Numerical Approach on Hydrogen Detonation: Fundamentals and Applications
-Part 2-

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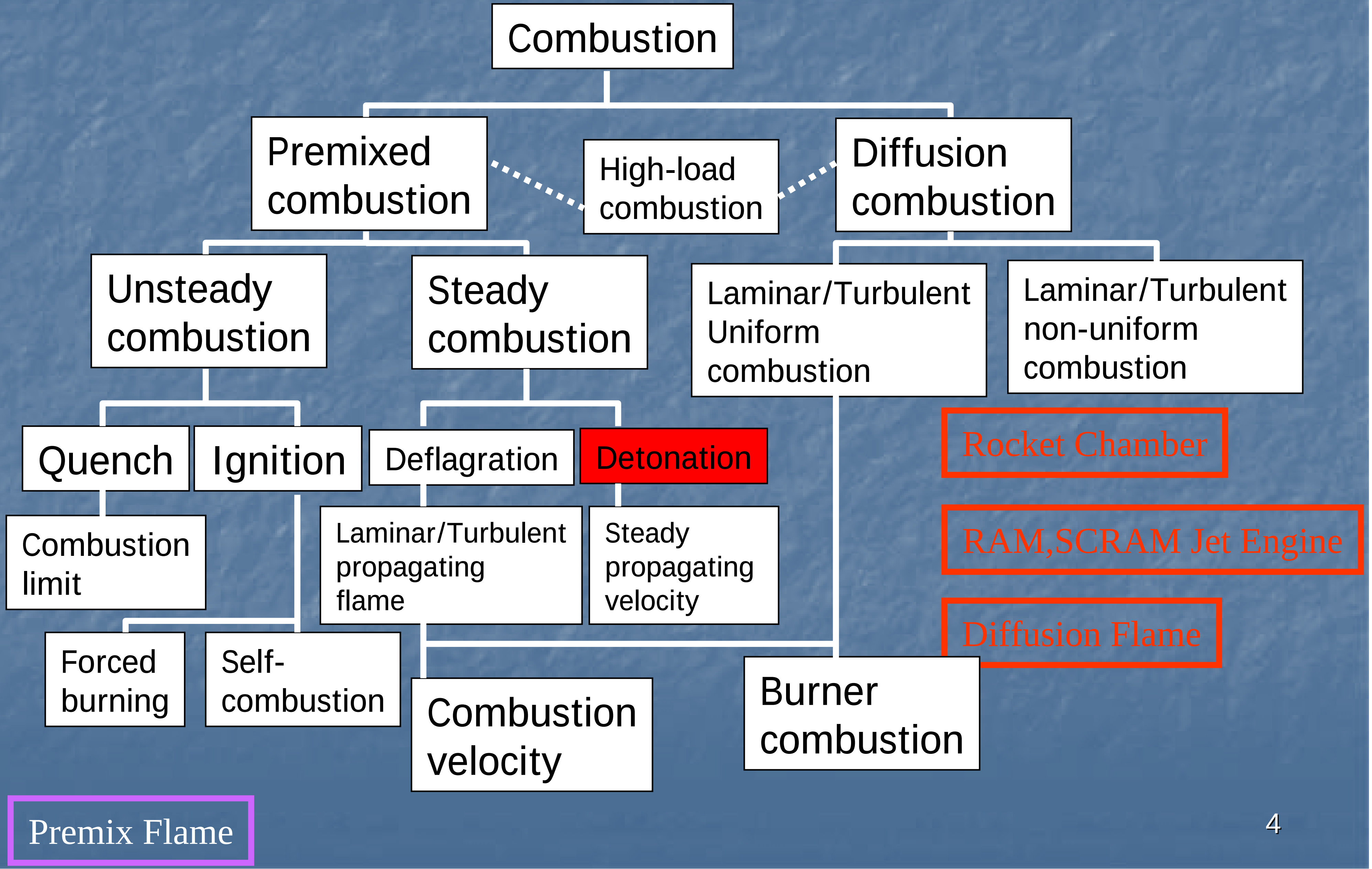
Overview

1. Motivations
2. Introduction of Detonation
3. History and Previous Research
4. Initial and Boundary Condition
5. Effects of Grid Resolutions
6. Detonation Structure by Numerical Simulations(2D,3D)
7. Remaining Tasks and Summary

Motivations

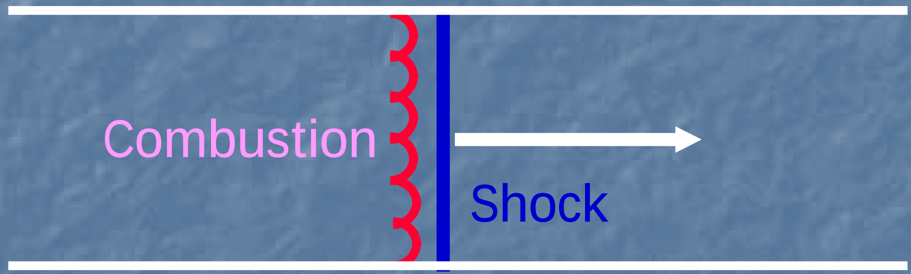
- Hydrogen/air mixture: detonable gas
- Detonation: shock induced combustion
  -Pressure behind detonation increases
    about 10 times ambient pressure
- Closed environment such as a tunnel causes serious accident.

What is Detonation?



What is Detonation?

- Detonation wave is combustion wave induced by shock wave

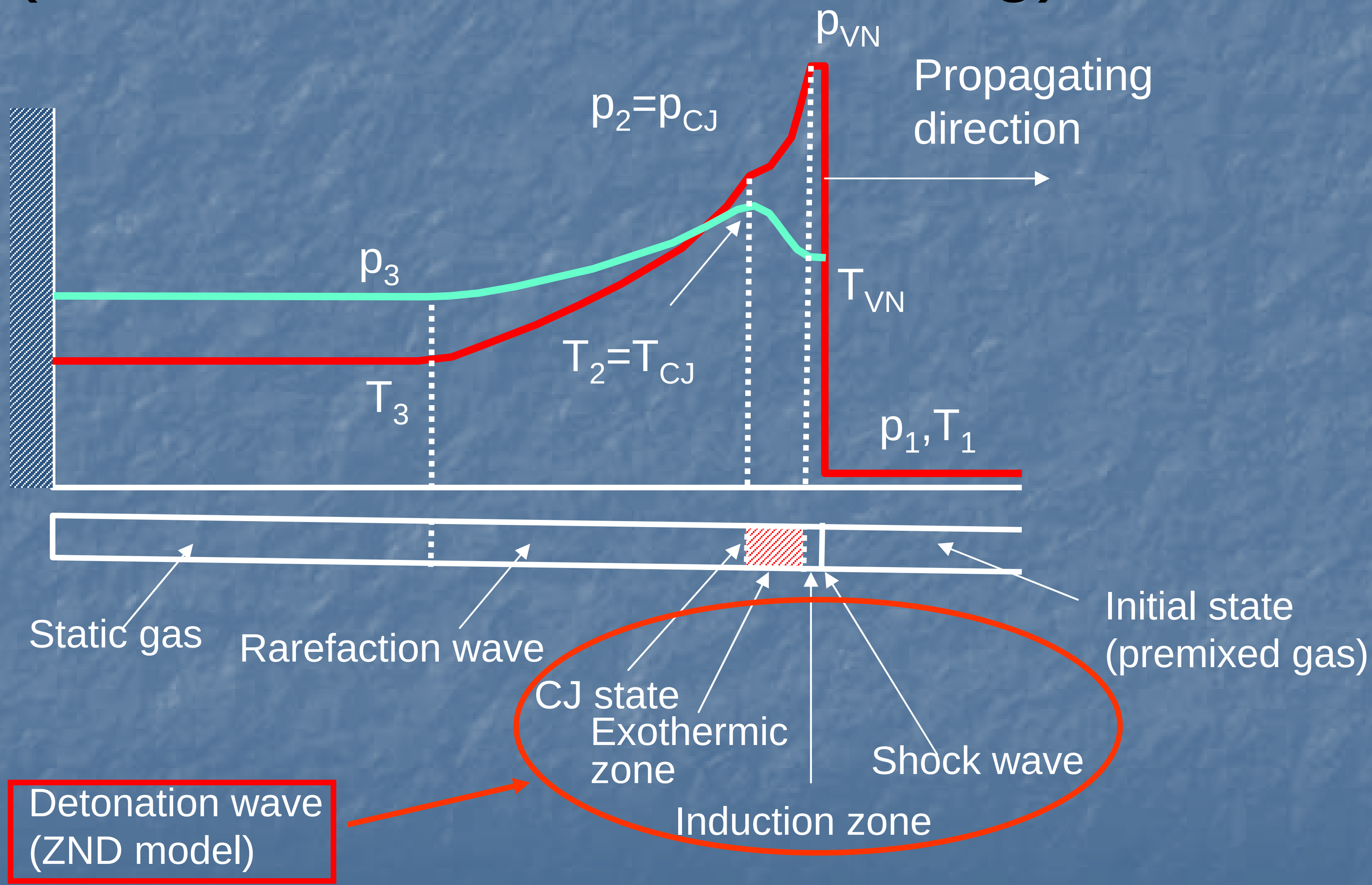


Detonation velocity:

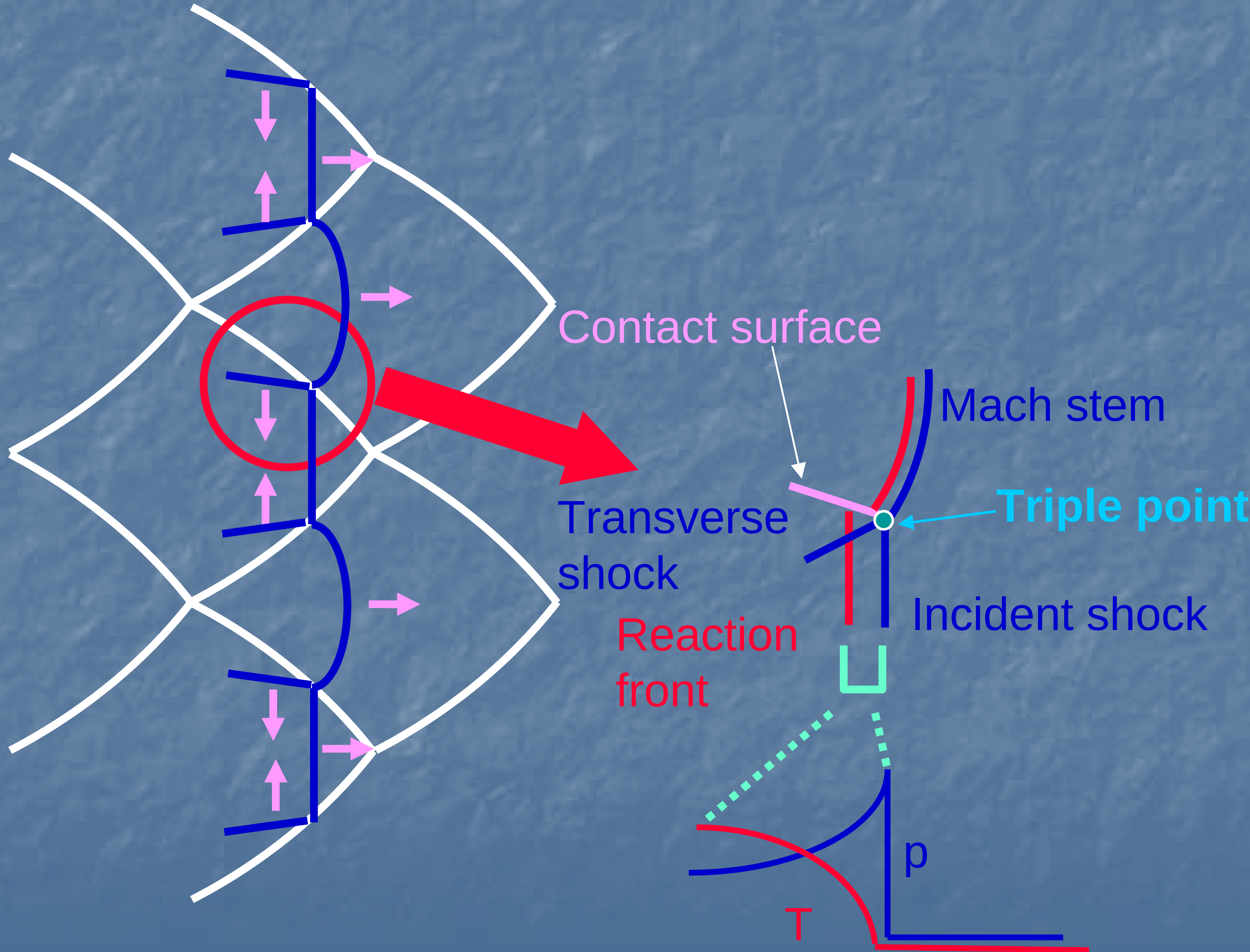
80%H2 20% O2 : 3,400m/s
66%H2 33.3%O2 : 2,850m/s
25%H2 75%O2 : 1,750m/s
CH4 + O2 : 2,600m/s

What is Detonation?

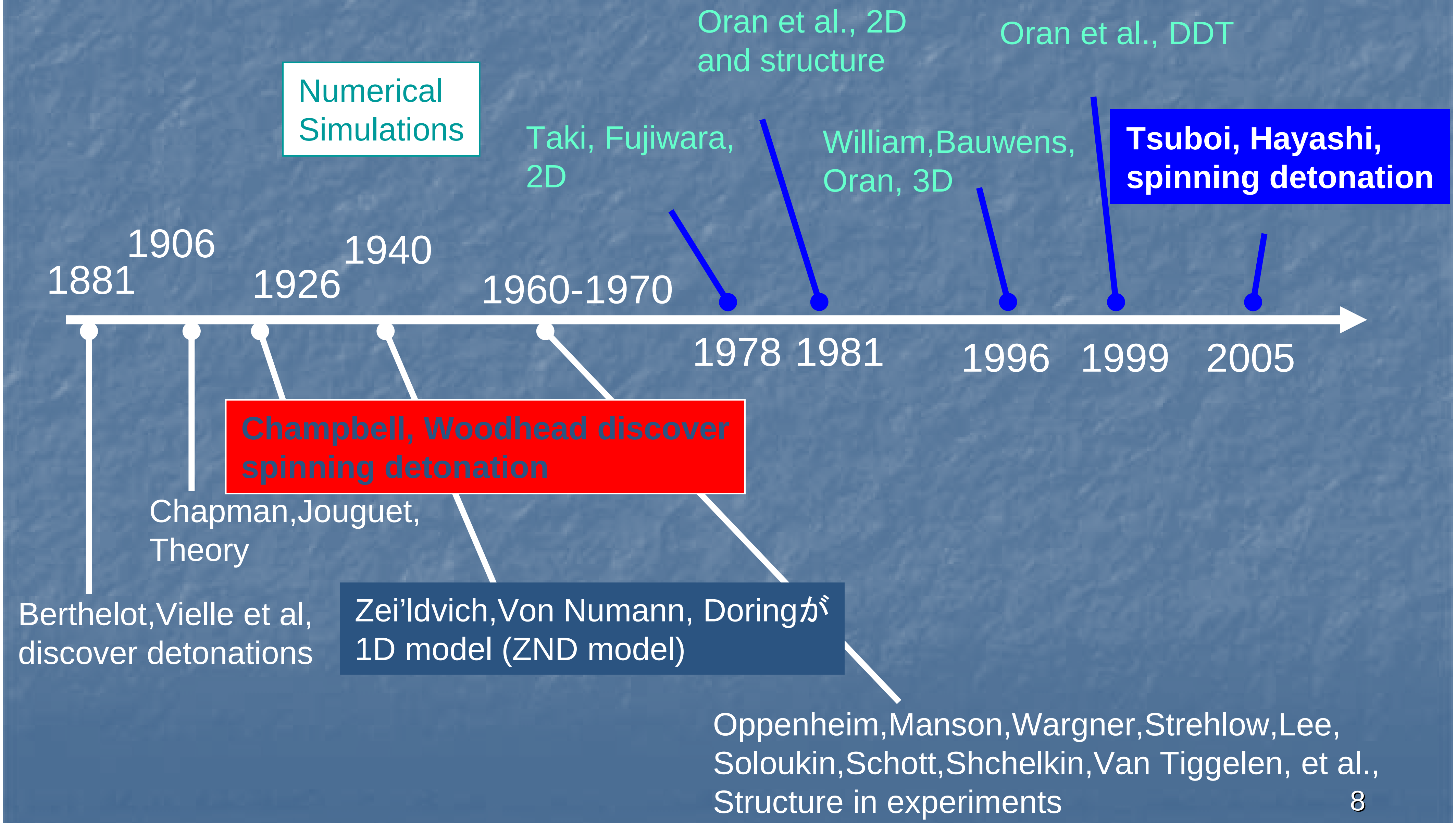
- ZND(Zeldovich-Neumann-Doering) model



What is Detonation?



History and Numerical Simulation



Initial and Boundary Conditions

Initial Conditions

- 1D : one wall is the boundary at a stationary coordinate system and a high pressure and temperature for ignition is initially imposed near the wall.
- 2D :

  -ZND or 1D results are used

  -Unburned premixed gas behind the detonation front
- 3D :

  -ZND or 1D results are used

  -Unburned premixed gas behind the detonation front

  -Optional initial condition is given to get a desired detonation pattern (square tube)

Boundary Conditions (2D,3D)

- Shock wave coordinate system for the constant tube cross section
- Upstream boundary : A premixed gas flows with CJ velocity
- Downstream boundary:

-A CJ pressure-fixed BC (transverse wave are reflects, slight overdriven detonation)

-An expansion BC proposed by Gamezo (expansion boundary: reflection of transverse wave can be weaken)

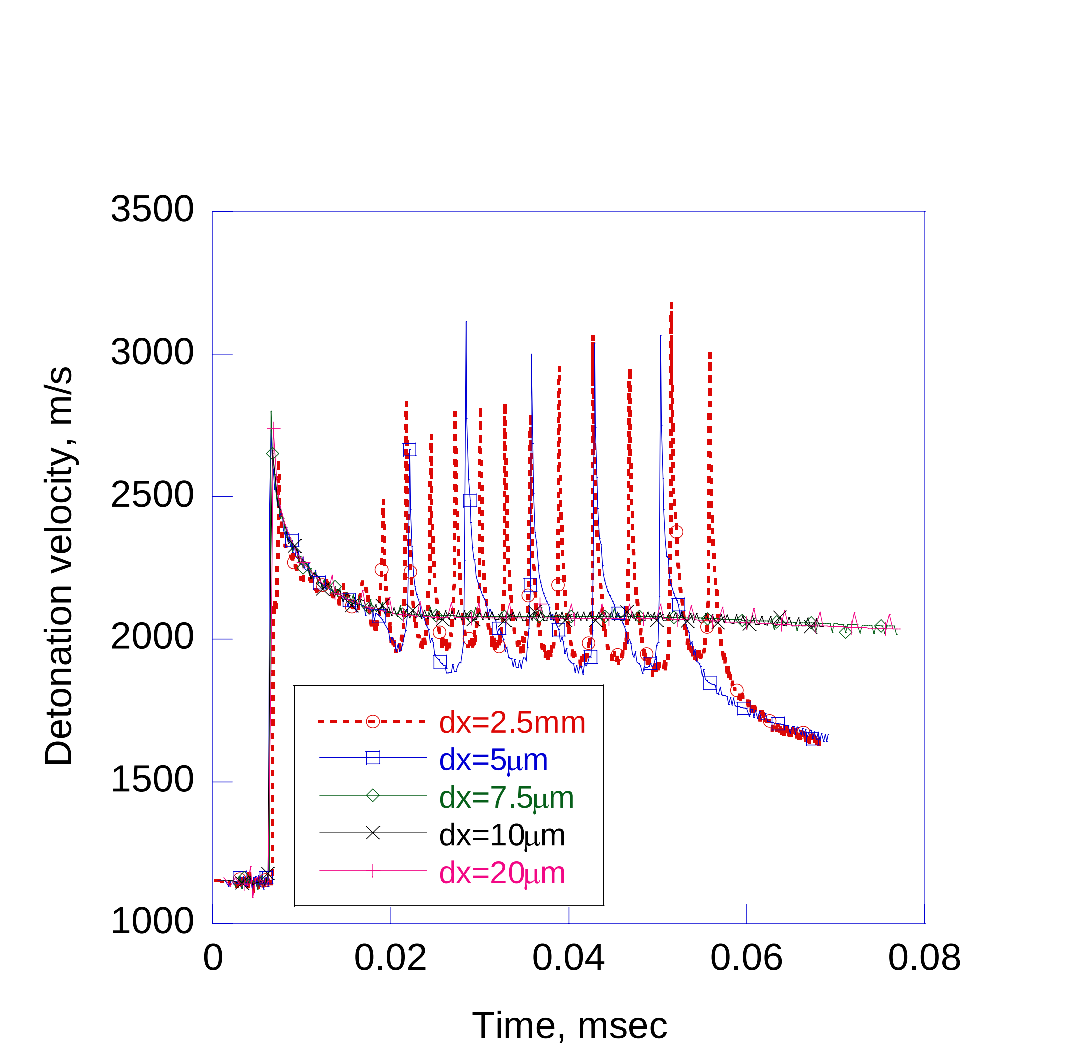
Effects of Grid Resolutions

Effects of Grid Resolutions on 1D Detonation

- The important index for grid resolutions is the grid number in the half reaction length of fuel.
- The half reaction length is calculated by ZND profile.
- Its value for stoichiometric H2/Air is about 160 micron and it is dependent on the (detailed) reaction model.
- At least 30 points are better.

Effects of Grid Resolutions on 1D Detonation Velocity

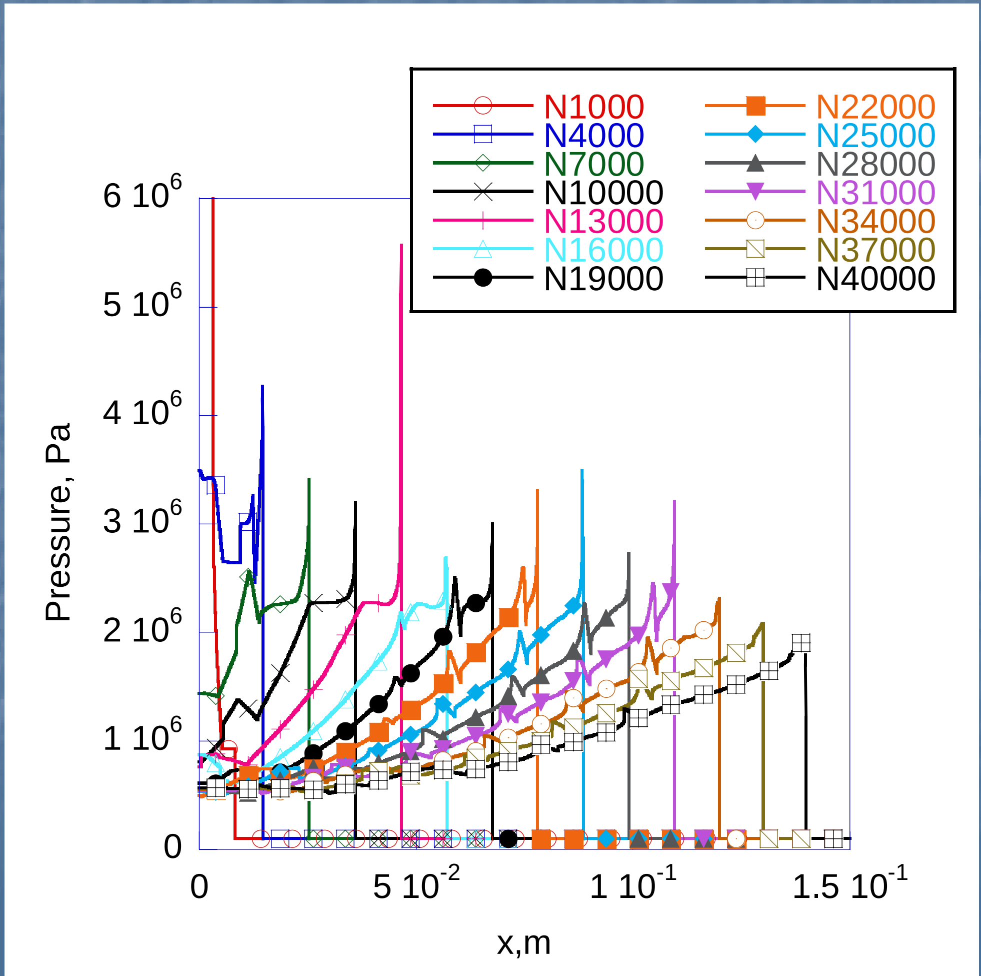
- Detonation velocity oscillates near CJ velocity for fine grid.
- Weakly “stable” overdriven detonation for coarse grid due to numerical dissipation.



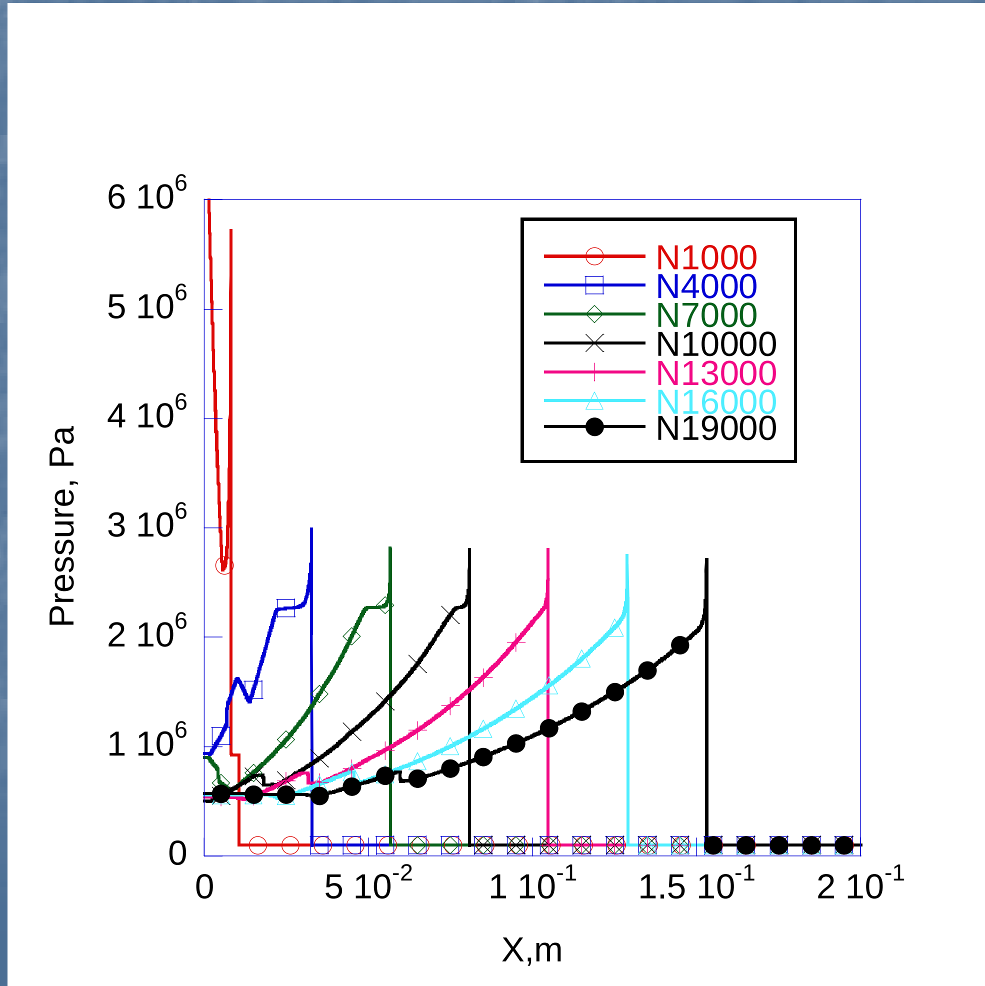
Stoichiometric H2/Air, 1atm, 300K

Effects of Grid Resolutions on 1D Instantaneous Pressure

- Detonation oscillates near CJ velocity for fine grid because combustion front separate or catch up with the shock periodically.
- Weakly "stable" overdriven detonation for coarse grid due to numerical dissipation



dx=5micron

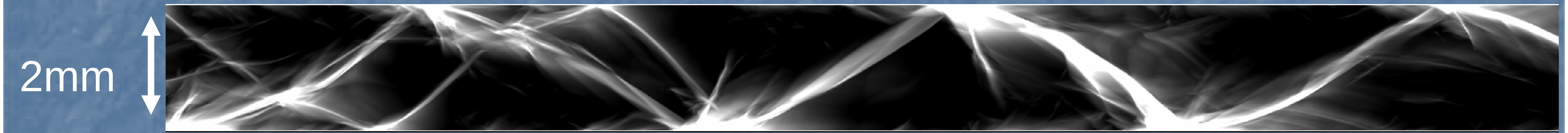


dx=10micron

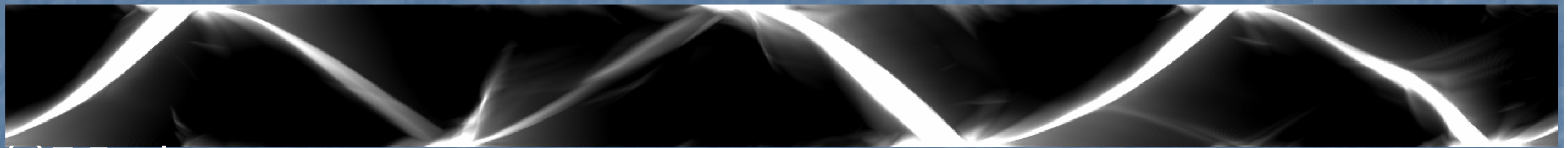
Effects of Grid Resolutions on 2D Detonation

- Cell structure becomes clearly unstable and large for finer grid

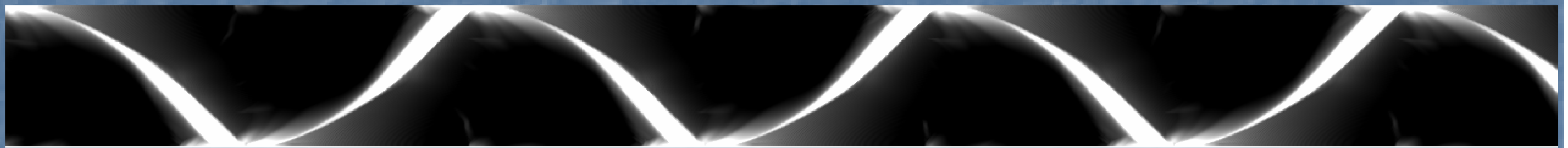
(a)2.5 micron



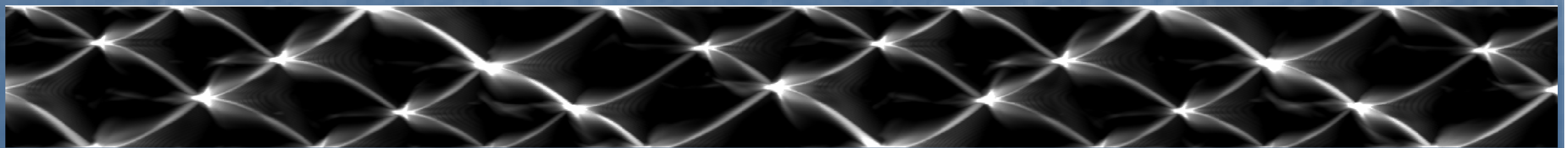
(b)5 micron

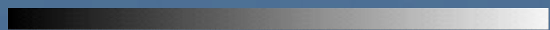


(c)7.5 micron



(d)10 micron

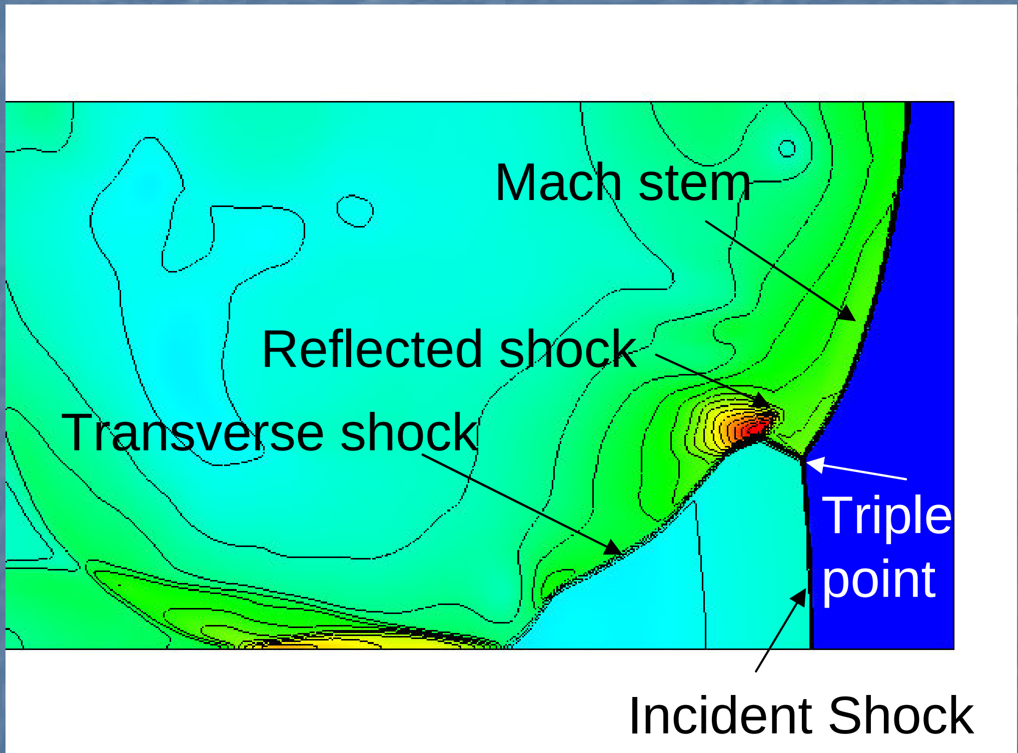




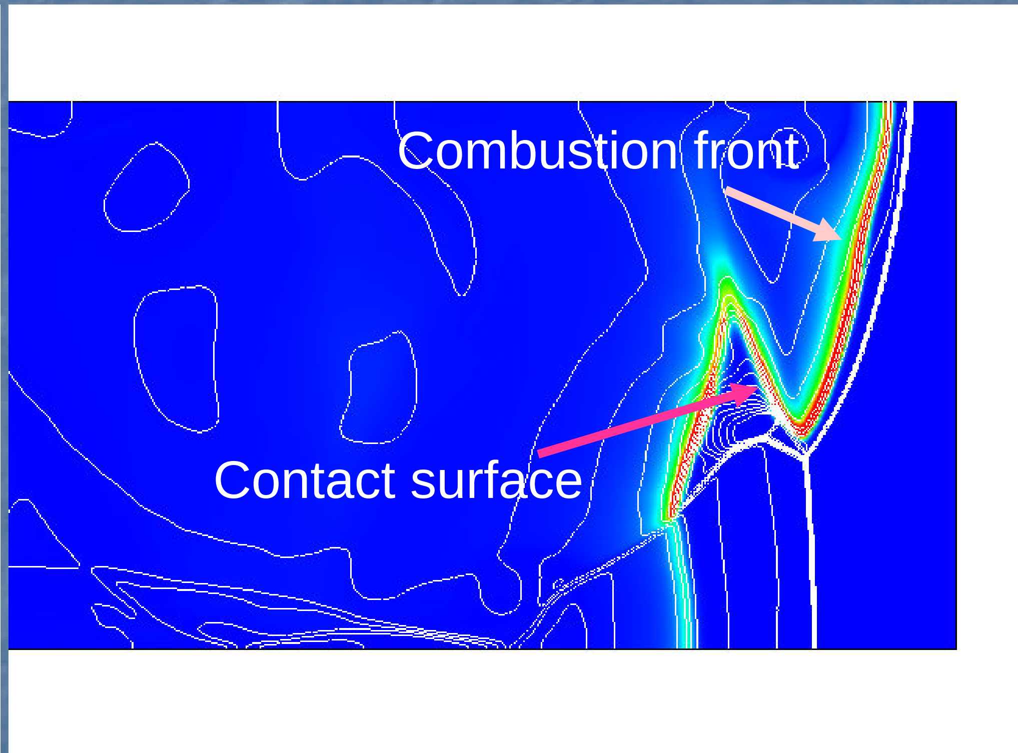
Detonation Structure by Numerical Simulations: 2D Detonation Structure

2D Detonation Structure

Maximum pressure history



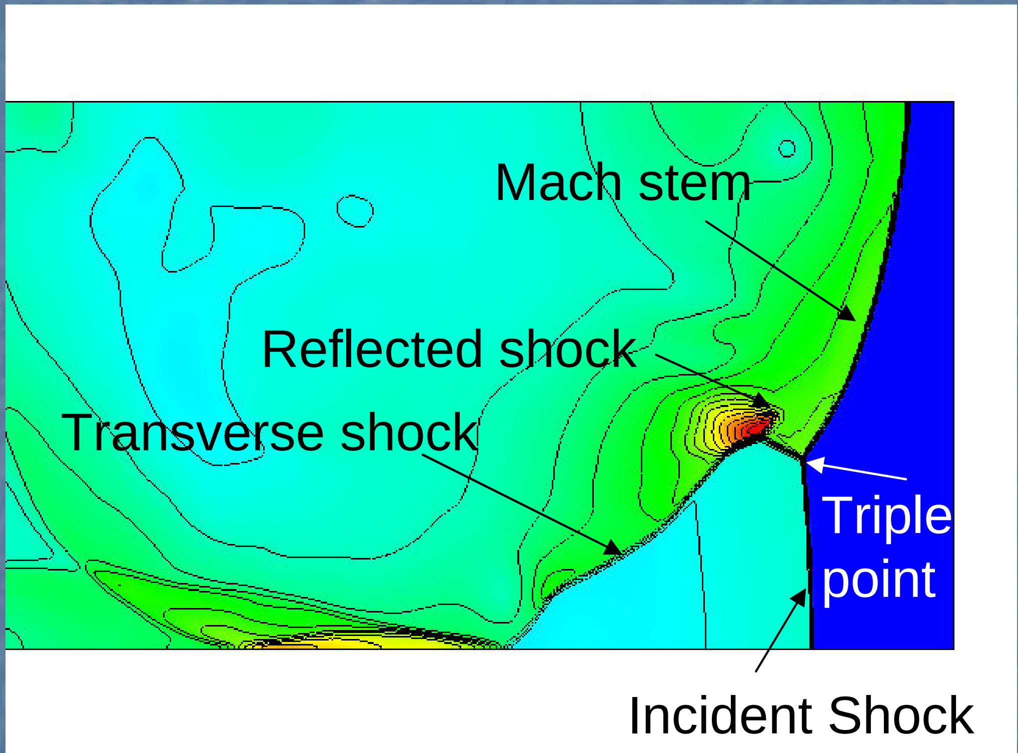
Pressure

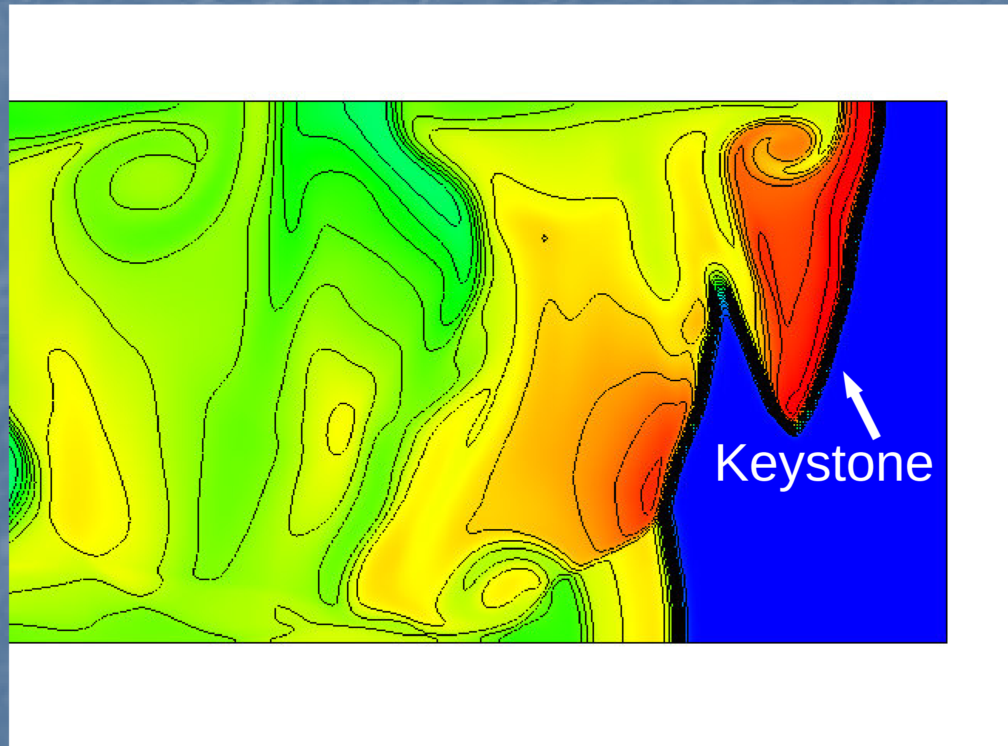


Density(white), specific energy release

2D Detonation Structure

- Keystone structure was observed experimentally by Pintgen et al.





Pressure

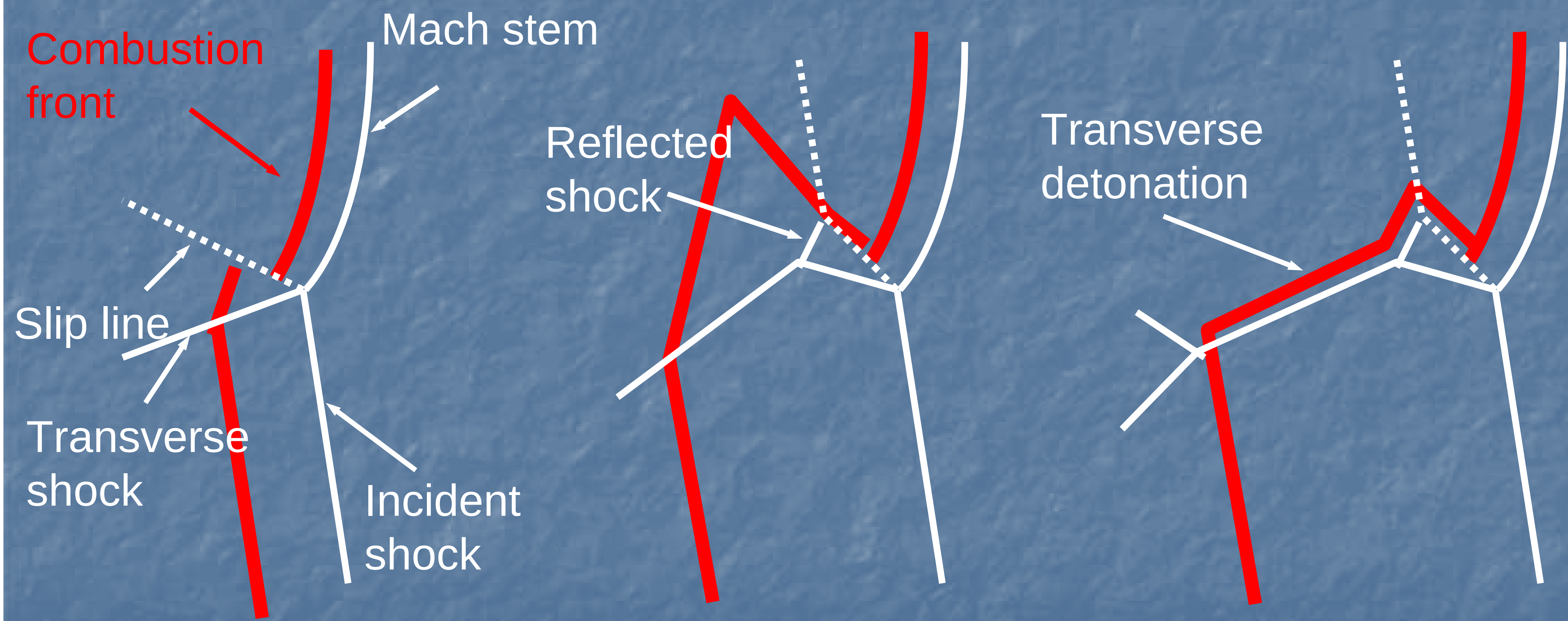
OH mass fraction

1 — 60 atm

0 — 0.03

2D Detonation Structure

- The schematic figure of the basic two-dimensional detonation proposed by Lefebvre et al.



(a)Single Mach reflection

(b)Double Mach reflection

(c)Complex Mach reflection

Detonation Structure by Numerical Simulations:
3D Detonation Structure
(Square Tube)

Simulation Conditions (Half Cell)

Computational grids

$\Delta x=5; \Delta y, \Delta z=10$ [μm]

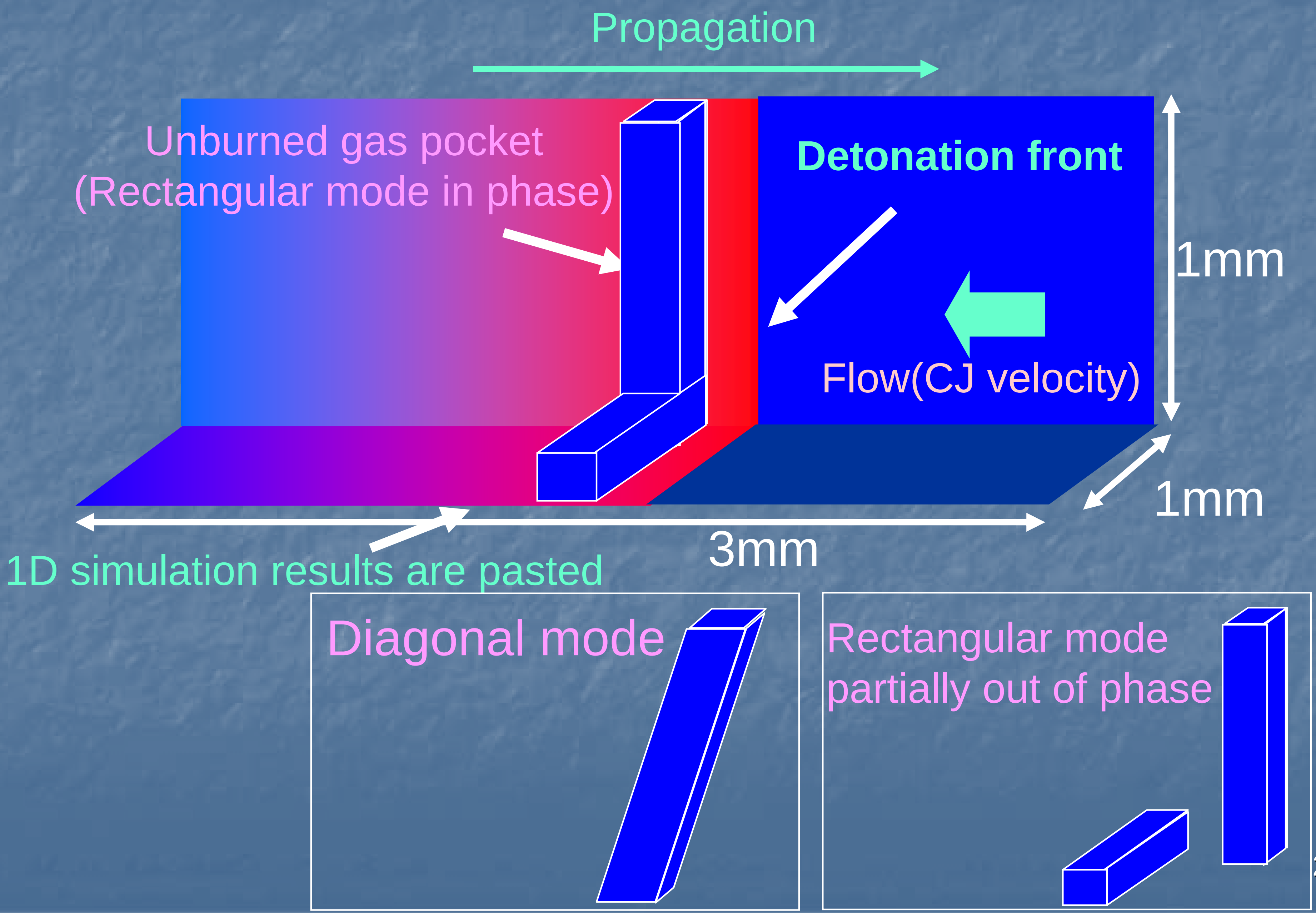
Grid points :601x101x101(uniform grid)

Total : 6 millions

Numerical conditions

- Gas composition: Stoichiometric H2/Air
- Pressure : 0.1 [MPa]
- Temperature : 298.15 [K]
- Initial condition : 1-D simulation results
- Iteration : 57,000
- CPU time: about 140 hours (on SX-6 (1node,8 CPU))

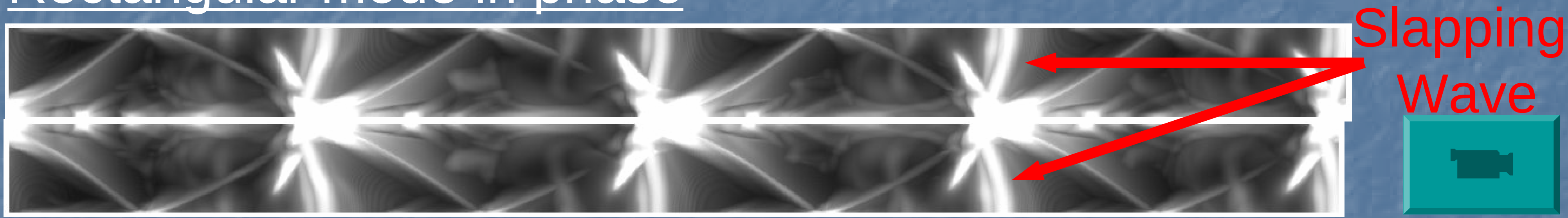
Initial Conditions (Half Cell)



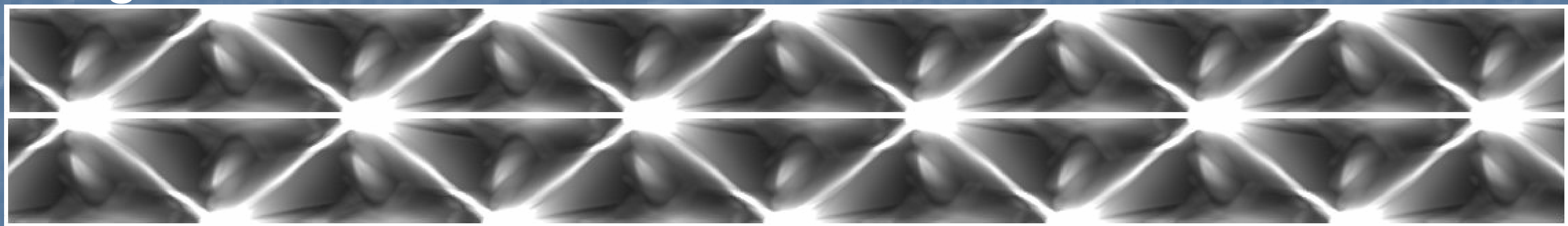
Maximum Pressure History (Half Cell)

2D

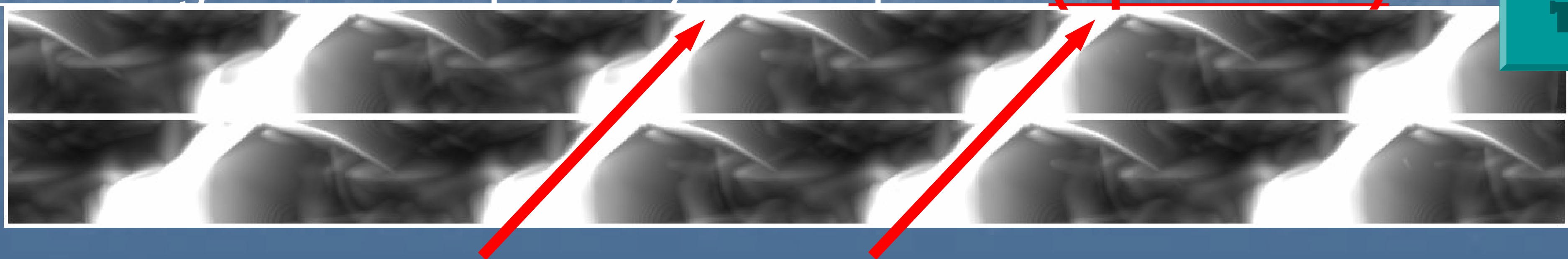
Rectangular mode in phase



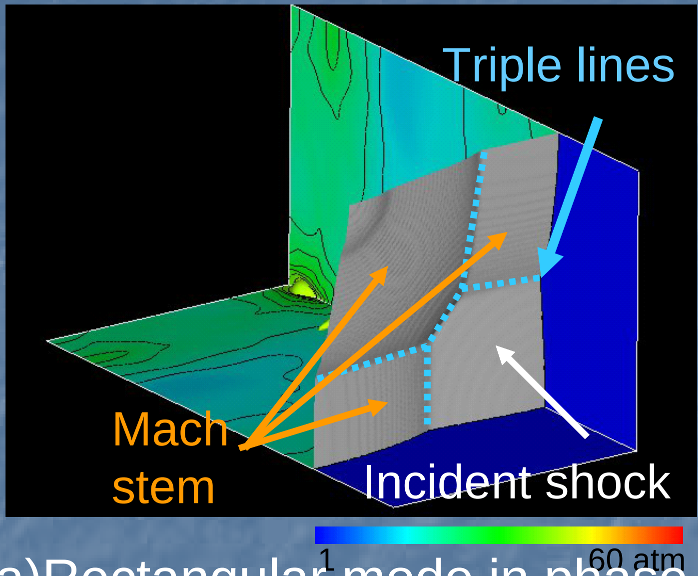
Diagonal mode



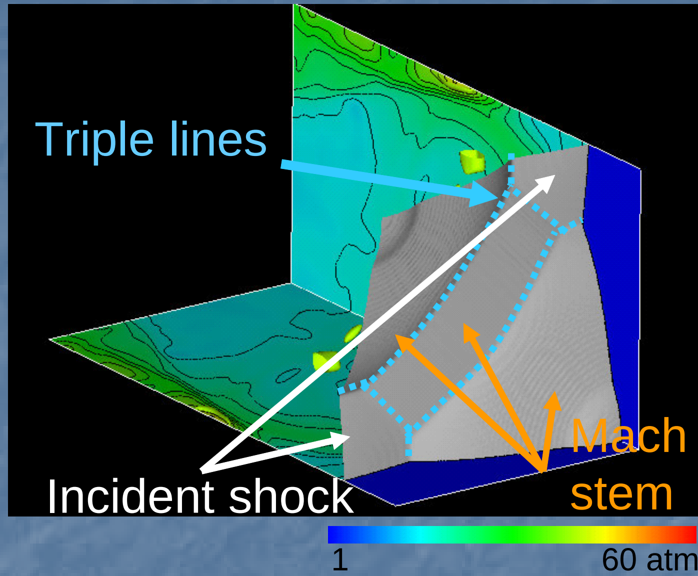
Rectangular mode partially out of phase **(Spin mode)**



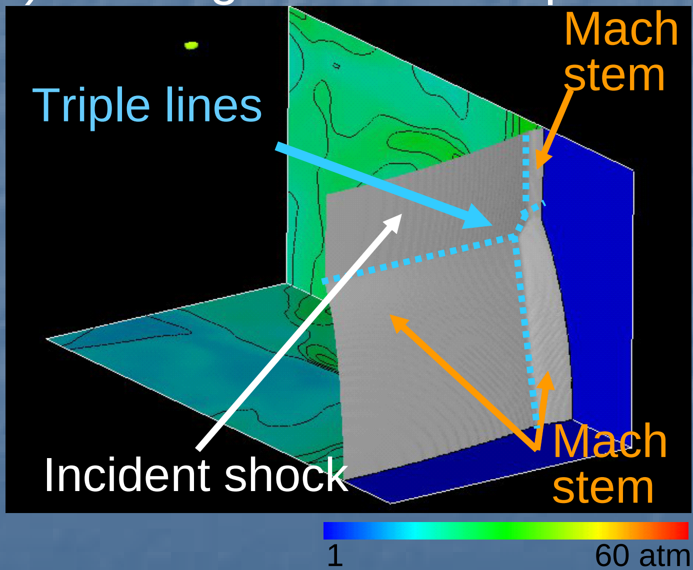
Instantaneous Pressure Contours (Half Cell)



(a)Rectangular mode in phase

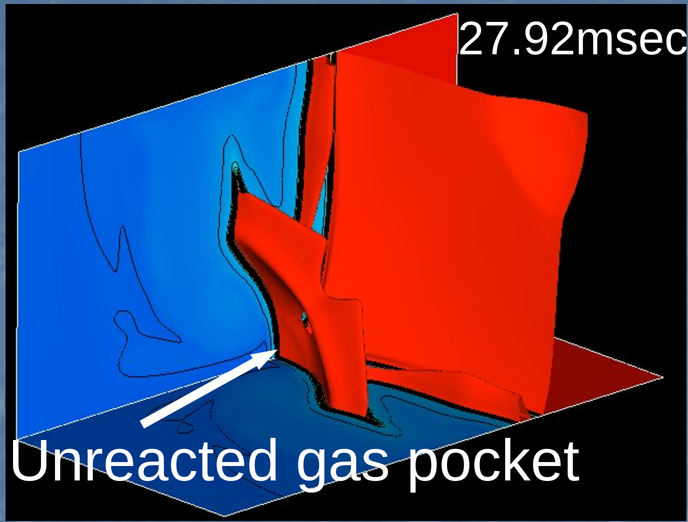


(b)Diagonal mode

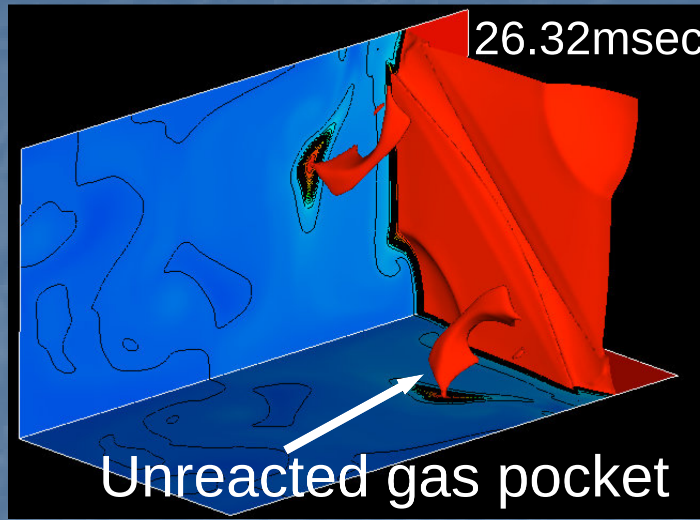


(c)Rectangular mode partially out of phase(spin mode)

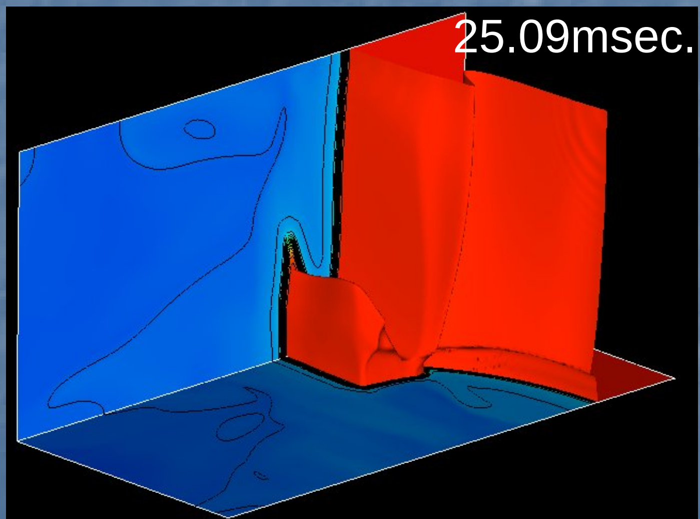
Instantaneous H2 Massfraction Contours (Half Cell)



(a)Rectangular mode in phase

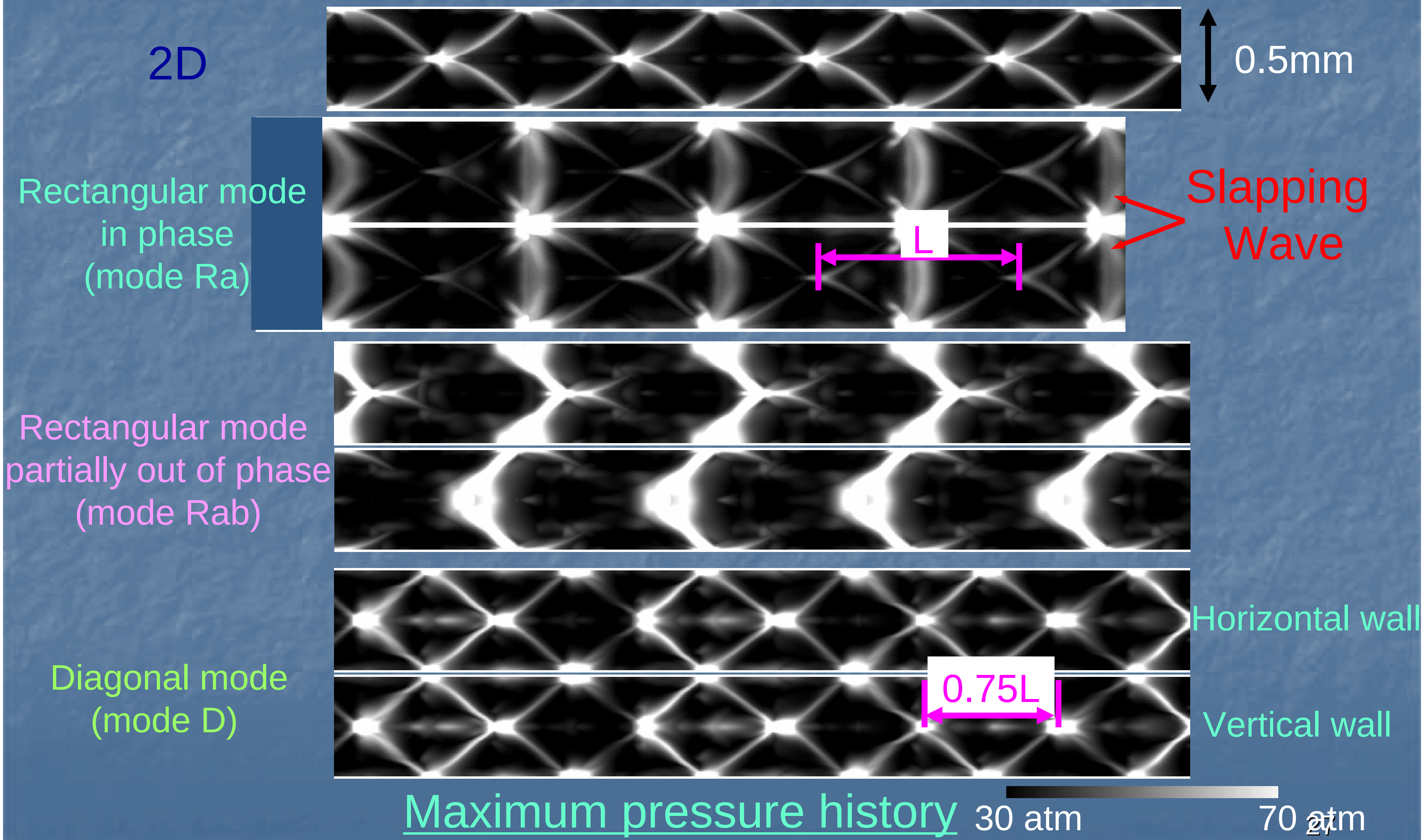


(b)Diagonal mode

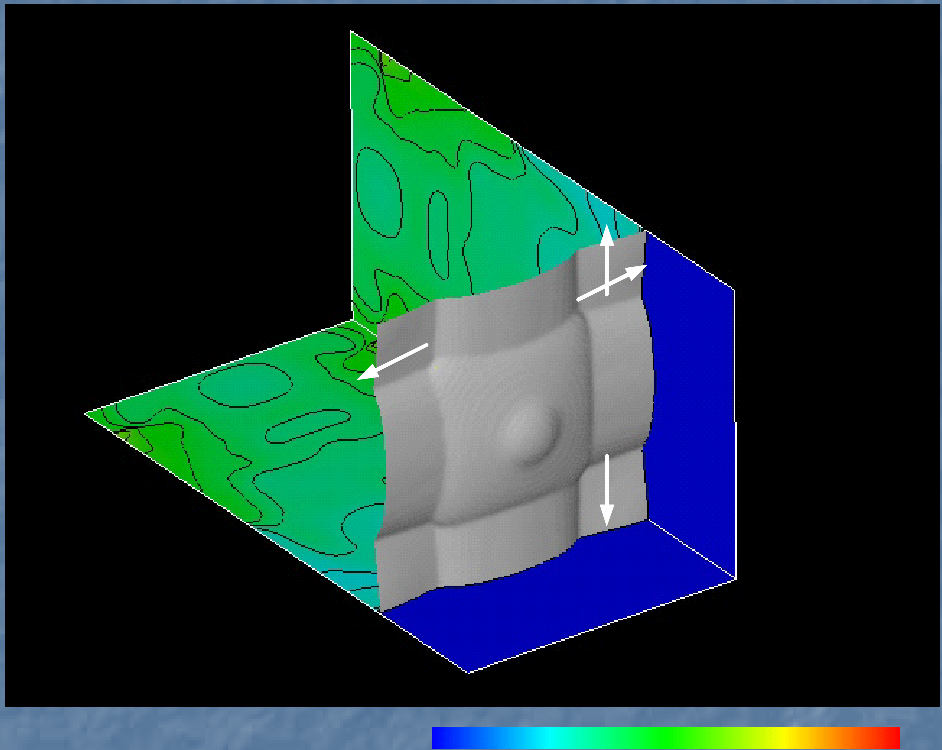


(c)Rectangular mode partially out of phase(spin mode)

Maximum Pressure History (One Cell)

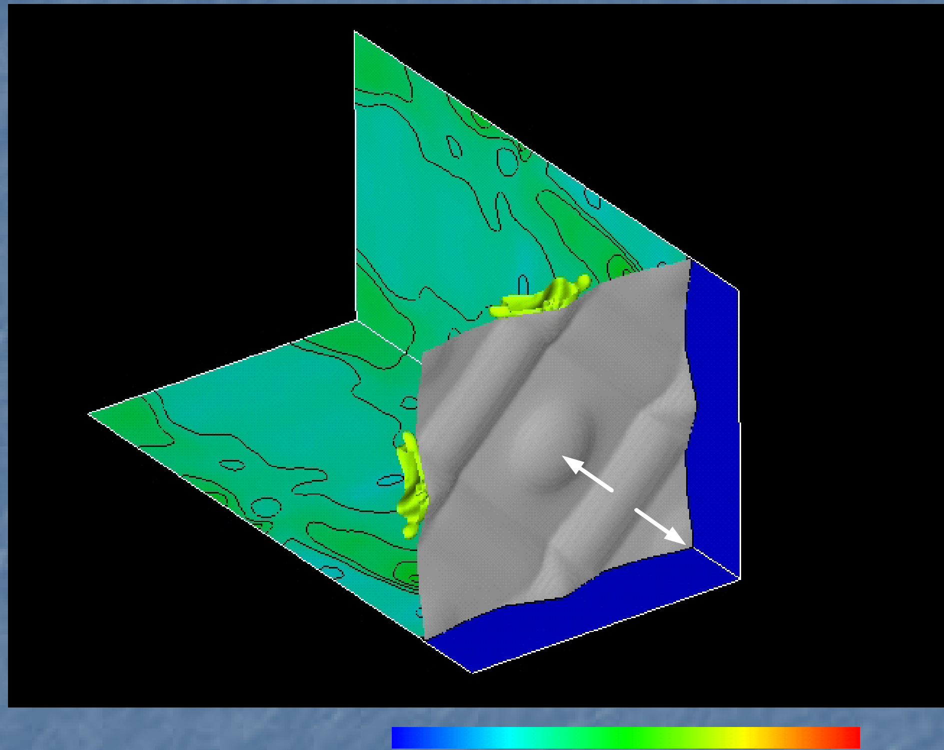


Instantaneous Pressure Contours (One cell)



1atm 60atm

(a)Rectangular mode in phase



1atm 60atm

(b)Diagonal mode

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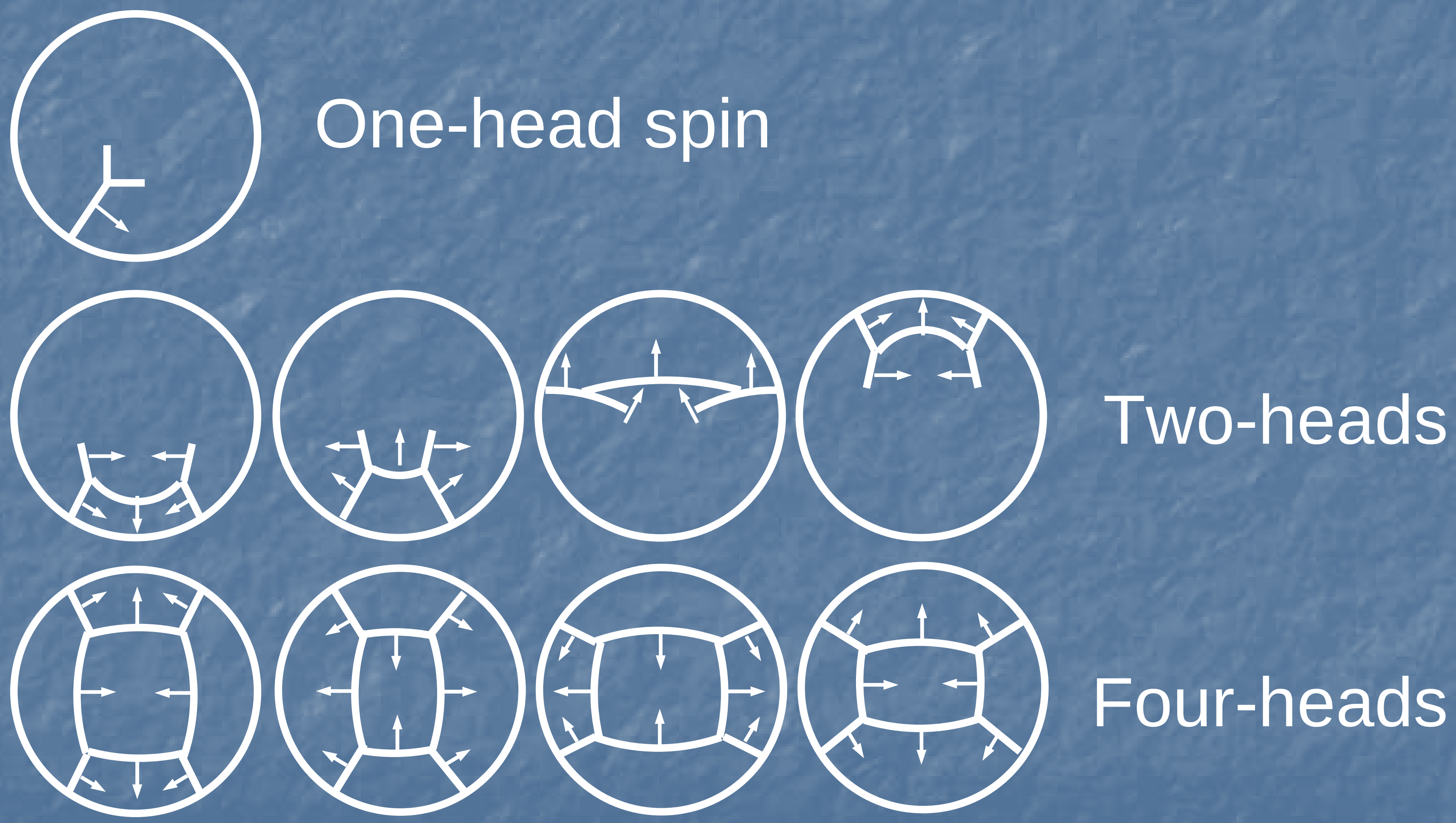
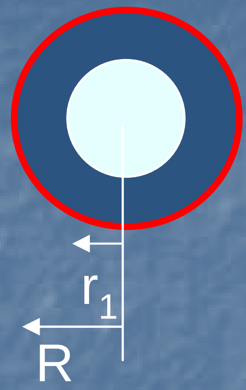
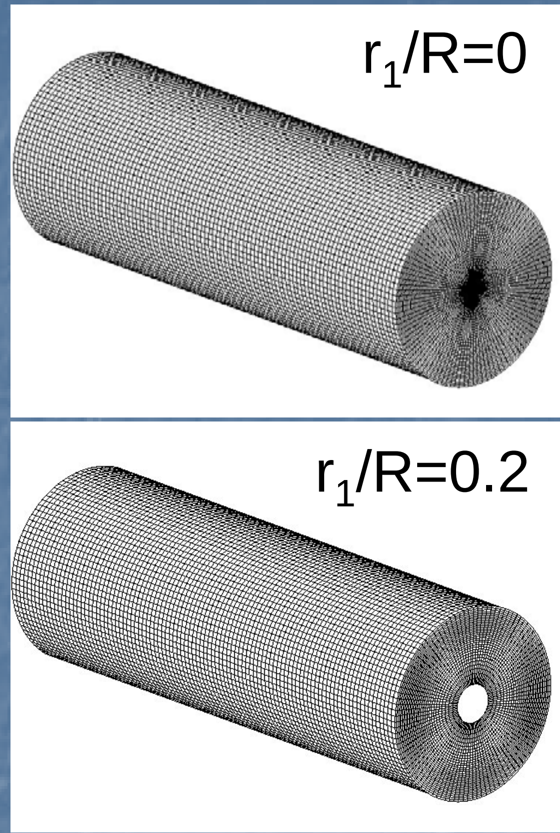
Detonation Structure by Numerical Simulations: 3D Detonation Structure (Circular Tube)

Diagram of Motion of Fronts in Plane of Cross Section



Simulation Conditions





Computational grids

$\Delta x=5;\ \Delta r=10\text{-}20,\ r\Delta\theta=15$ [μ m]

(5 μ m=1/33 of half reaction length of H2 (167.3μm))

Grid points : 601x41x213(max)

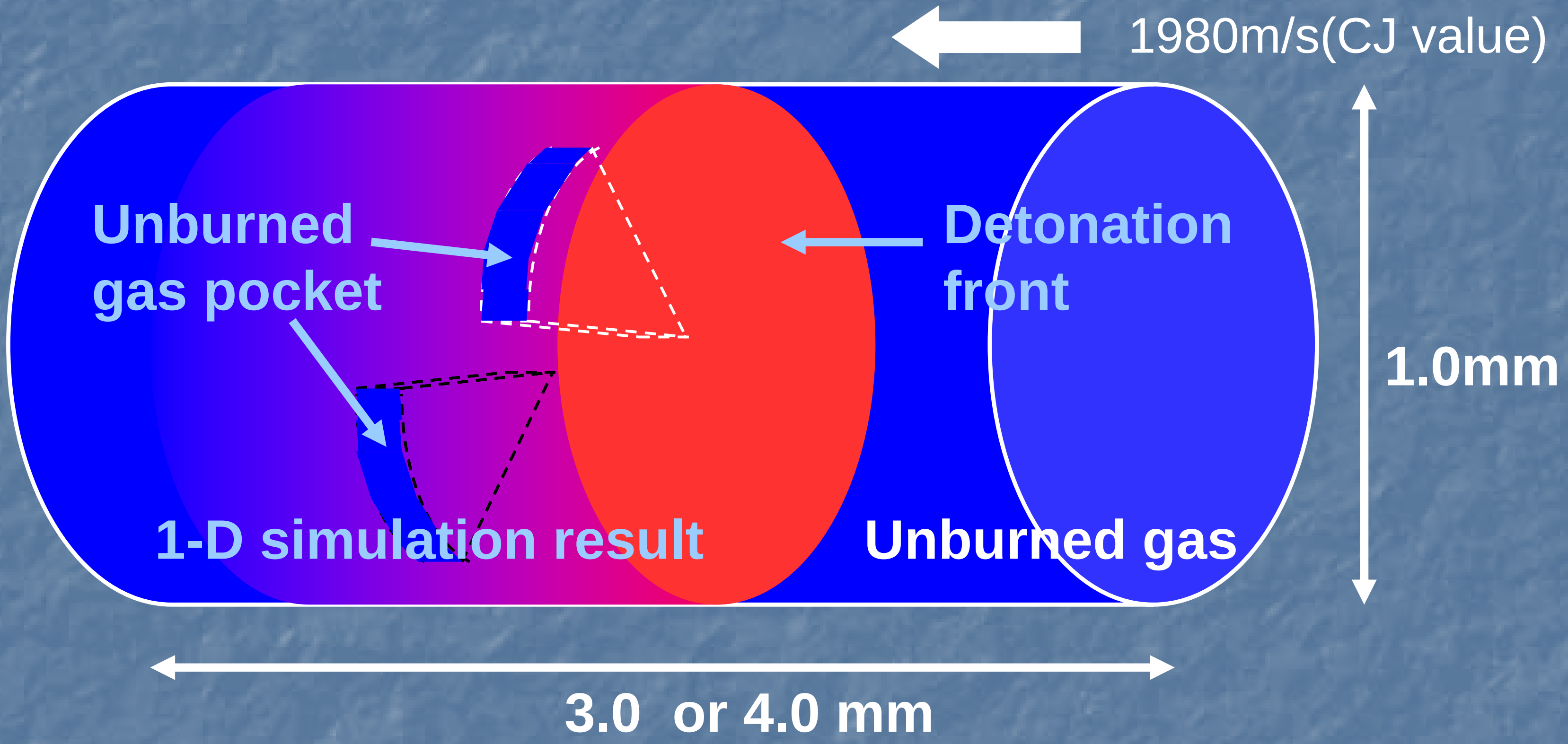
Total : 5.2 millions(max)

r_1/R : 0, 0.2

Numerical conditions

- Gas composition: Stoichiometric H2/air
- Pressure : 0.1 [MPa]
- Temperature : 298.15 [K]
- Initial condition : 1-D simulation results
- CPU time (max) : 200 hours (on SX-6 (1node,8 CPU))

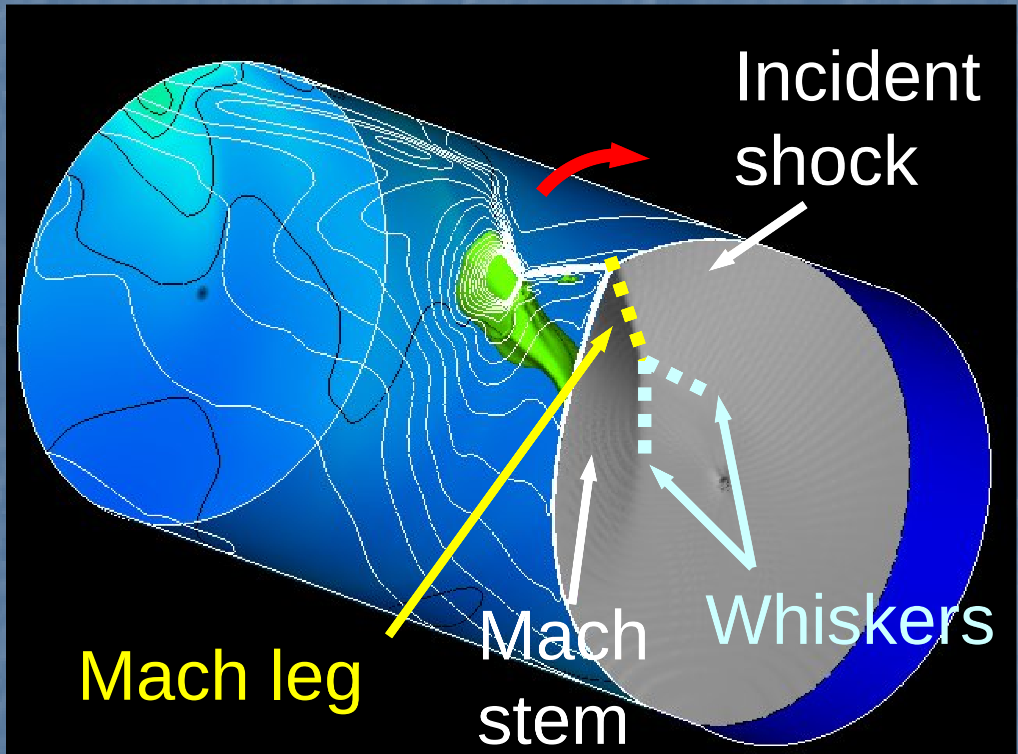
Initial Conditions

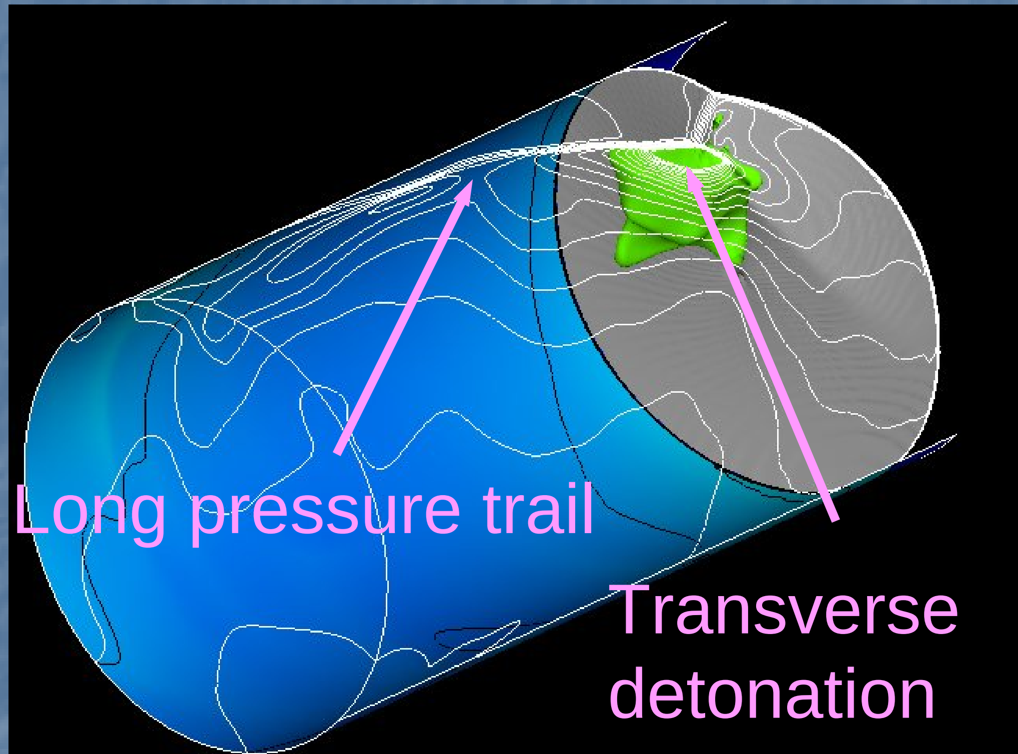


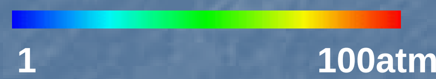
Initial conditions: the result of 1-D simulation.

Initial disturbance: unburned gas pocket
asymmetrically added on the radial direction.

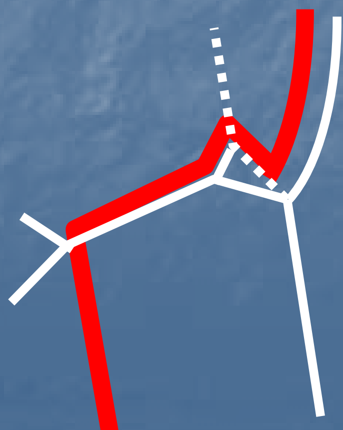
Instantaneous Pressure Contours (Spinning Mode)



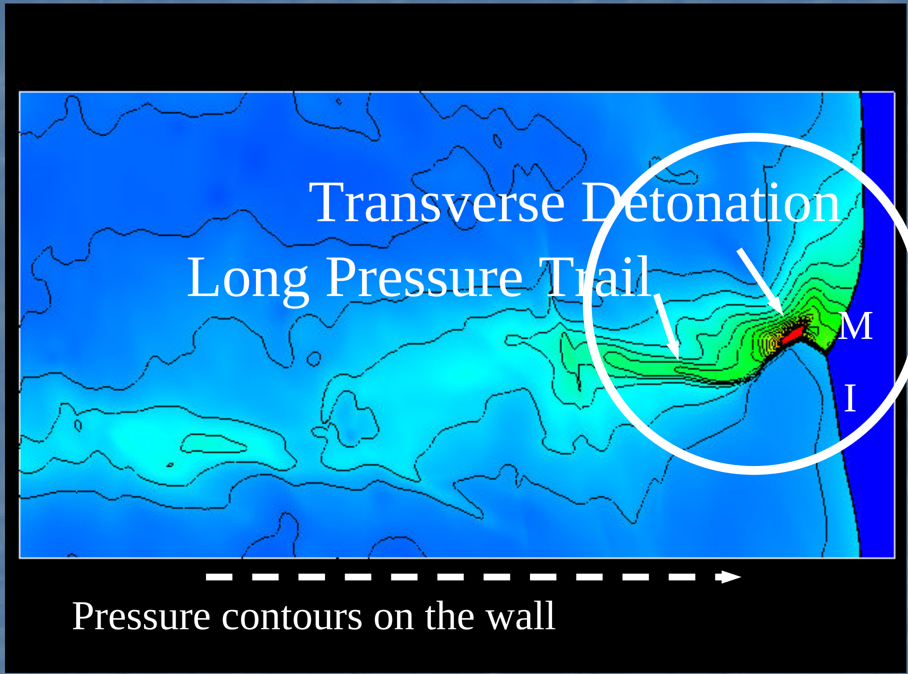


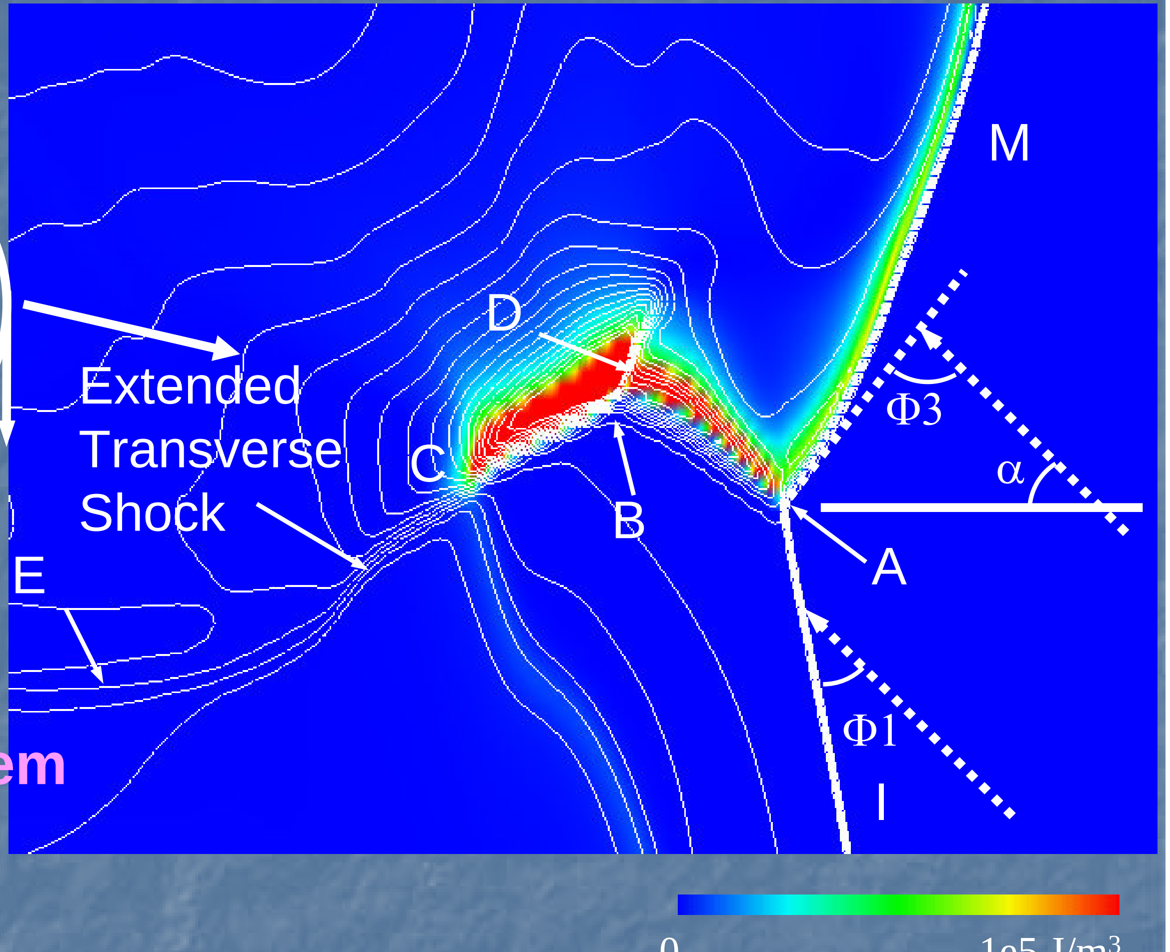


Shock wave structure:
Complex Mach reflection

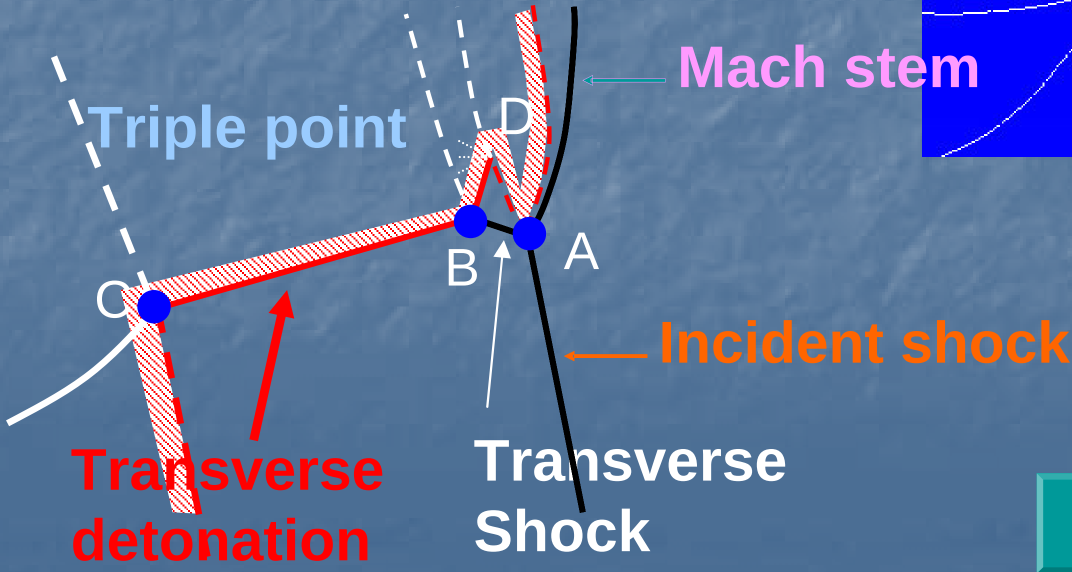


Instantaneous Pressure Contours on Wall (Spinning Mode)

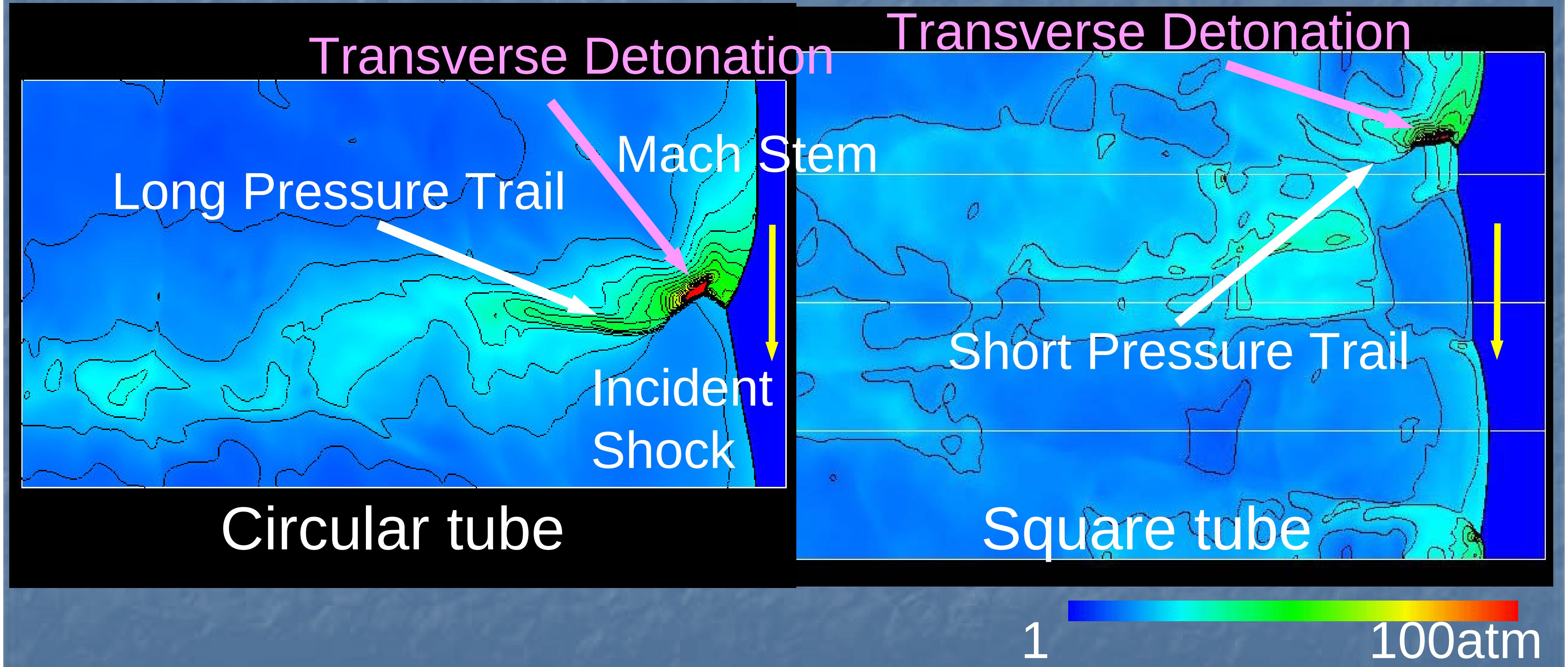




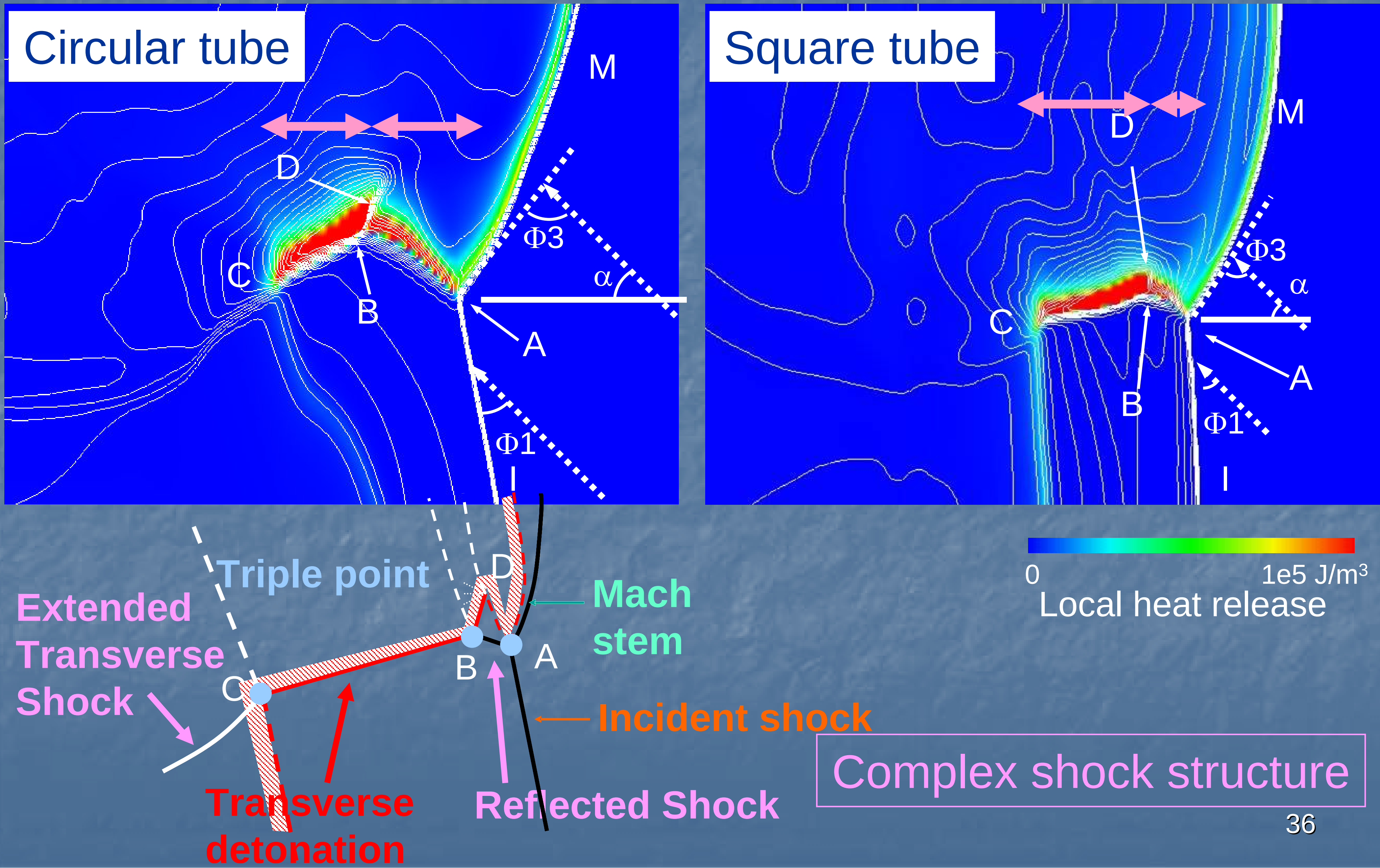
heat release contours +density contours(white)



Instantaneous Pressure Contours on Wall (Spinning Mode: Circle vs. Square)



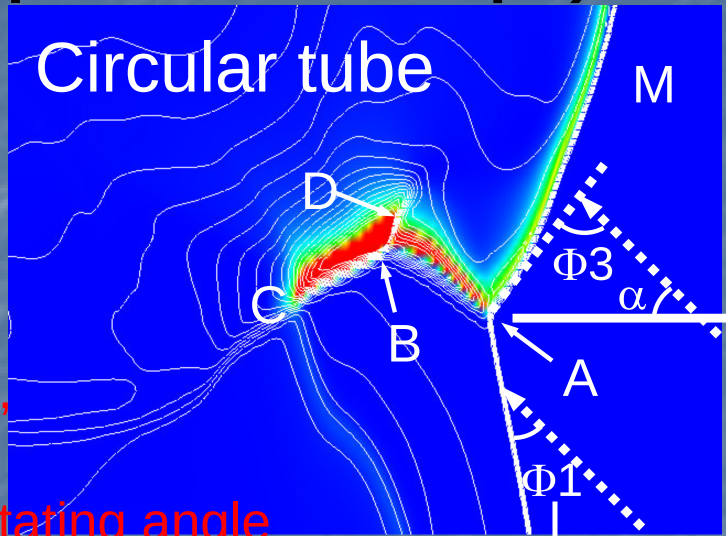
Shock Structure on Wall (Spinning Mode: Circle vs. Square)



Complex shock structure

Shock Angle on Wall
(Spinning Mode: Circle vs. Square vs. Exp.)

Table 1. The flow incident angle of the Mach stem Φ3 using the experimental value of the flow angle of the incident shock Φ1;
^a Nikolaev et al, ^b Voytsekhovsky et al;
^c Huang et al., ^d Ul'yanitskii, ^e This work(Cylinder),
^f Bone et al., ^g Lee et al, h^ This work(Square).



Rotating angle

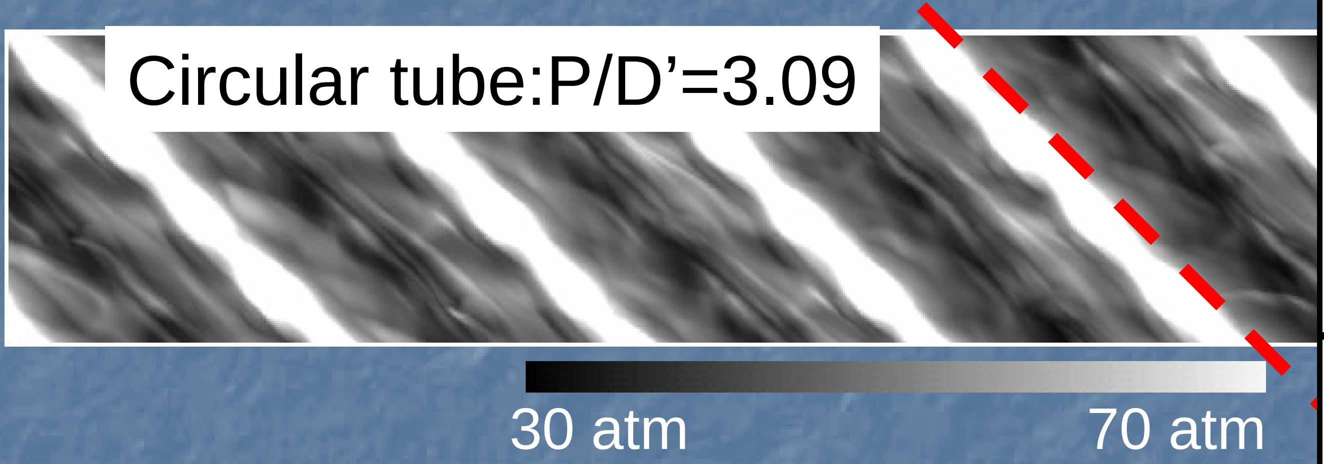
Mixture	Tube diameter(mm)	Initial pressure(Torr	Detonation velocity(m/s	Track angle α	Φ1, deg.	Φ3, deg.
C2H2 + 1.5O2 + 12.5Ar^a	21	45	1637	49	29.2	89.6
2H2 + O2^a	21	48	2688	47	27.8	89.8
2H2 + O2 + 3Ar^a	21	40	1816	46	34.2	87.6
2CO + O2 + 5%H2^a	21	80	1760	45	33.6	87.8
2CO + O2 + 3%H2^b	27	76	1700	44.2	35.6	87.1
1.5H2 + 1.5O2 +7Ar^c	90	22	1325	46.8	30	89.9
C2H2 + 7.58O2 + 34.3 Ar^c	90	30	1227	48.7	32	88.9
H2+Air(Stoich.)^d	40	53	1690	46.6		
2H2 + O2 + 3.76N2^e	1	760	1980	45	35	83
2CO+O2^f	12		1760	49.5		
C2H2 + 1.43O2 + 5.9Ar^g	19	21.4		49		71
2H2 + O2 + 3.76N2^h	1	760	1980	51	43	71

45-49

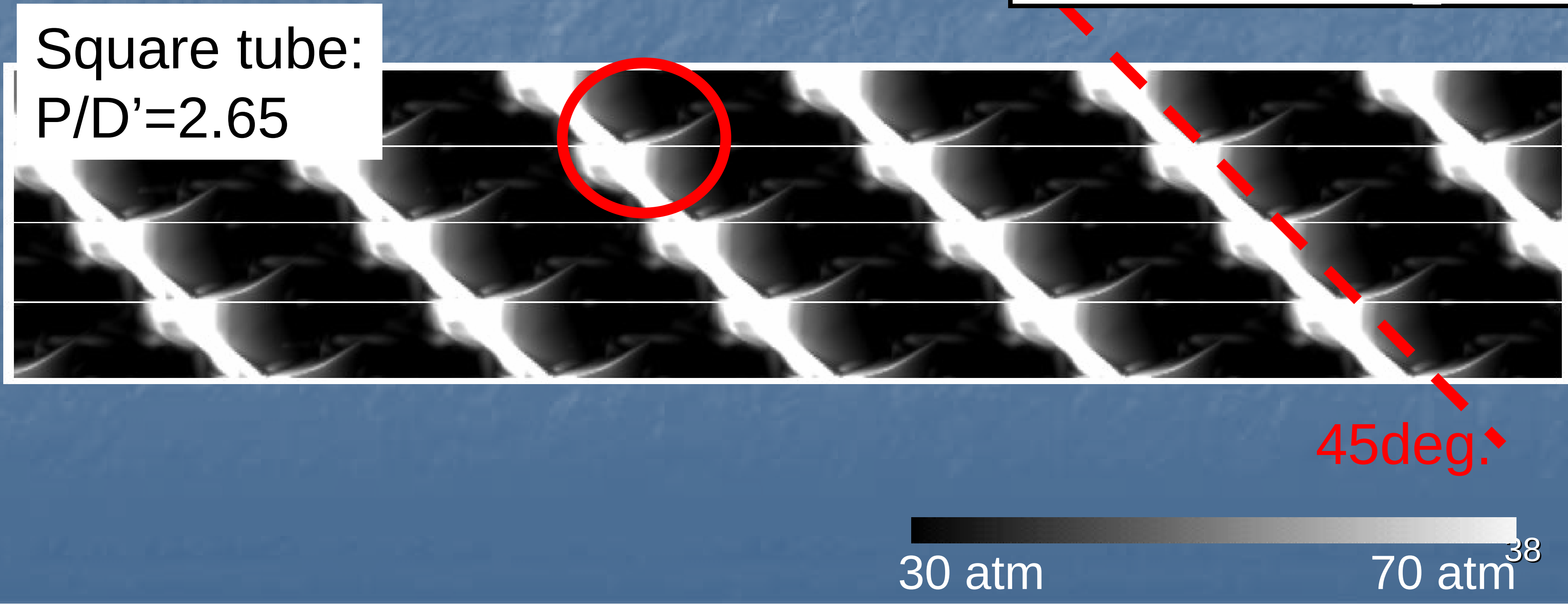
83-90

49-51

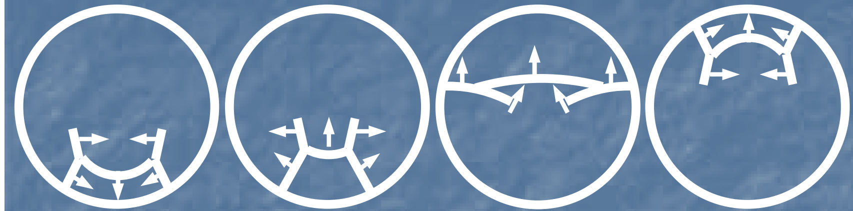
Max. Pressure History
(Spinning Mode: Circle vs. Square vs. Exp.)



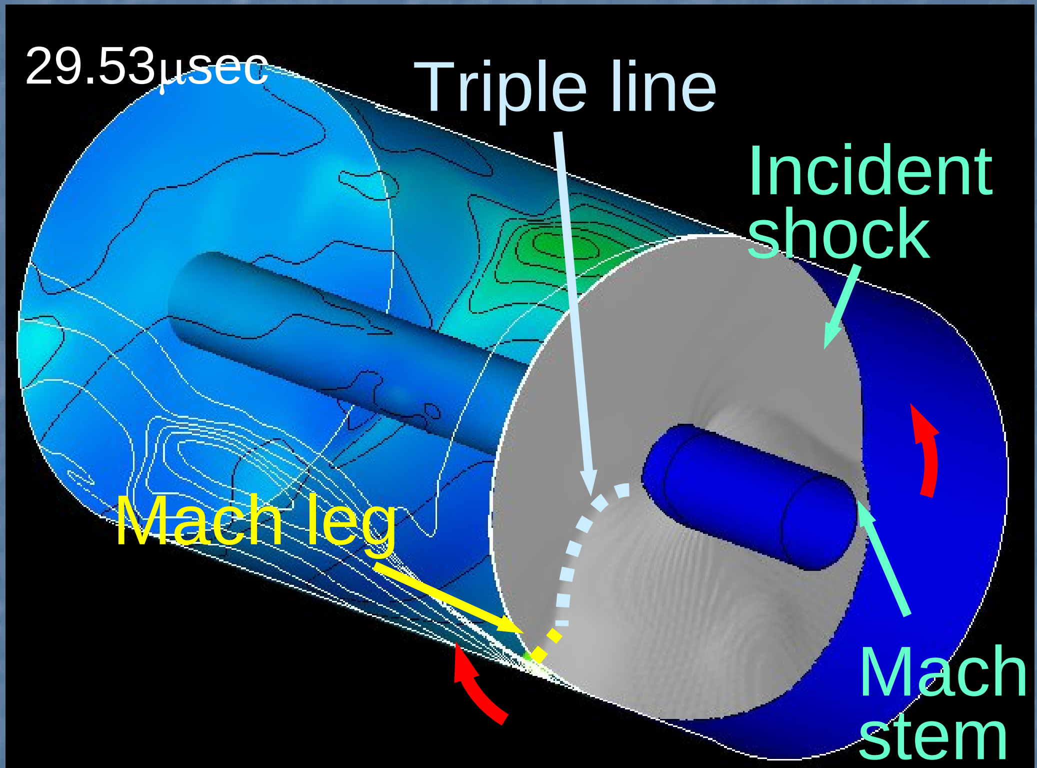
Mixture	P/D’	
C2H2 + 1.5O2 + 12.5Ar^a	2.73	2.7-3.1
2H2 + O2^a	2.93	
2H2 + O2 + 3Ar^a	3.03	
2CO + O2 + 5%H2^a	3.14	
2CO + O2 + 3%H2^b	3.23	
1.5H2 + 1.5O2 +7Ar^c	2.95	
C2H2 + 7.58O2 + 34.3 Ar^c	2.76	
H2+Air(Stoich.)^d		
2H2 + O2 + 3.76N2^e	3.09	
2CO+O2^f	2.69	2.6
C2H2 + 1.43O2 + 5.9Ar^g	2.61	
2H2 + O2 + 3.76N2^h	2.65	

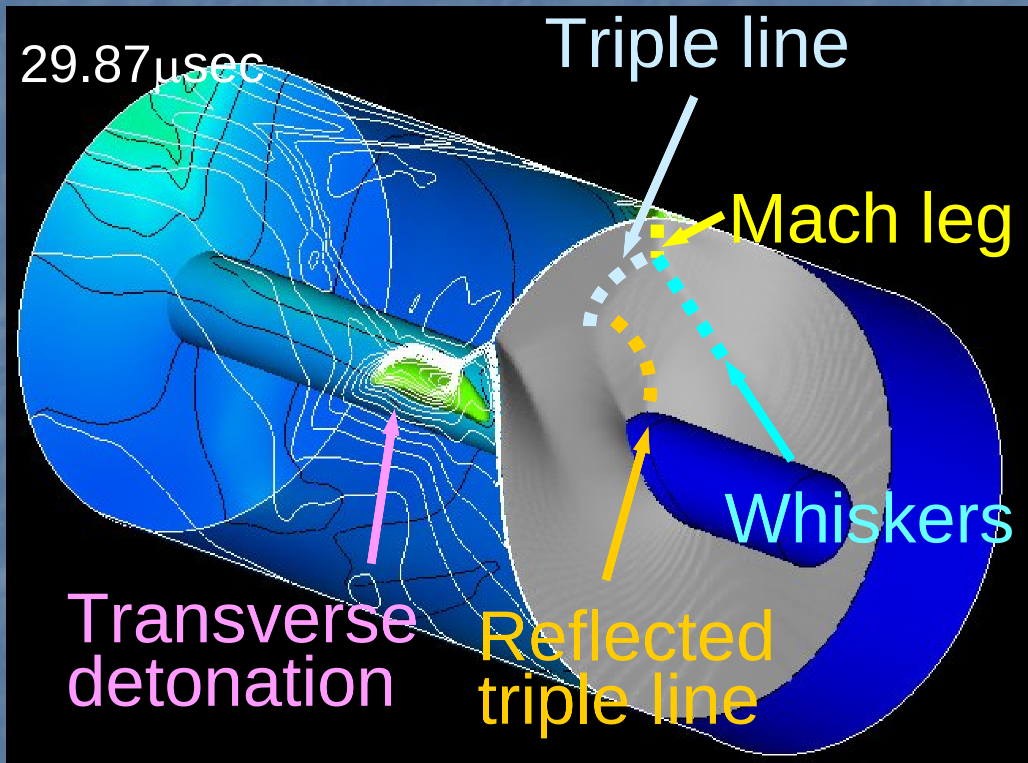


Instantaneous Pressure Contours (Two-headed Mode)



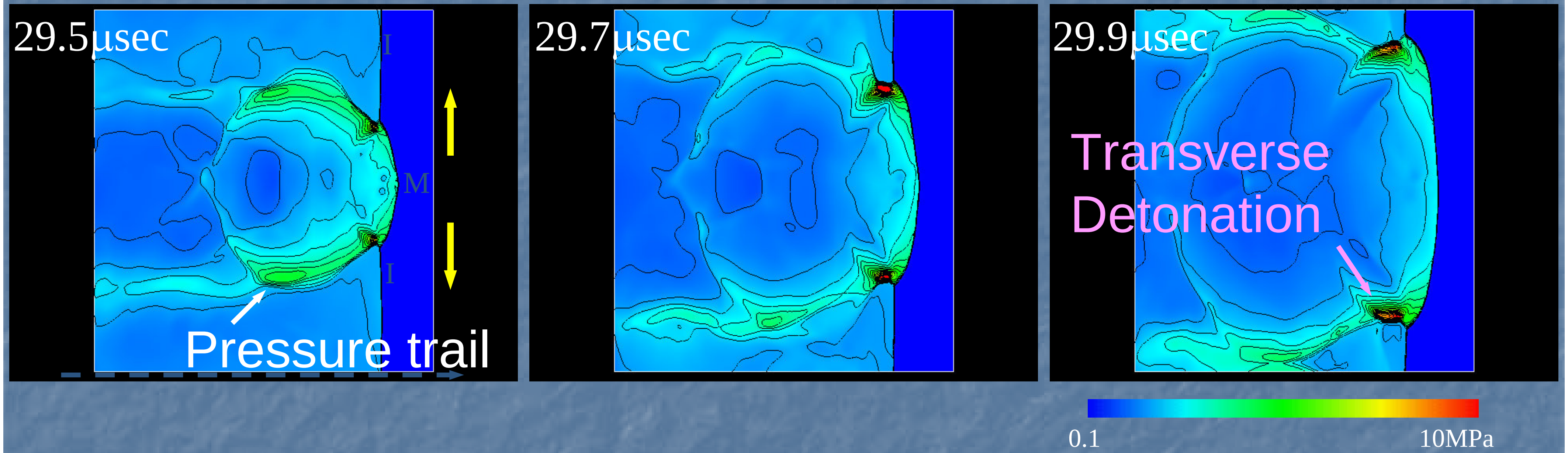
Two-heads



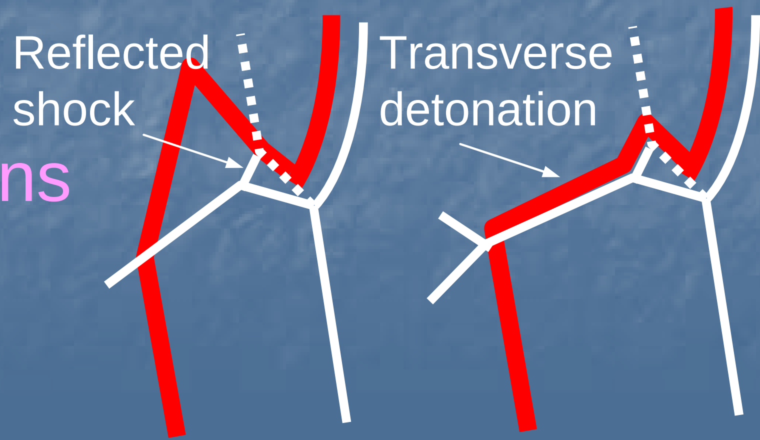


Pressure isosurface and contours

Instantaneous Pressure Contours on Wall (Two-headed Mode)



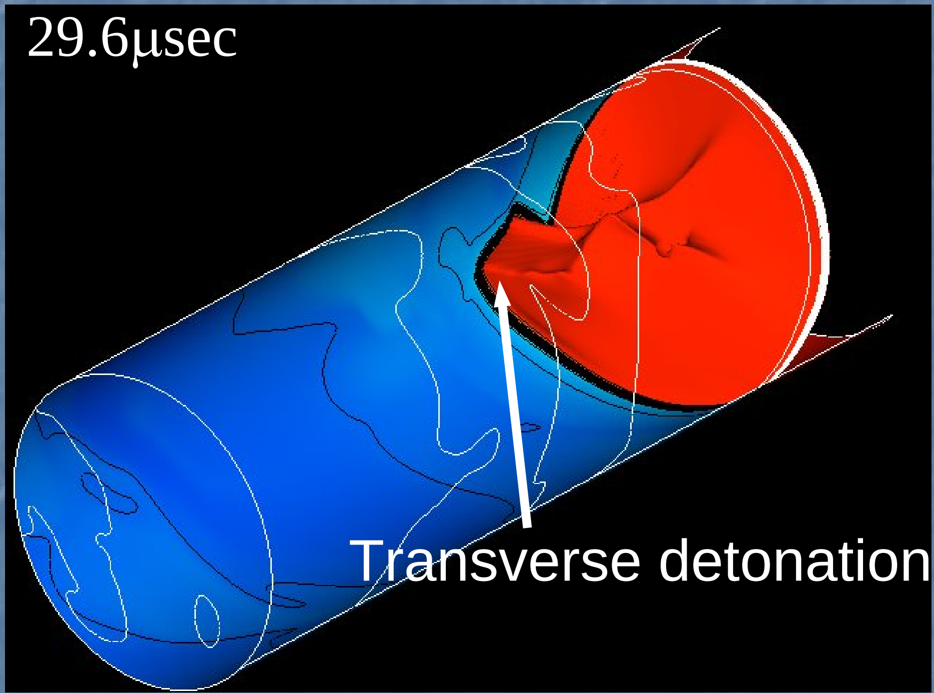
Shock wave structure:
Single, Double Mach reflections
-> Complex Mach reflection

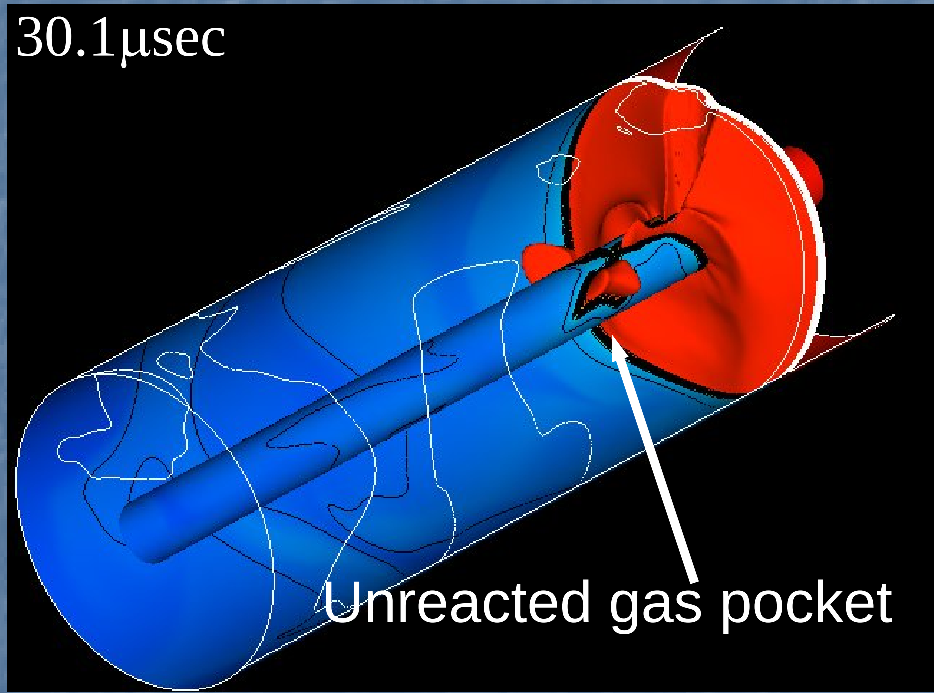


(b)Double Mach reflection (c)Complex Mach reflection

Unburned Gas Pocket (Spinning vs. Two-headed Mode)

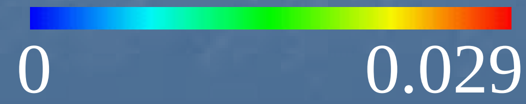
No unburned gas pocket





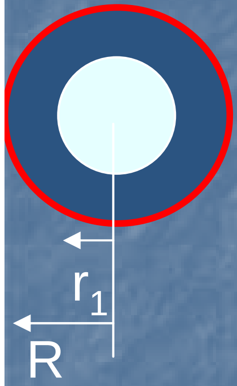
(a)$r_1/R=0$
Spinning mode

(b)$r_1/R=0.2$
Two-headed mode

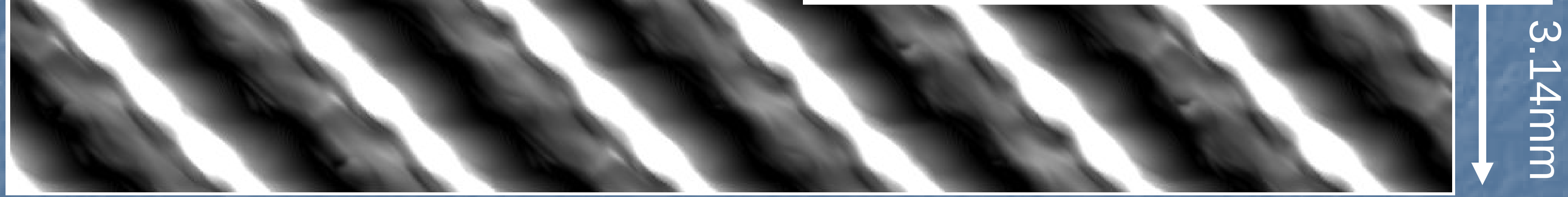


H2 Mass Fraction Contours

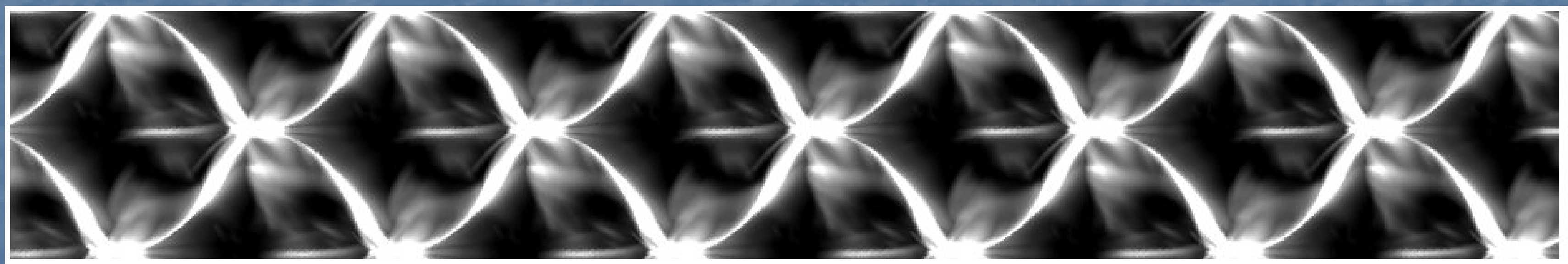
Max. Pressure History (Spinning vs. Two-headed)



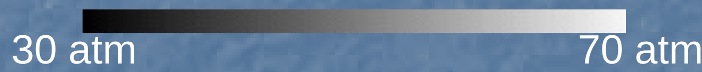
Pitch/Diameter=3.14



(a) $r_1/R=0$: Single Spinning mode (Periodically Irregular)



(b) $r_1/R=0.2$: Two-headed mode



Summary of 3D Simulations

- Numerical results about spinning detonation can be comparable with experimental data.

Spinning detonation has

- No unburned gas pockets
- Complex Mach reflection

Two headed detonation has

- Unburned gas pockets
- Single, double, and complex Mach reflections

Remaining Task and Summary

- 3D phenomena except for special cases
- High grid resolution and stiff problems for detailed reaction models
- Chemical reaction model including high pressure dependence
- Turbulent effects and DDT

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