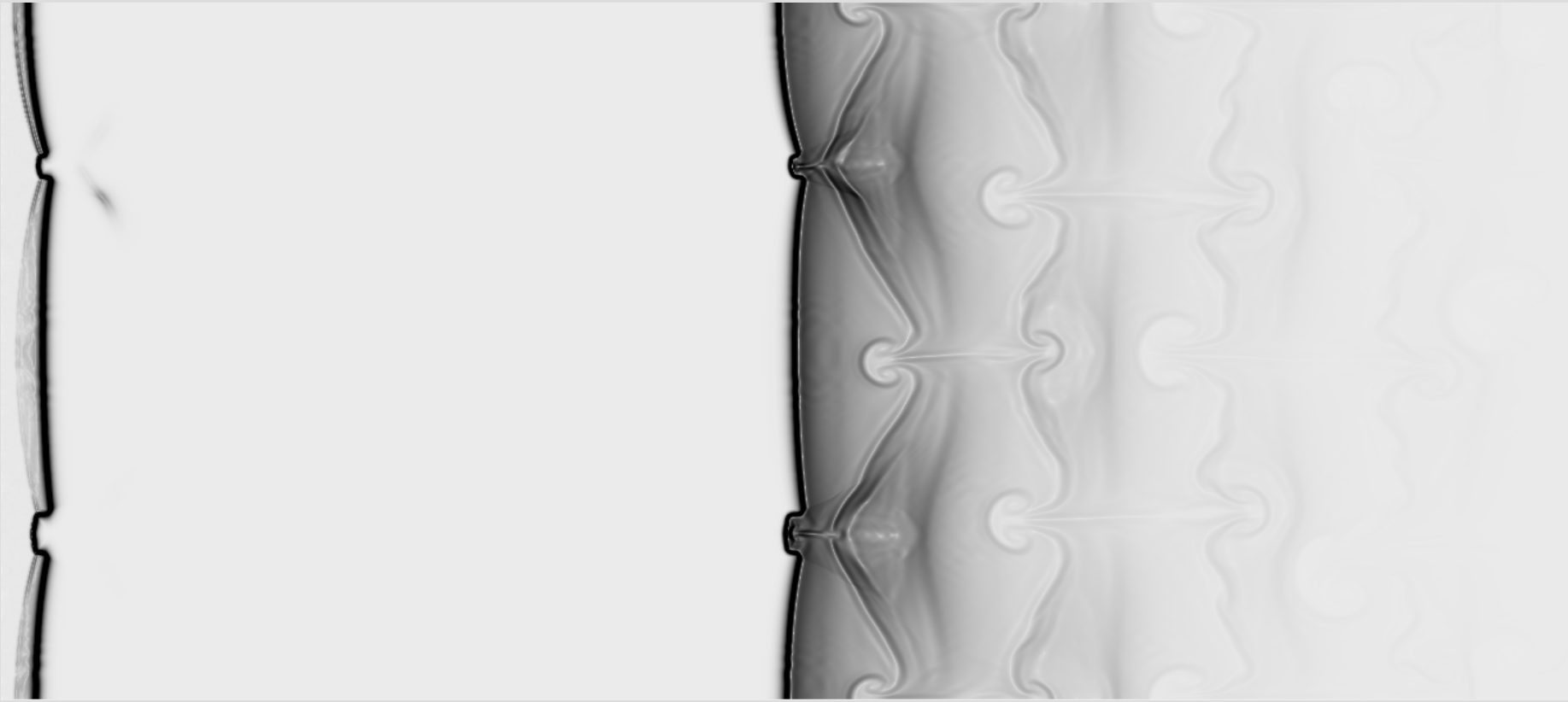
2-D Cells (4)

2-D Cells (5)
(Liang & Bauwens, 3 step chain-branching)





2-D Cells (6)



2-D Cells (7)

- Marginal detonation movie (Gamezo et al. 2000)
  - When leading front overdriven: secondary cells
  - Transverse detonations also unstable
  - With single step Arrhenius

2-D Cells (8)

- 2-D structure reasonably well understood
  - Pair of triple points moving sideways along front
  - Source of transverse shock and slip line (shear)
  - Collision -> Hot spot -> explosion -> Mach stem
  - Mach stem weakens
  - Next collision: Mach stem -> incident wave
  - Incident wave further weakens
  - Reaction front decouples. R-T unstable?
  - Slip line: K-H unstable

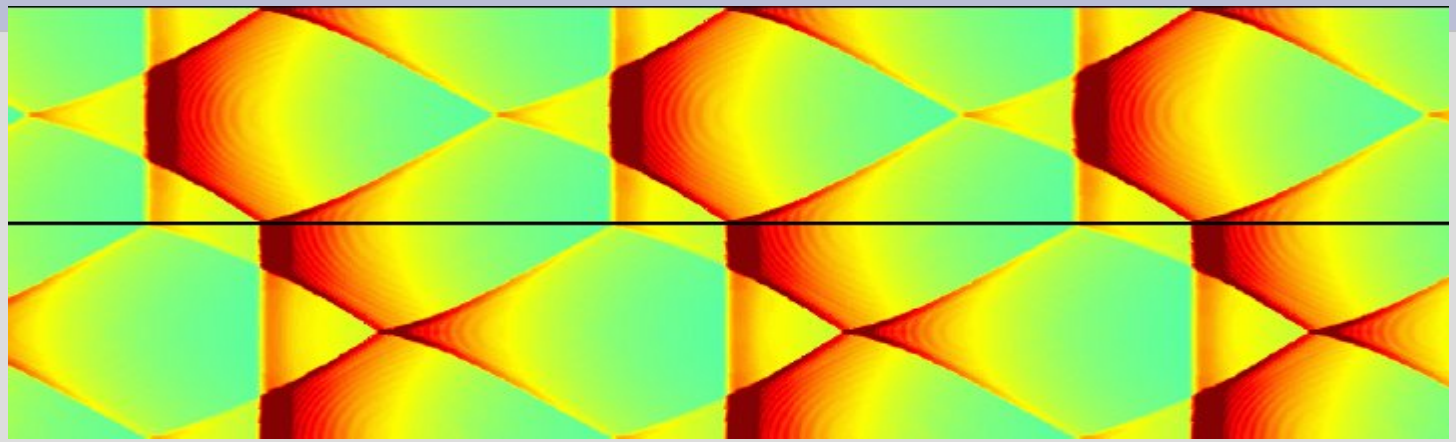
2-D Cells (9)

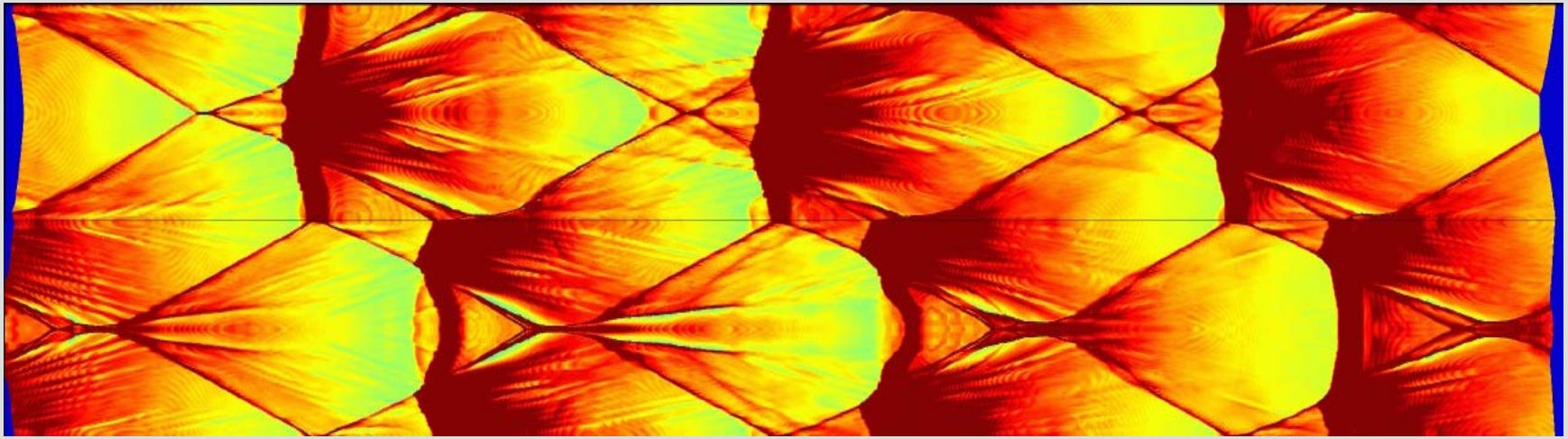
- But why cells?
  - Instability: known since Zaidel & Erpenbeck.
  - But physical understanding?
- What determines the cell size?
  - A chemical length
  - Kinetics: many scales + temperature
  - Critical widths >> Cells >> ZND half length!
  - Stability wavelengths closest?

2-D Cells (10)

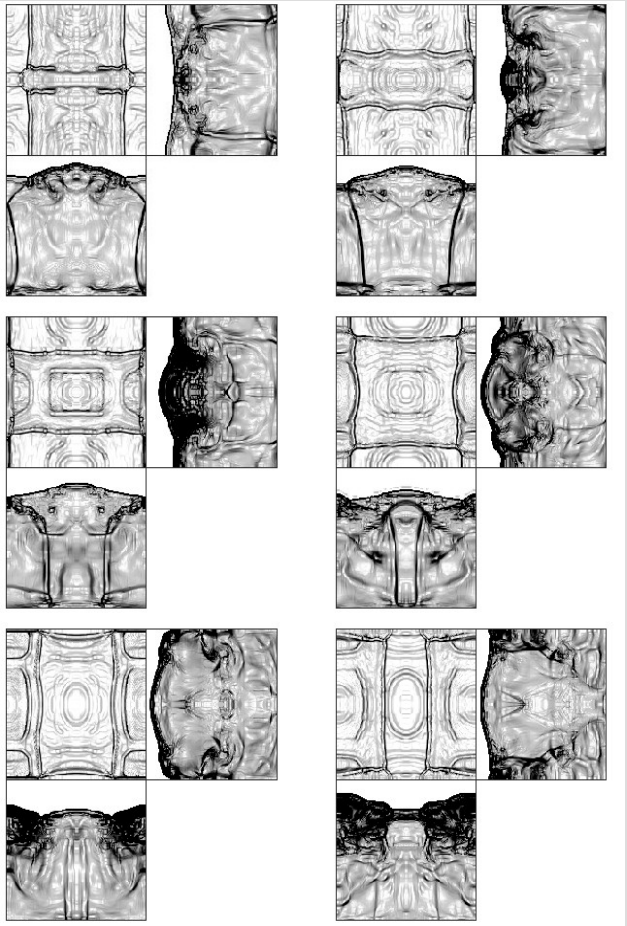
- Support mechanism?
  - Planar CJ wave ends at sonic (CH) plane
  - But 1st order termination -> ZND length infinite
  - Kinetic energy in vortices: how long to dissipate? Forever? Perhaps not relevant?
  - Is there an unsteady equivalent to CJ plane?
  - Sonic: frame of ref. dependent. But shock unsteady
  - Front dynamics (Yao & Stewart) + “explosion within explosion” (Urtiew & Oppenheim)?”

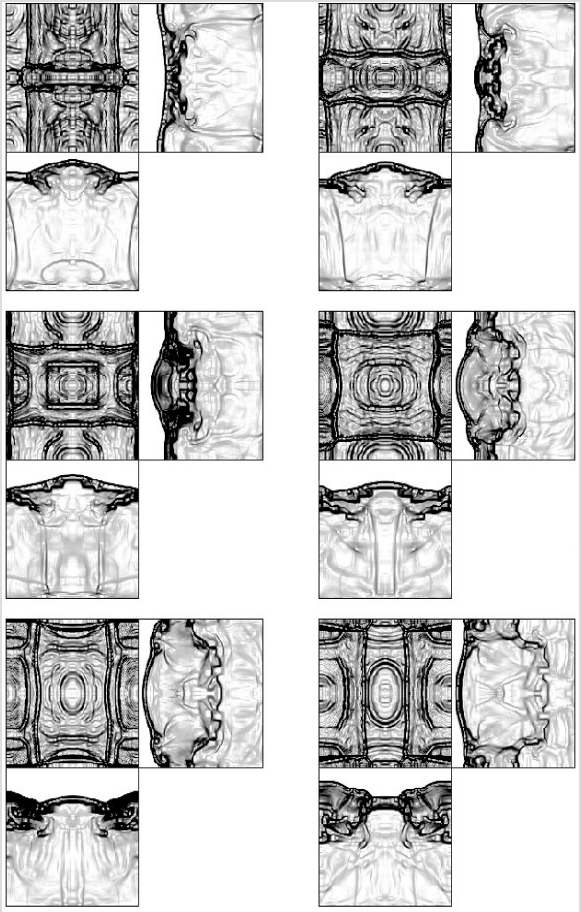
3-D Cells: Smoke foils





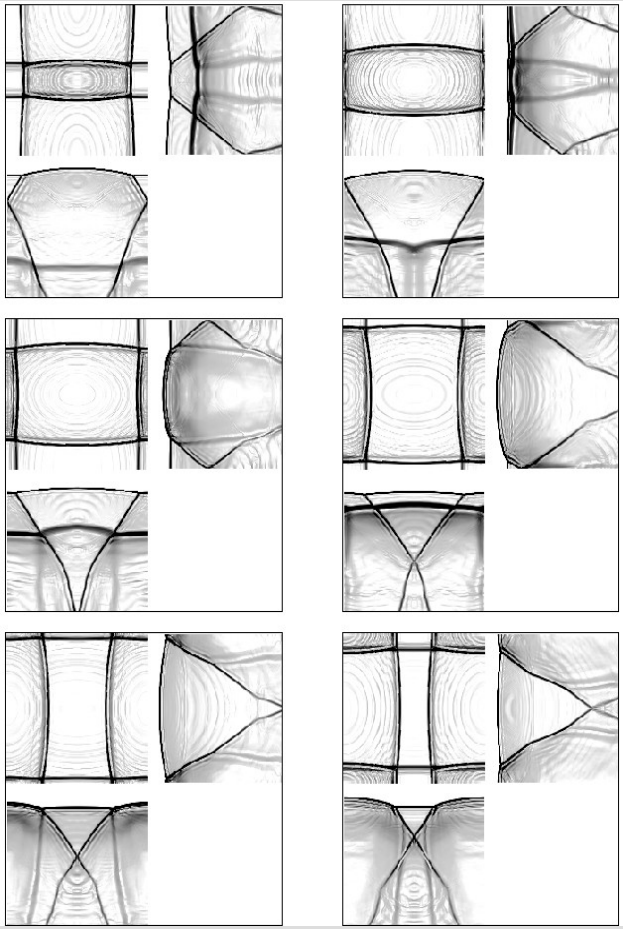
3-D Cells: Instantaneous frames
(Williams D.N, Bauwens, Oran 1996)

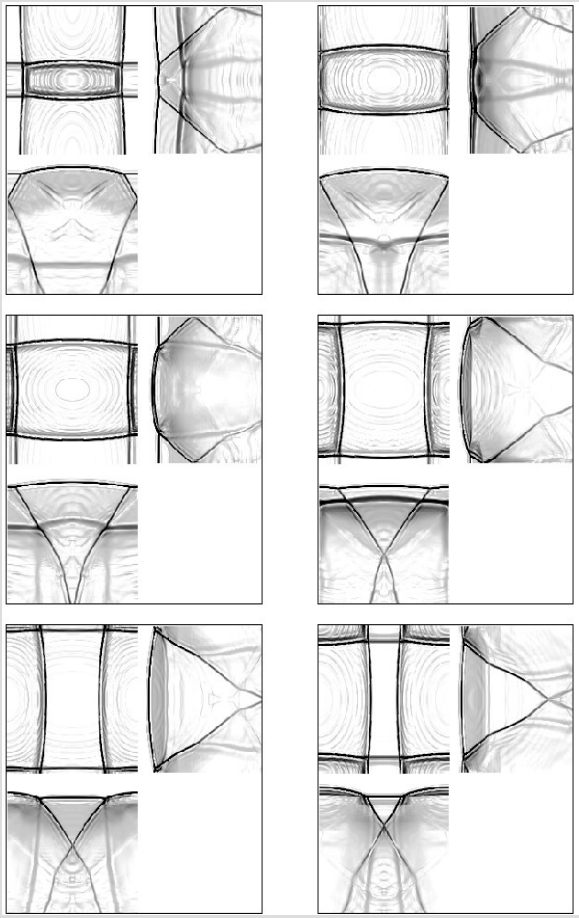




- Density and pressure gradients

3-D Cells: Instantaneous frames
(Williams D.N, Bauwens, Oran 1996)

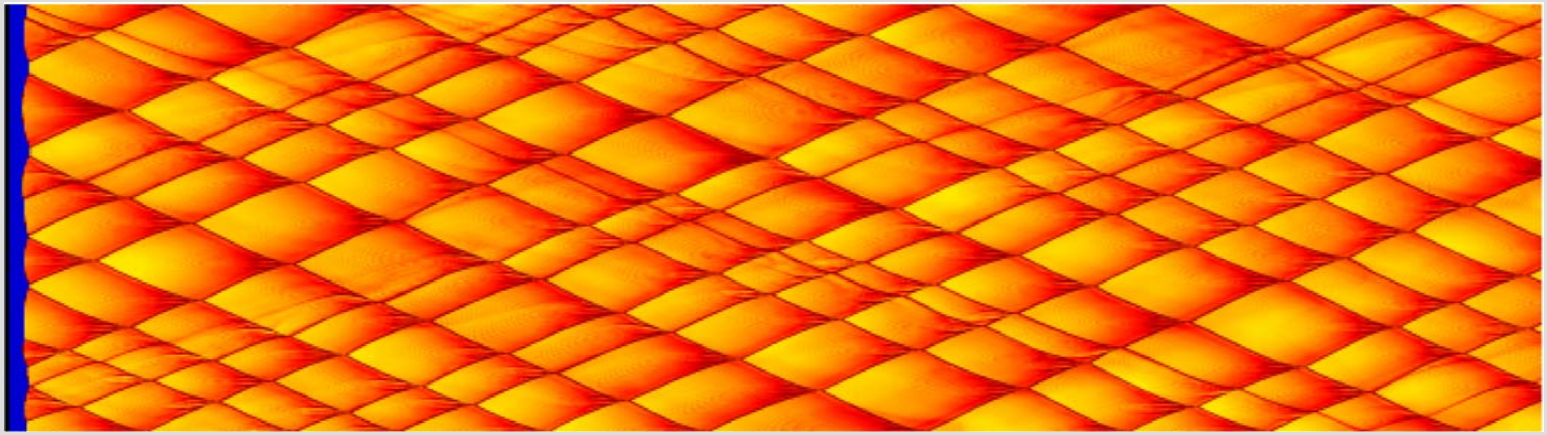




- Density and pressure gradients

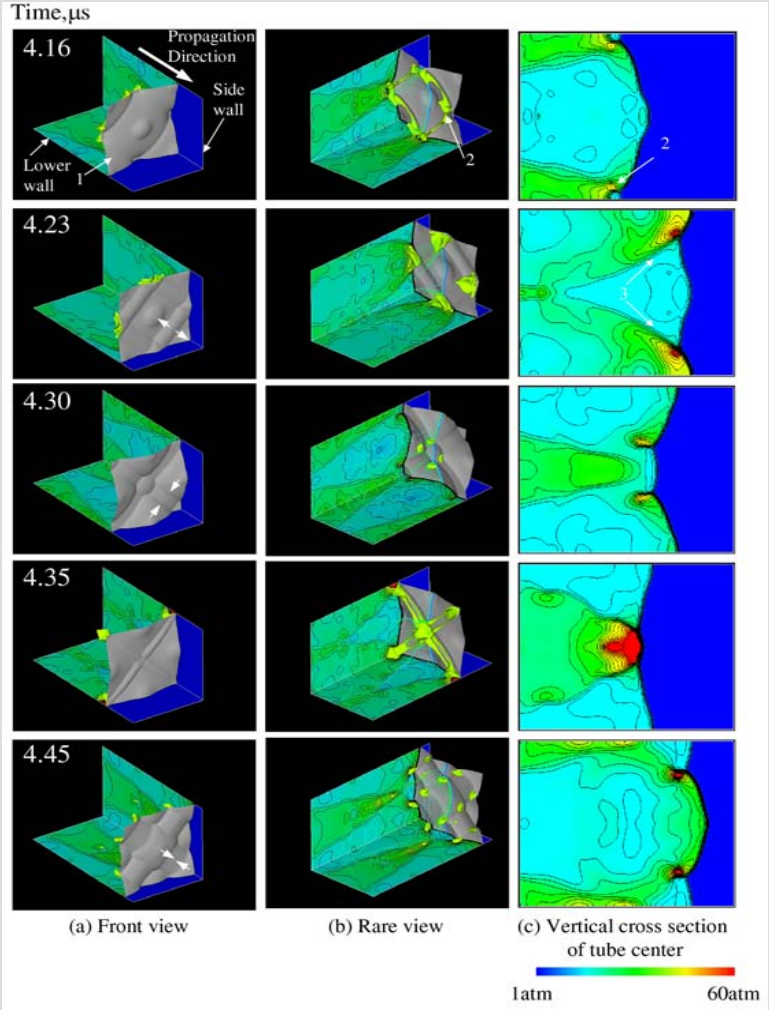
3-D Cells: Smoke foils

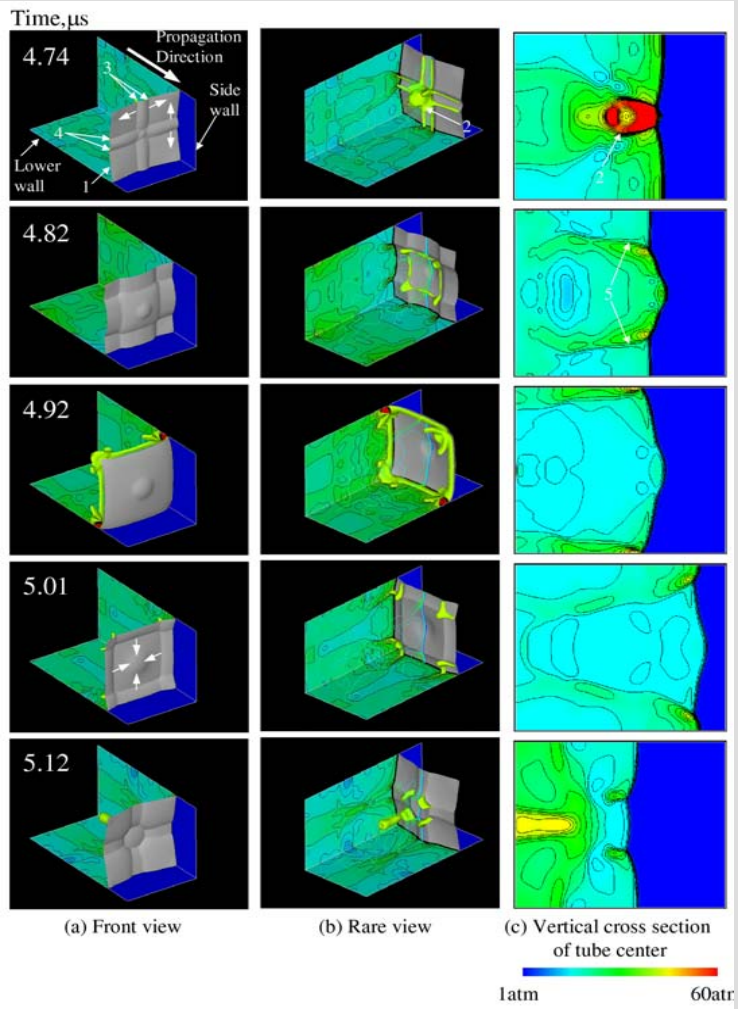
- Our results: single step, two cases, both γ_0 = 1.2, respectively f=1.1, Q=2, E=20 and f=1.2, Q=50, E=10
- First is “well-behaved,” regular cells. Second is irregular (using domain wide enough)



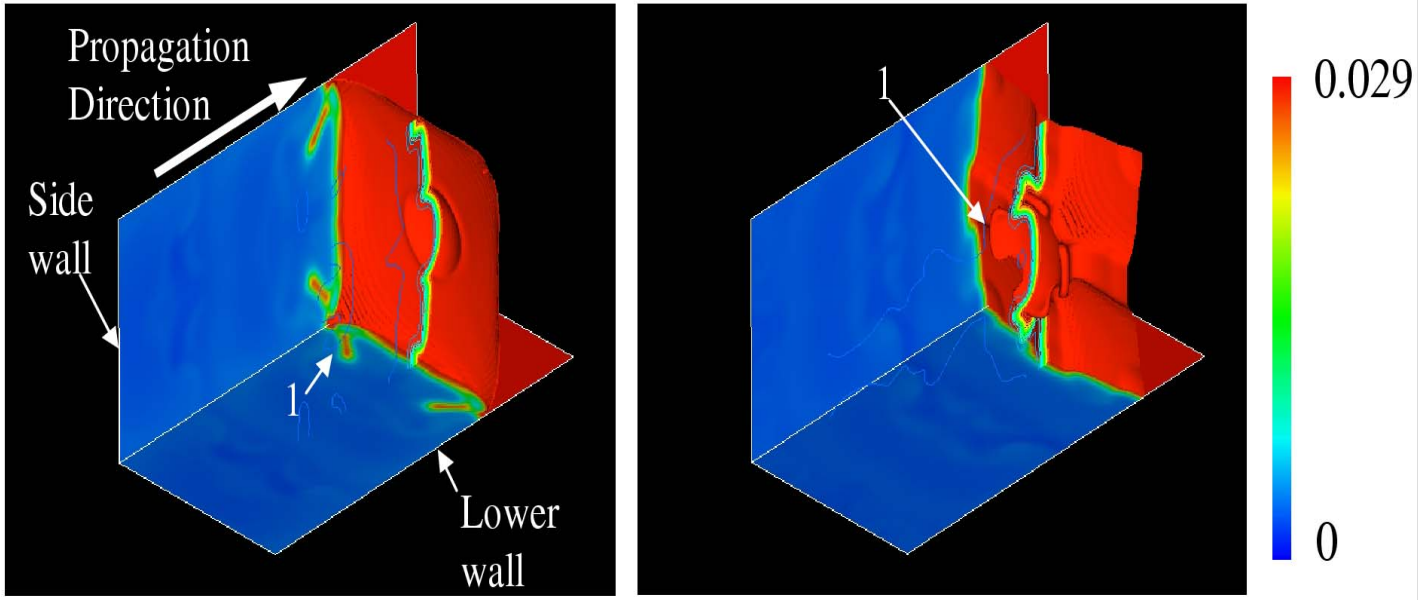
- Compared with two-D:
  - 2 sets of modes in 2 directions (hence slapping wave)
  - Vortex structure fully connected

3-D Cells
(Tsuboi & Hayashi, complex kinetics)





3-D Cells: Smoke foils
(Tsuboi & Hayashi, complex kinetics)



(a) 4.92 μs (b) 5.12 μs

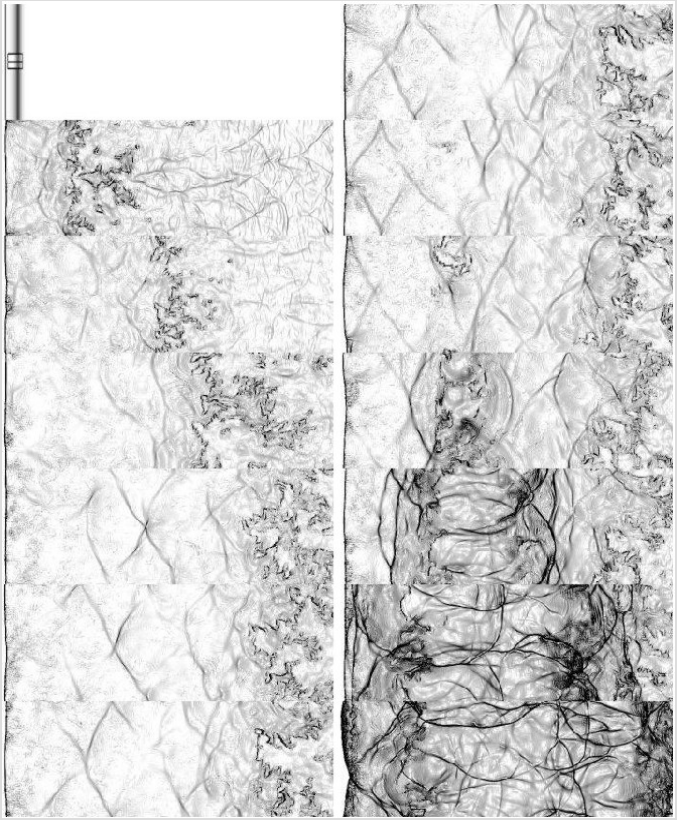
3-D Cells
(Tsuboi & Hayashi, complex kinetics)

- Phase between 2 orthogonal modes can be controlled (Hanana et al. 2001)
- Complex kin -> computation 10 x bigger
- So, resolution still an issue
- Cell size?
- Otherwise, seems similar to 2-D

Chemistry
(Details in other talk)

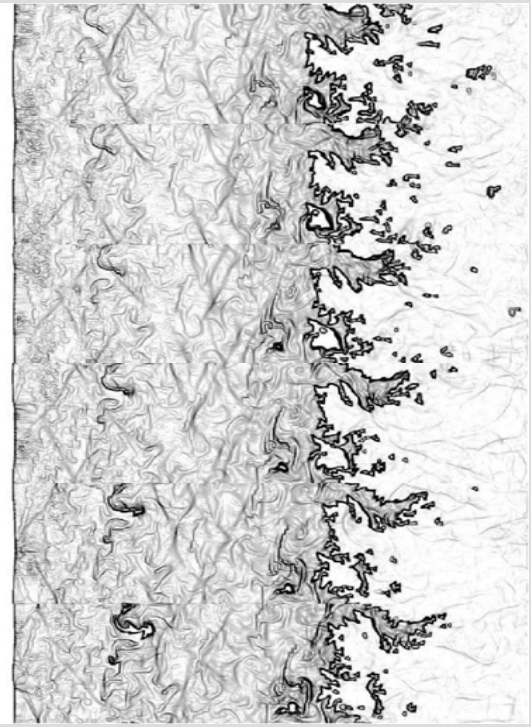
- Hydrogen-oxygen: simplest kinetics
- Even so, detailed schemes still uncertain
- Particularly at high pressure
- Stiffness problem fundamental
- Chain-branching is crucial: resolution?

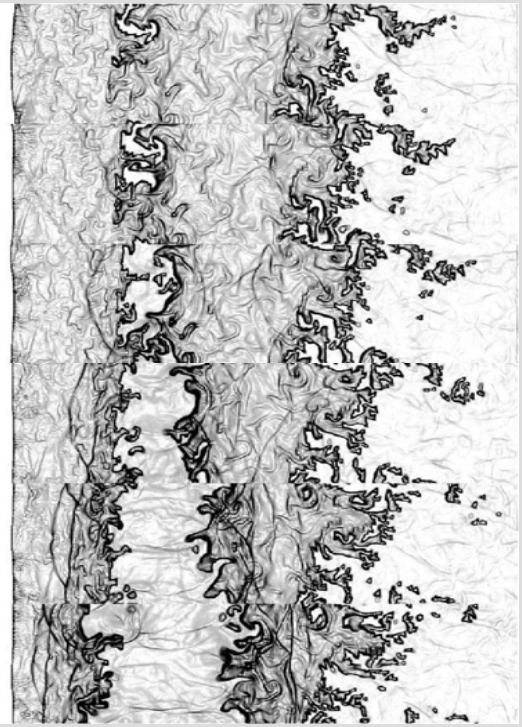
Hot Spots/DDT



- Pressure and temperature gradients
- (Williams D.N., Bauwens, L. & Oran, E.S, 1996.)

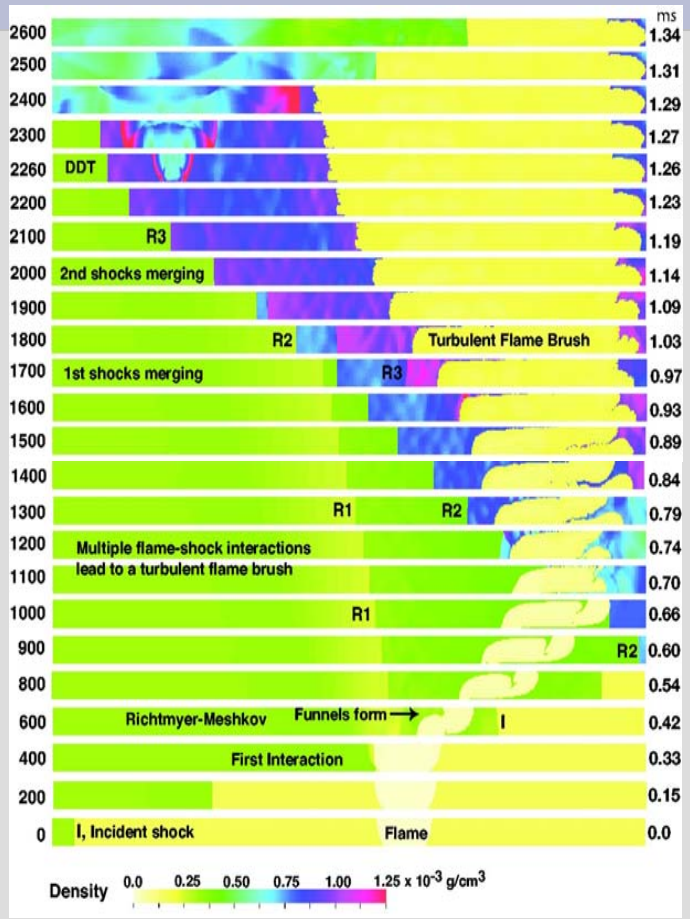
Hot Spots/DDT





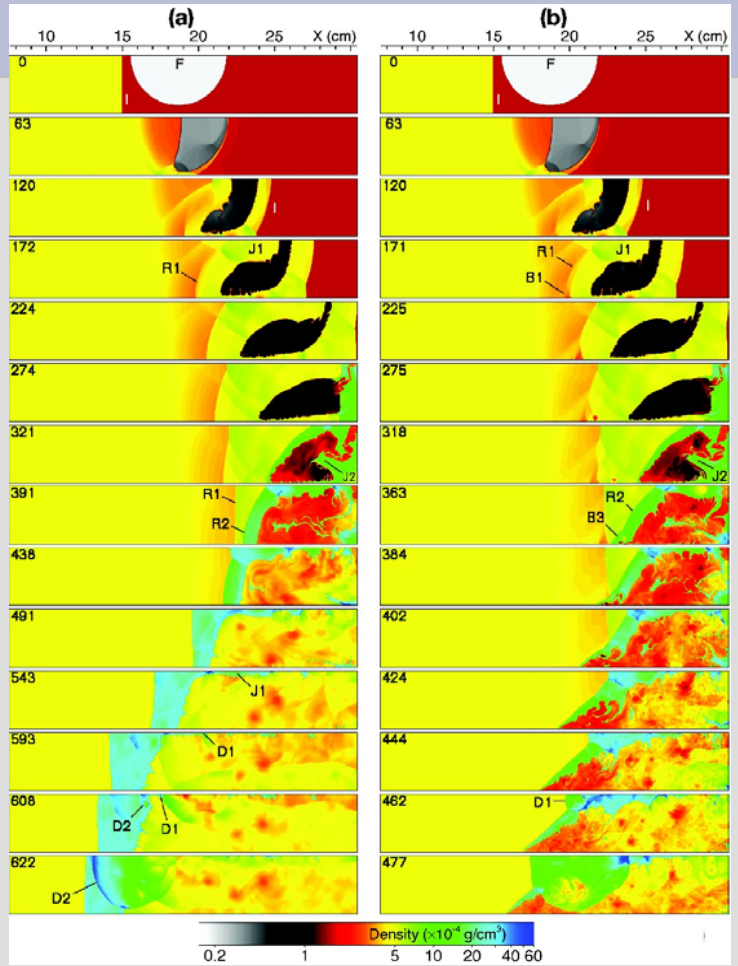
- Density gradients (Williams D.N., Bauwens, L. & Oran, E.S, 1996.)

DDT



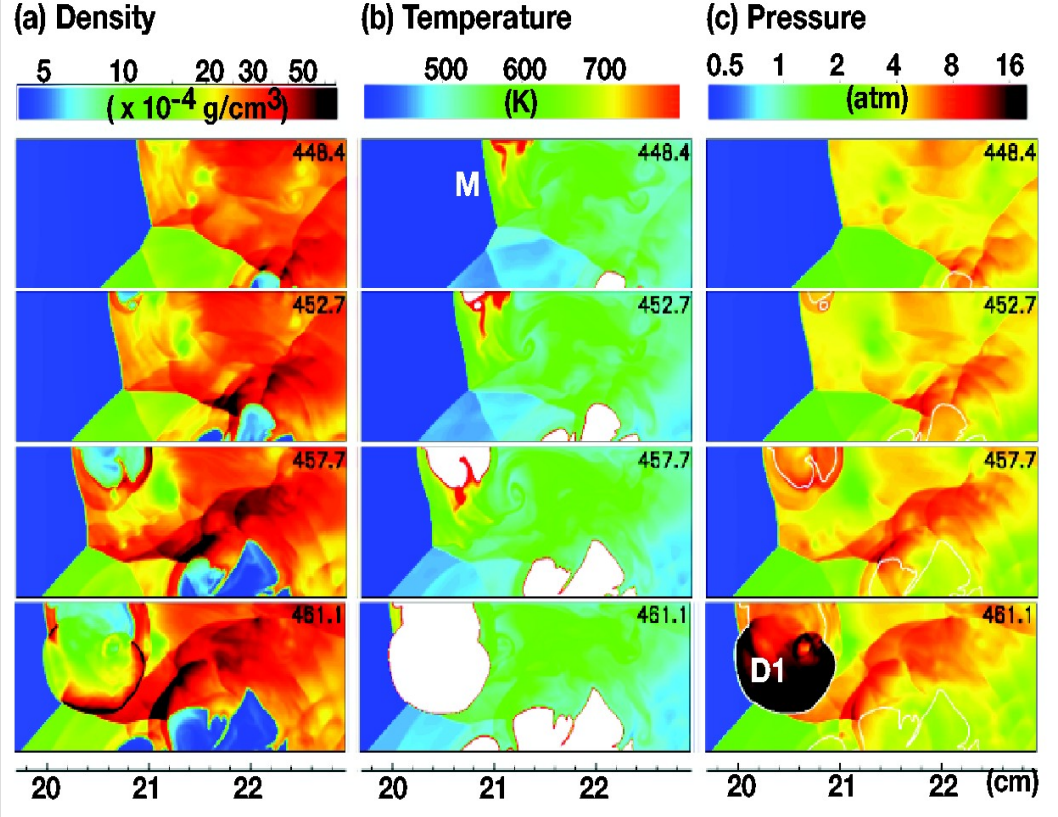
- (Oran & Gamezo, in press 2006)

DDT (effect of boundary layer)



- (Oran & Gamezo, in press 2006)

Hot Spots/DDT



- (Oran & Gamezo 2006, in press)

Hot Spots/DDT

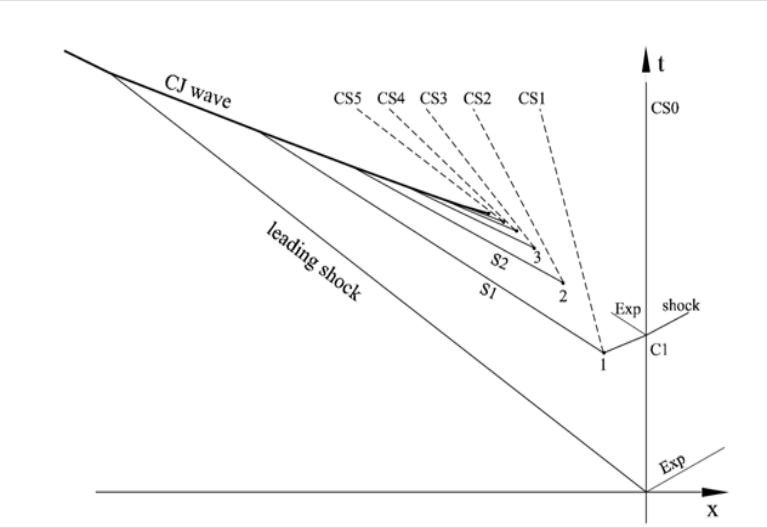
- Show movie (Gamezo et al. 2006)
  - Flame acceleration over obstacles
  - Turbulent combustion/recirculation
  - Rayleigh-Taylor?
  - Hot spot in corner (repeated shock heating)
  - Eventually strong enough: strong explosion
  - But observe: ahead of the flame

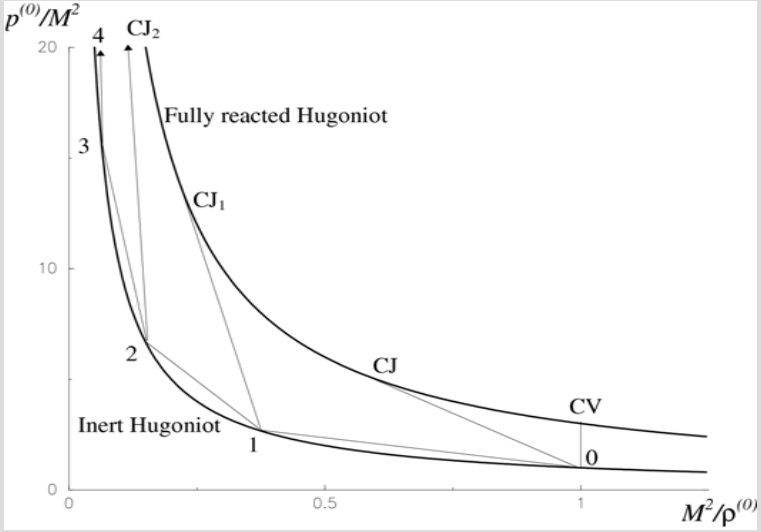
Hot Spots/DDT

- Current theories (spontaneous flame, Zel'dovich; SWACER, Lee...) unsatisfying (See Kapila et al. 2002)
- Why huge peak hence retonation?
- 1-D inviscid, non-conducting: peak higher on finer grid (further refinement -> floating point exception?)

Hot Spots/DDT

- Theory (Bauwens 2000, B & Liang 2002) -> embedded sequence of explosions (inviscid, non-conducting)





Hot Spots/DDT
(a bit of speculation)

- Starts with shock heating and hot spot
- Inviscid: peak to infinity on curve?
- Actually: limited by diffusion and/or non-equilibrium?
- Need theory
  - without Newtonian approx
  - More realistic chemistry

Summary

- We have come a long way
- Chemistry/stiffness still an issue
  - Schemes?
  - Stiffness (or better multiscales) is fundamental
- Currently
  - either high res. 3D
  - or more or less detailed kinetics
  - Still no real quantitative match with measurements

Summary (continued)

- However, great insight on physics
- Situation is better than for example
  - turbulent combustion
  - hydrogen dispersion
- Much closer to actual physics

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