Lecture 5

Detonation simulation

Course *Block-structured Adaptive Finite Volume Methods in C++*

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Outline

Outline

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Planar ZND Structure

Steady situation under Galilean transformation:

$$\frac{\partial}{\partial x'}(\rho u') = 0$$

$$\frac{\partial}{\partial x'}(\rho u'^2 + p) = 0$$

$$\frac{\partial}{\partial x'}(u' \rho H) = 0$$

$$\frac{\partial Y_i}{\partial x'} = \frac{W_i \dot{\omega}_i \left(\rho \frac{Y_1}{W_1}, \ldots, \rho \frac{Y_K}{W_K}, T\right)}{\rho u'}$$

CJ-detonation of $\mathrm{H_2} : \mathrm{O_2} : \mathrm{Ar}$ with molar ratios $2 : 1 : 7$ at $T_0 = 298\,\mathrm{K}$ and $p_0 = 6.67\,\mathrm{kPa}$, $d_{CJ} \approx 1627\,\mathrm{m/s}$.

$t_{ig} \approx 3.55\,\mu\mathrm{s}$, $u'_{vN} \approx 395.5\,\mathrm{m/s}$, $l_{ig} \approx 0.14\,\mathrm{cm}$.

Cf. `code/amroc/doc/html/apps/clawpack_2applications_2euler__chem_21d_2ModelDetonation_2src_2Problem_8h_source.html`

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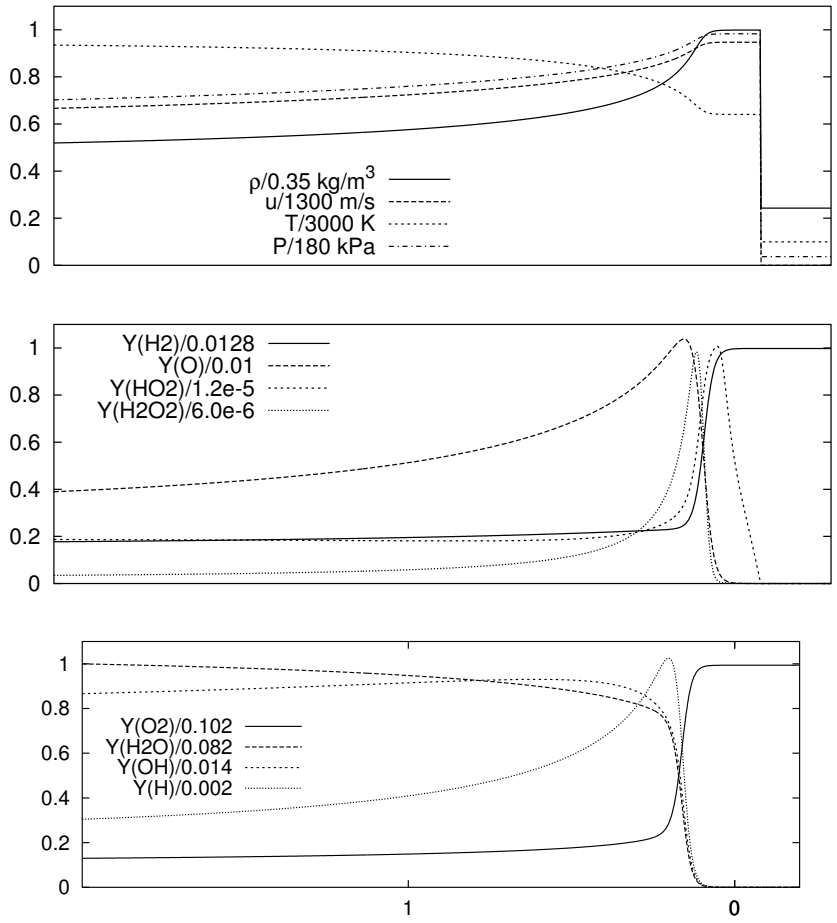

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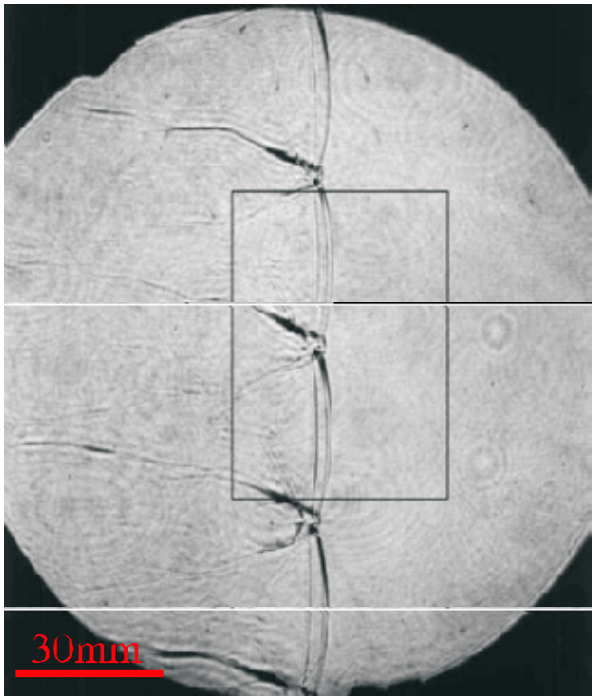
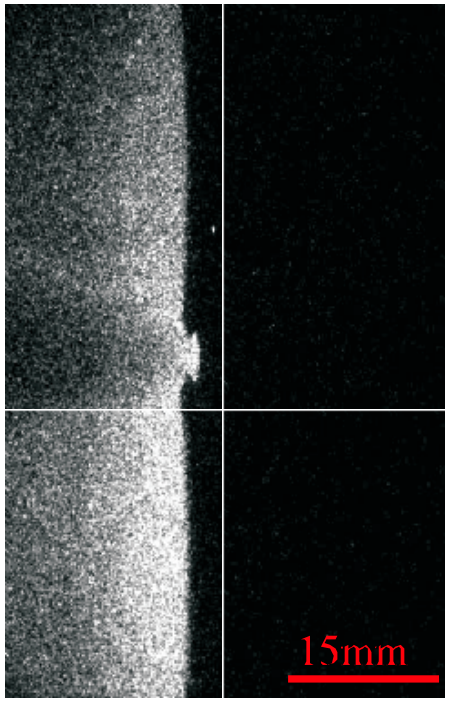
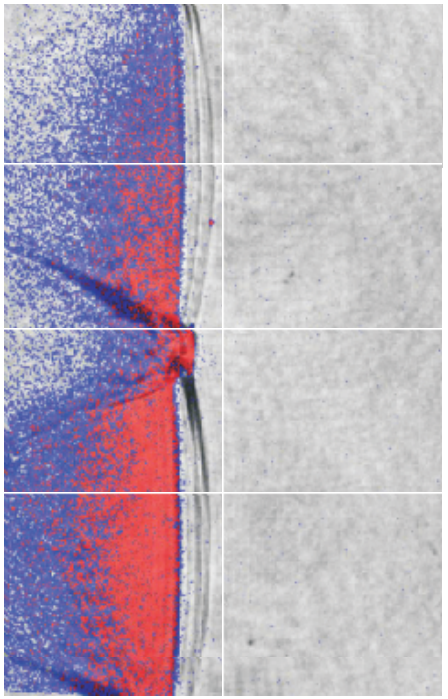
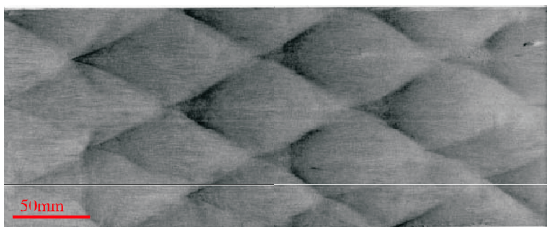
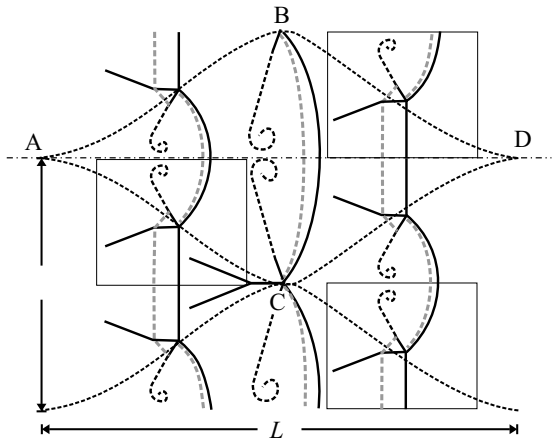
Detonation cell structure in 2D - Regular instability

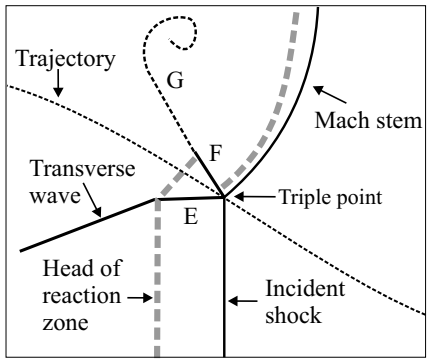






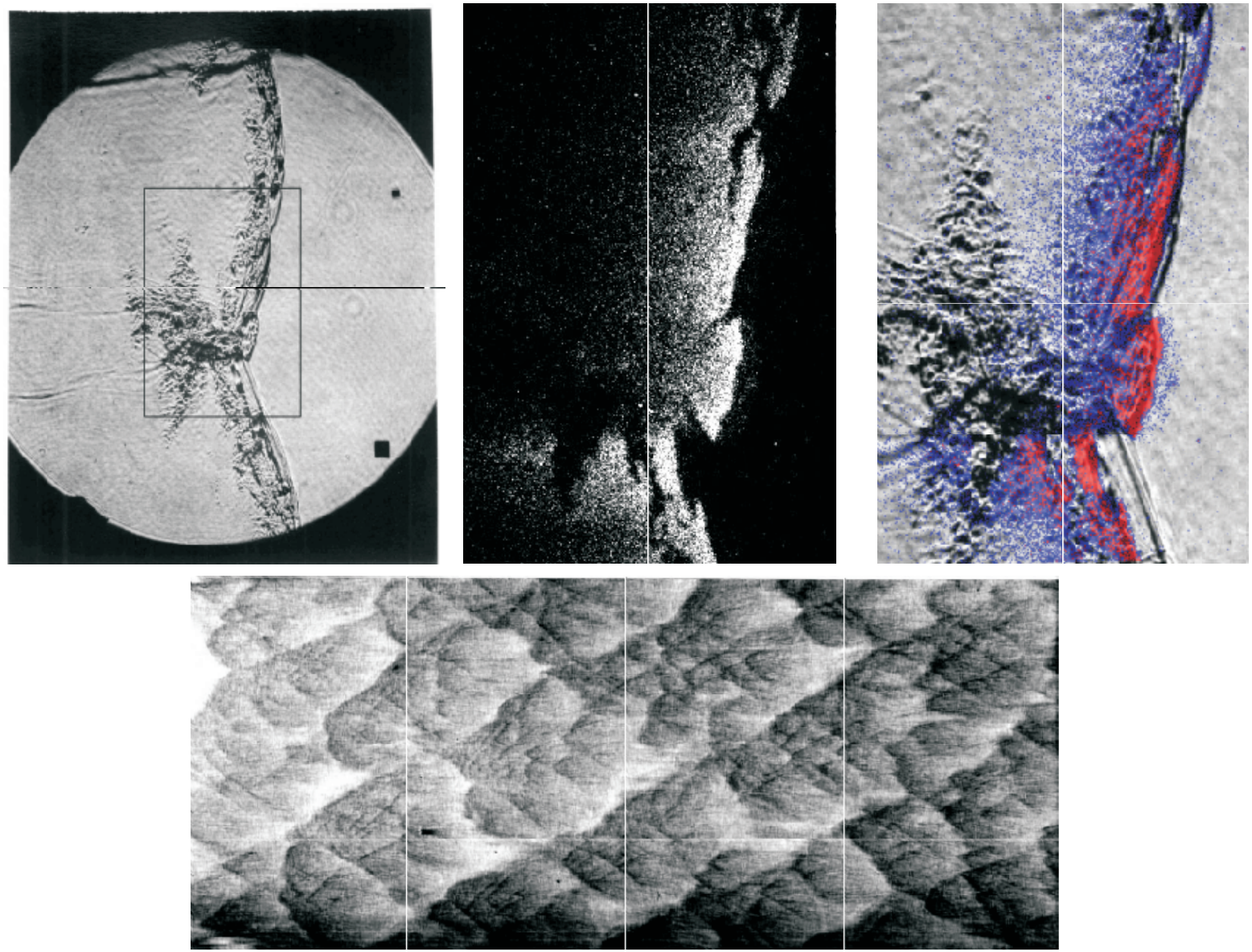






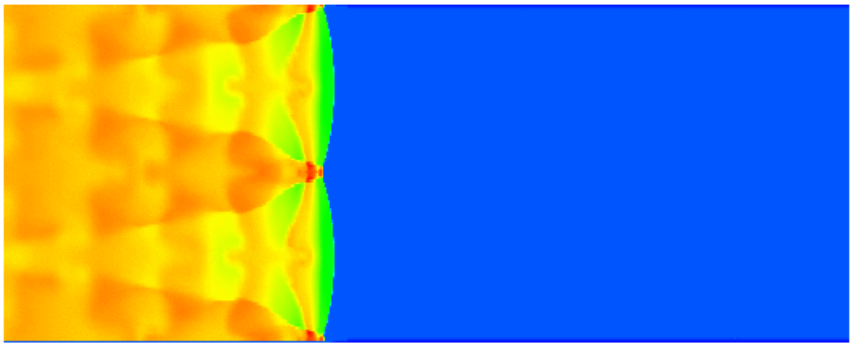
E: Reflected shock. F: Slip line. G: Diffusive extension of slip line.

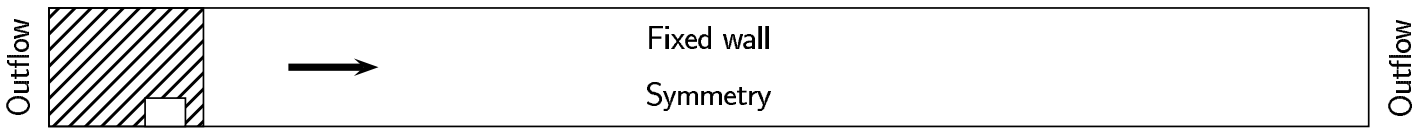
Transverse detonation structure - irregular instability



Simulation of regular structures

- CJ detonation for $H_2 : O_2 : Ar$ (2:1:7) at $T_0 = 298\,\mathrm{K}$ and $p_0 = 10\,\mathrm{kPa}$, cell width $1.6\,\mathrm{cm}$
- Perturb 1d ZND solution with unreacted high-pressure pocket behind front
- Triple point trajectories by tracking max $|\omega|$ on auxiliary mesh shifted through grid with CJ velocity. $\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$
- SAMR simulation with 4 additional levels (2,2,2,4), $67.6\,\mathrm{Pts}/l_{ig}$
- Configuration similar to Oran et al., J. Combustion and Flame 113, 1998.





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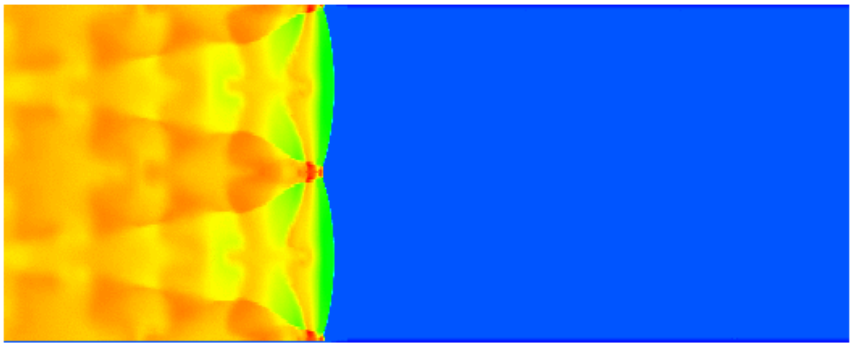

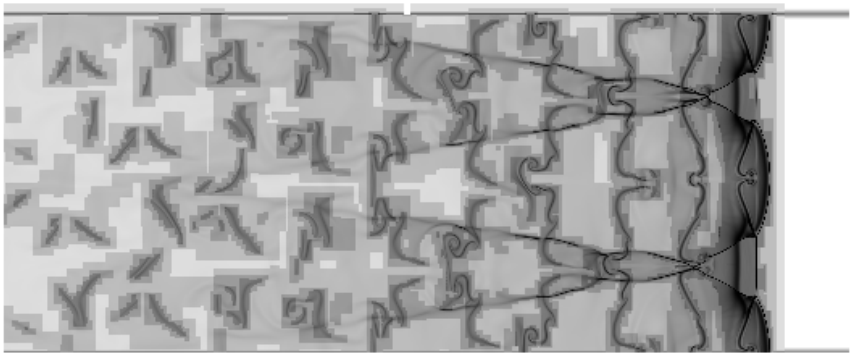

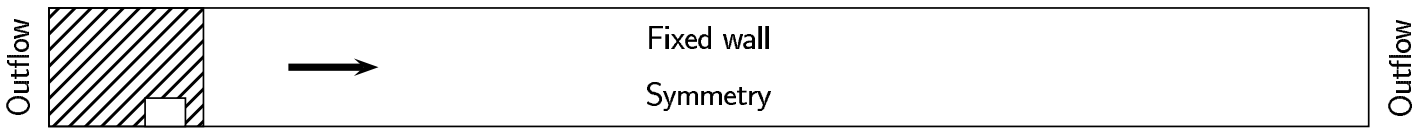

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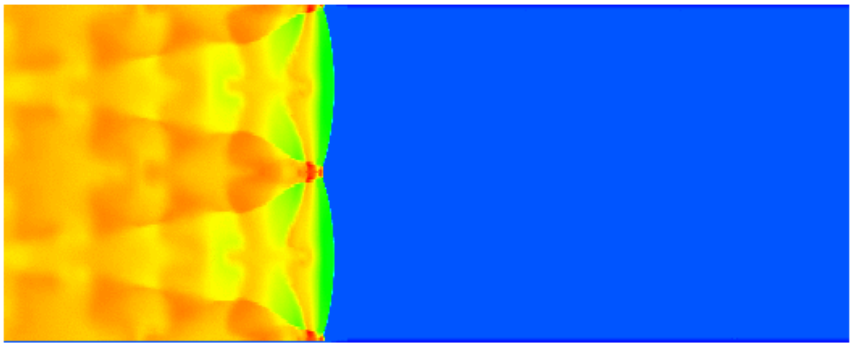

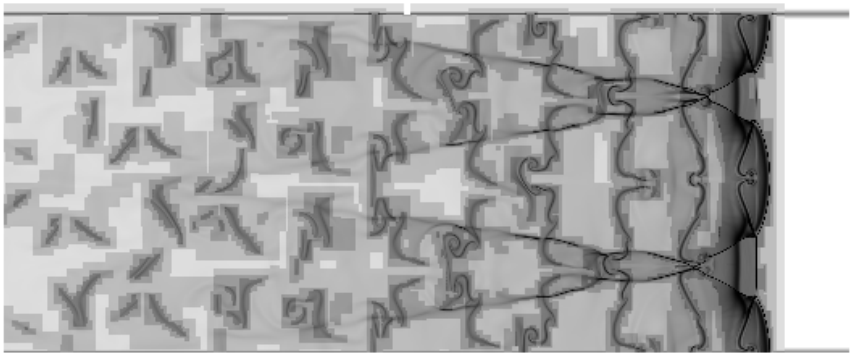

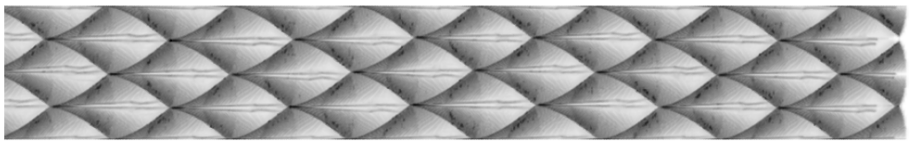

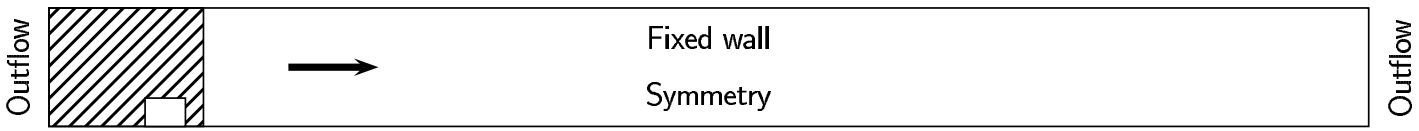

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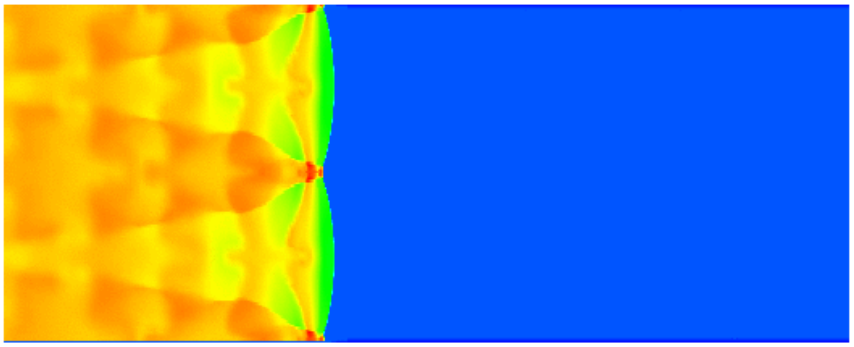
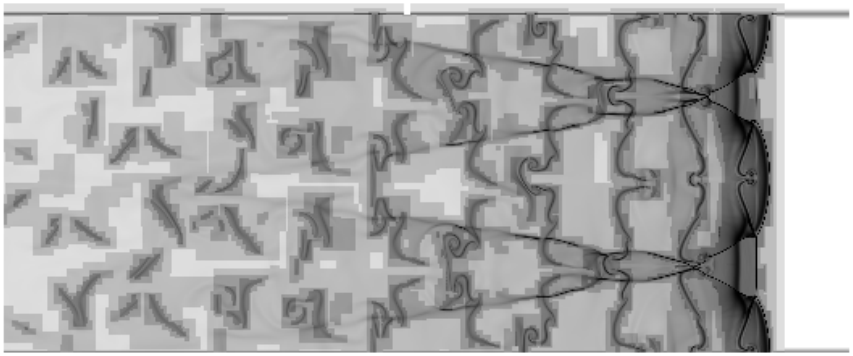
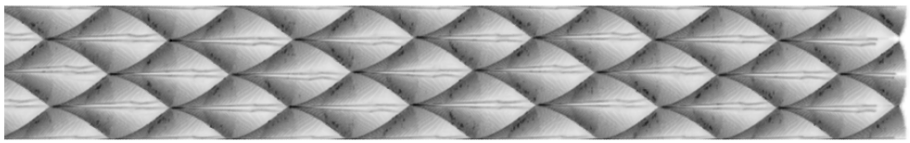
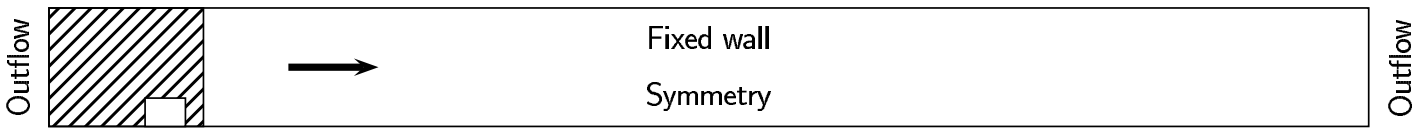




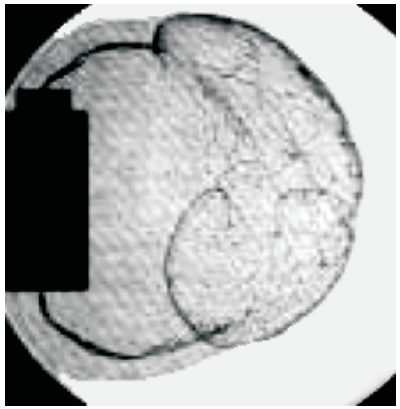




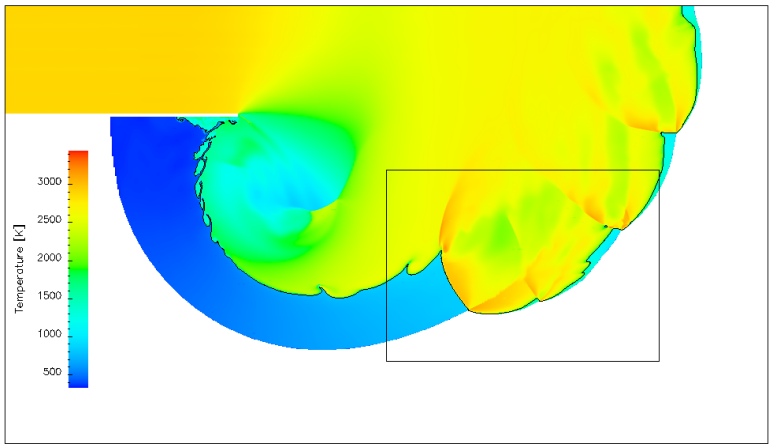
code/amroc/doc/html/apps/clawpack_2applications_2euler__chem_22d_2StrehlowH2O2_2StatDet_2src_2Problem_8h_source.

Detonation diffraction

- CJ detonation for $H_2 : O_2 : Ar/2 : 1 : 7$ at $T_0 = 298\,\mathrm{K}$ and $p_0 = 10\,\mathrm{kPa}$. Cell width $\lambda_c = 1.6\,\mathrm{cm}$
- Adaption criteria (similar as before):
  1. Scaled gradients of ρ and p
  2. Error estimation in Y_i by Richardson extrapolation
- $25\,\mathrm{Pts}/l_{ig}$. 5 refinement levels (2,2,2,4).
- Adaptive computations use up to $\sim 2.2\,\mathrm{M}$ instead of $\sim 150\,\mathrm{M}$ cells (uniform grid)
- $\sim 3850\,\mathrm{h}$ CPU ($\sim 80\,\mathrm{h}$ real time) on 48 nodes Athlon 1.4GHz

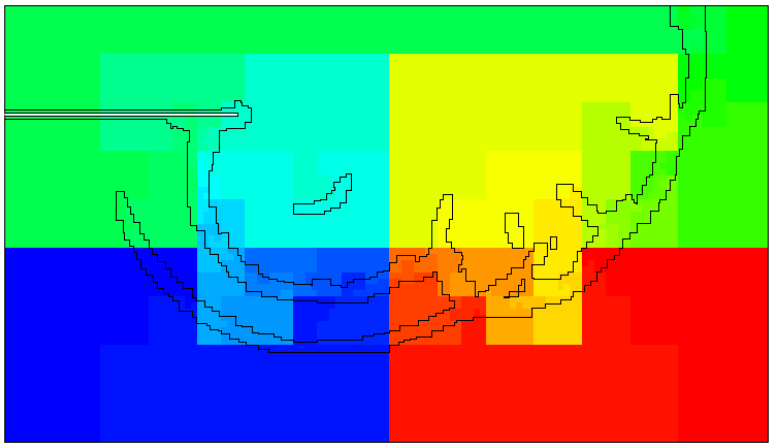


E. Schultz. *Detonation diffraction through an abrupt area expansion*. PhD thesis, California Institute of Technology, Pasadena, California, April 2000.



Detonation diffraction - adaptation

Final distribution to 48 nodes and density distribution on four refinement levels



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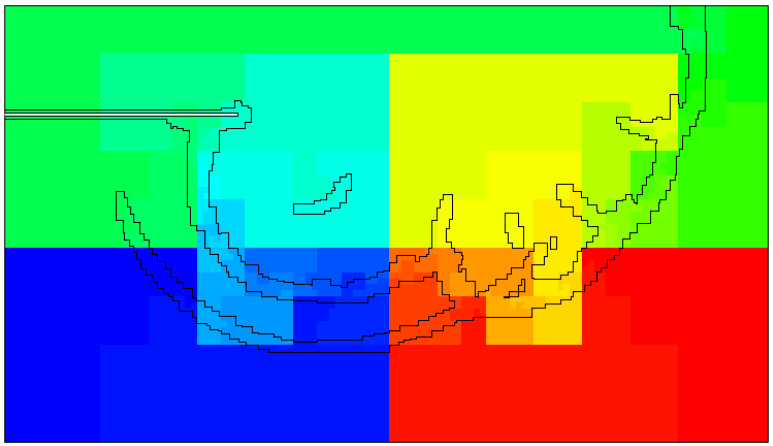

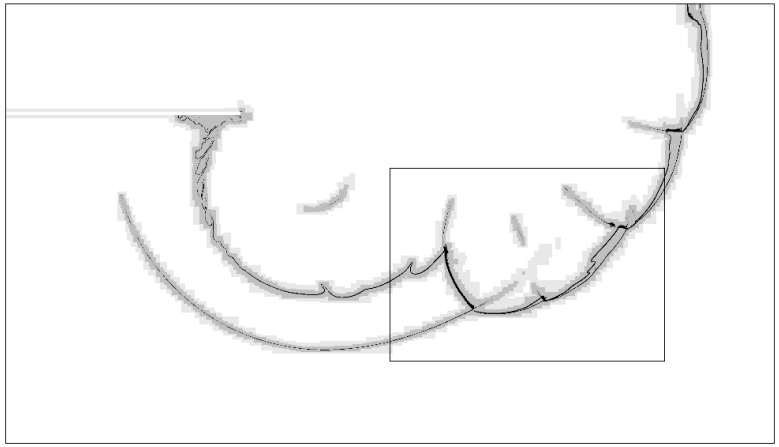

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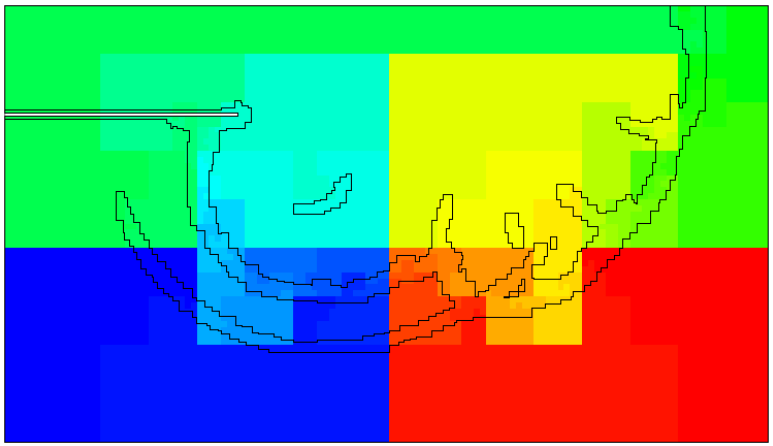

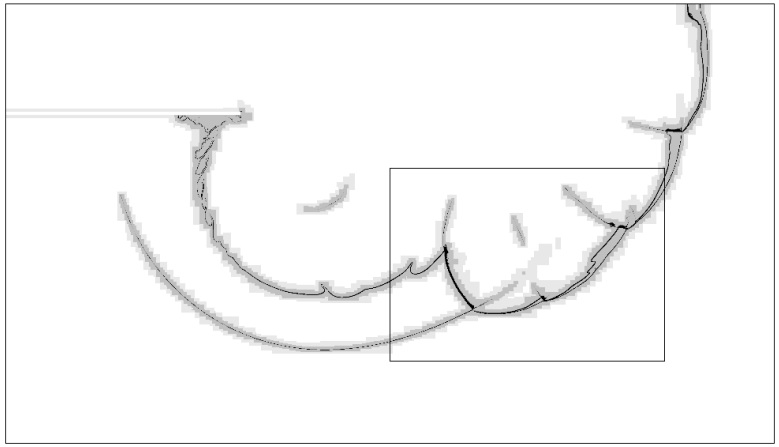

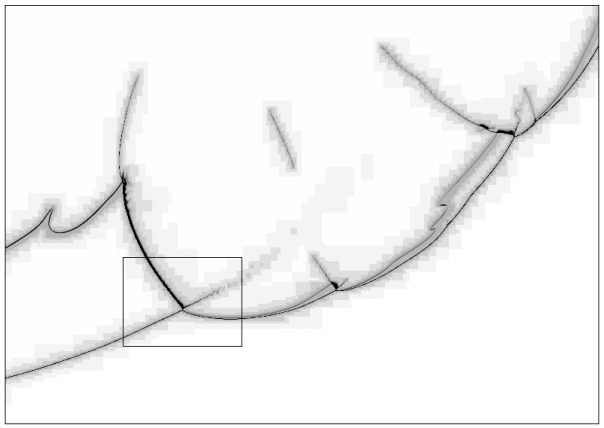

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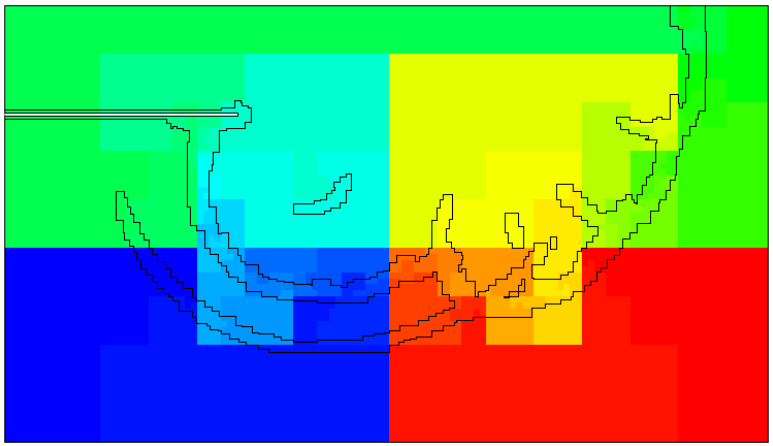

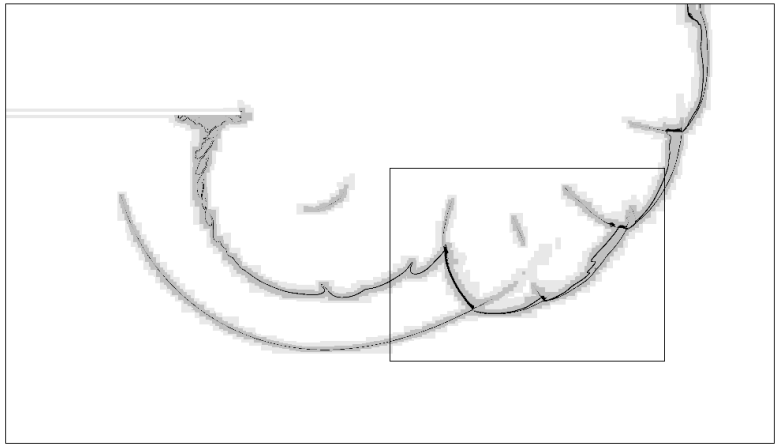

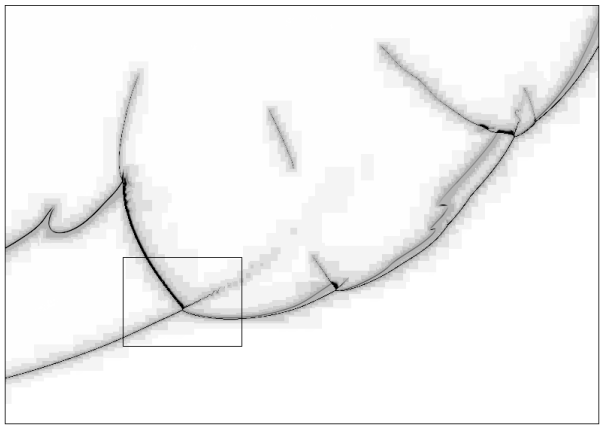

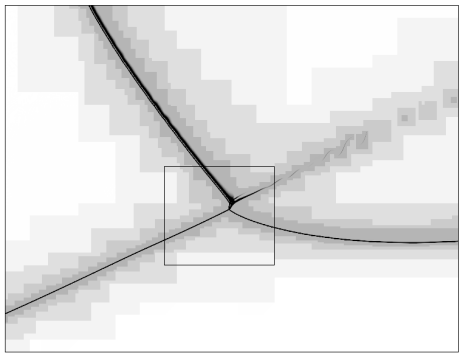

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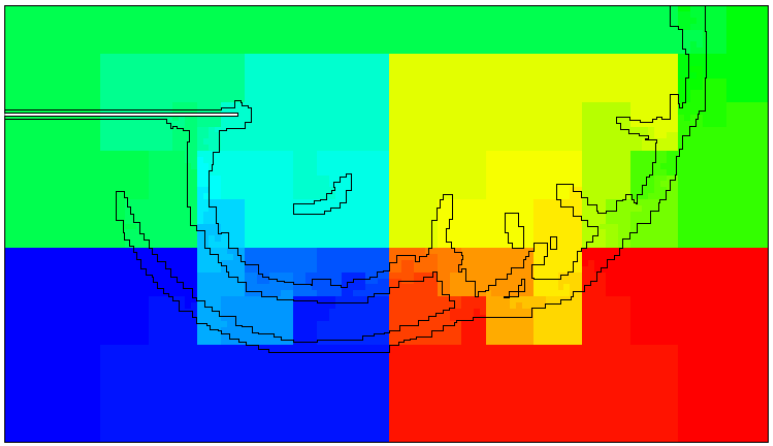

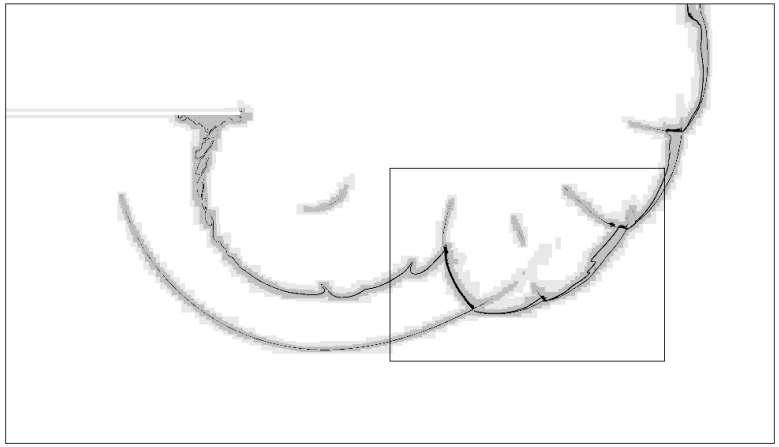

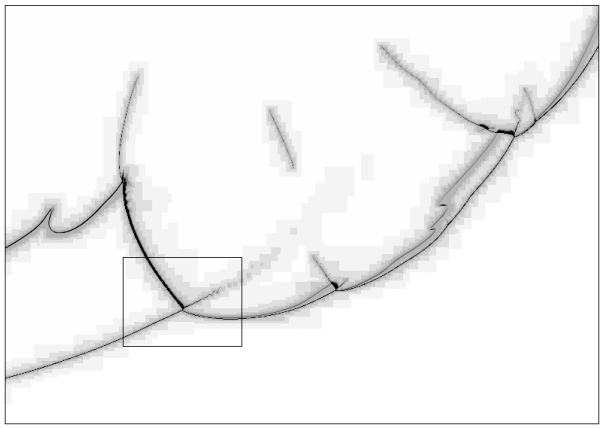

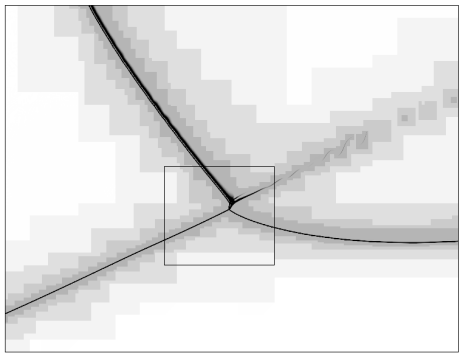

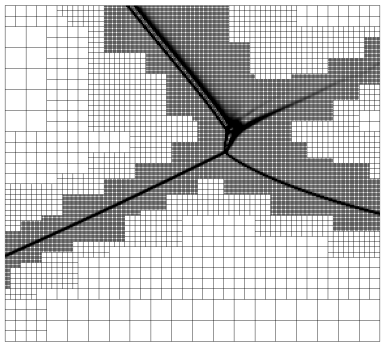

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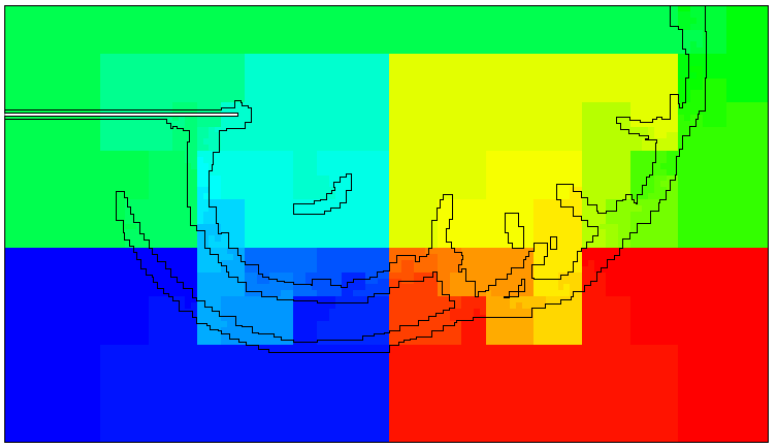

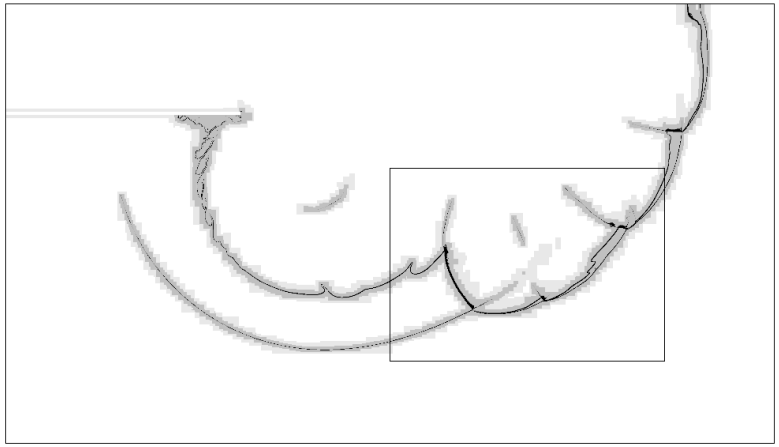

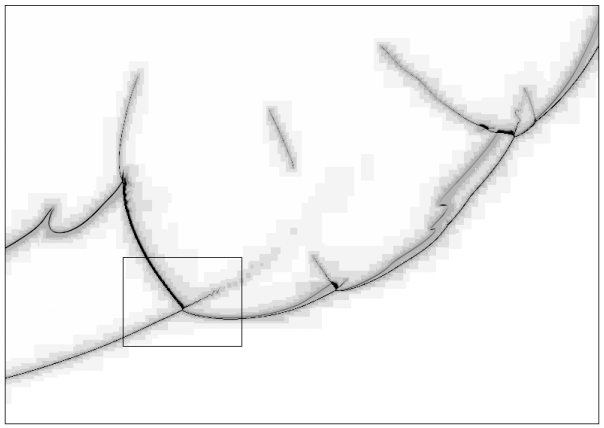

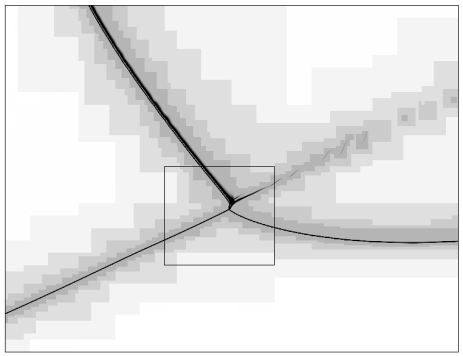

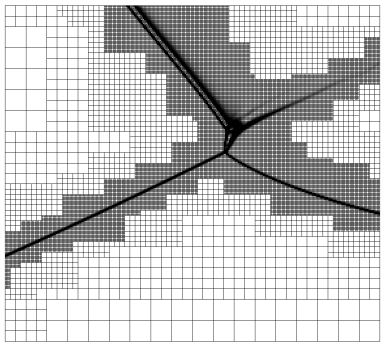

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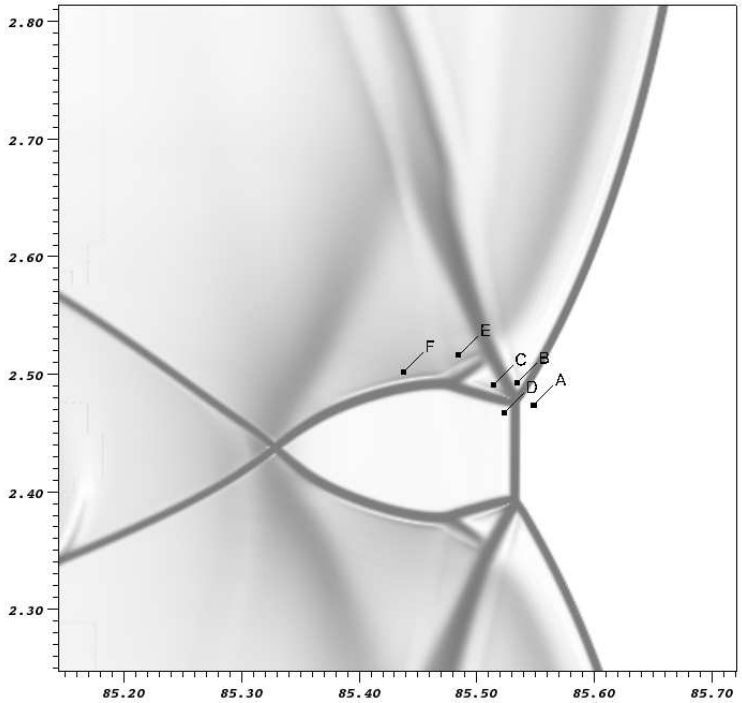
Triple point analysis

Double Mach reflection structure shortly before the next collision



	p/p_0	ρ/ρ_0	T [K]	u[m/s]	M
A	1.00	1.00	298	1775	5.078
B	31.45	4.17	2248	447	0.477
C	31.69	5.32	1775	965	1.153
D	19.17	3.84	1487	1178	1.533
E	35.61	5.72	1856	901	1.053
F	40.61	6.09	1987	777	0.880

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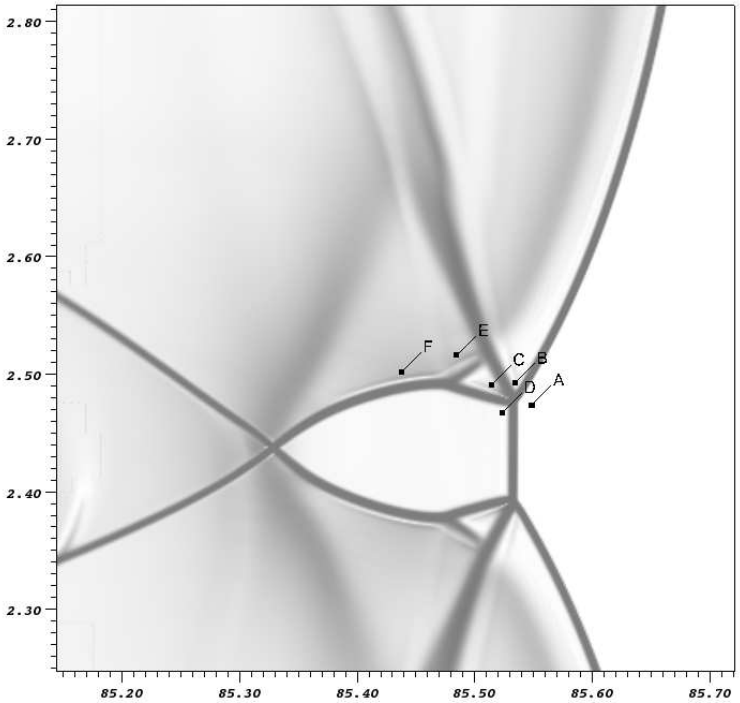
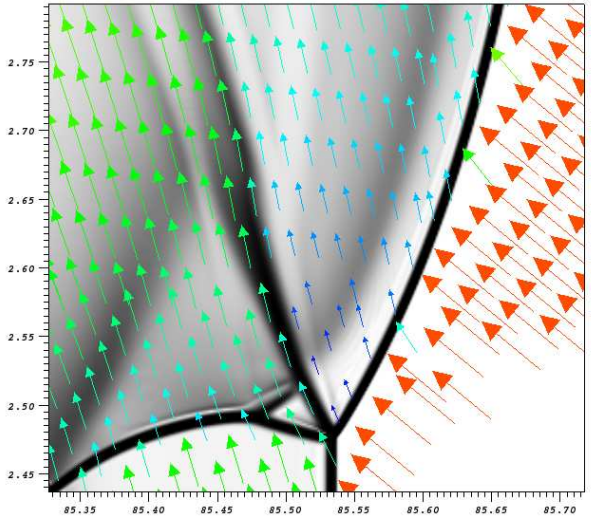
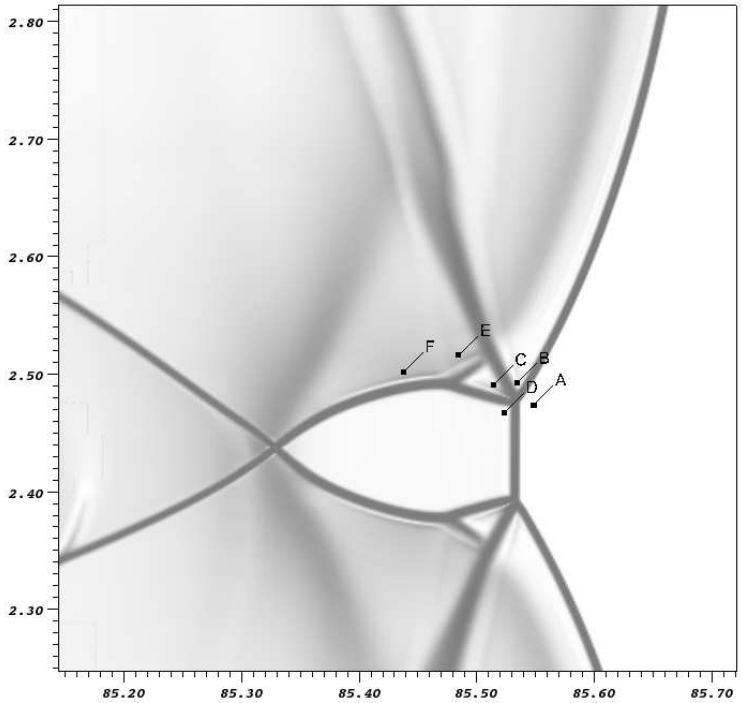


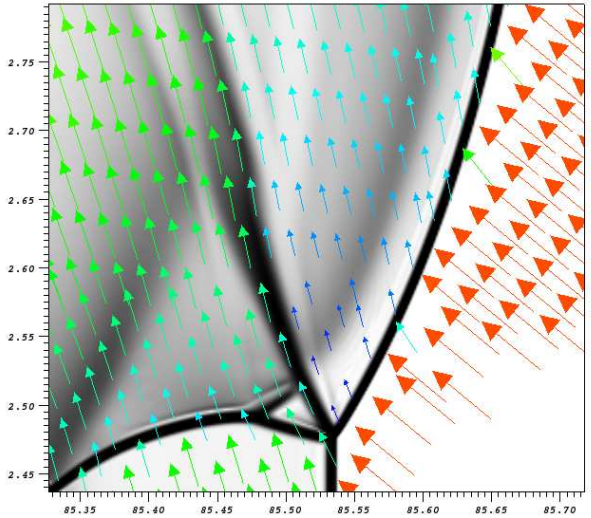


	p/p_0	ρ/ρ_0	T [K]	u[m/s]	M
A	1.00	1.00	298	1775	5.078
B	31.45	4.17	2248	447	0.477
C	31.69	5.32	1775	965	1.153
D	19.17	3.84	1487	1178	1.533
E	35.61	5.72	1856	901	1.053
F	40.61	6.09	1987	777	0.880

Triple point analysis

Double Mach reflection structure shortly before the next collision





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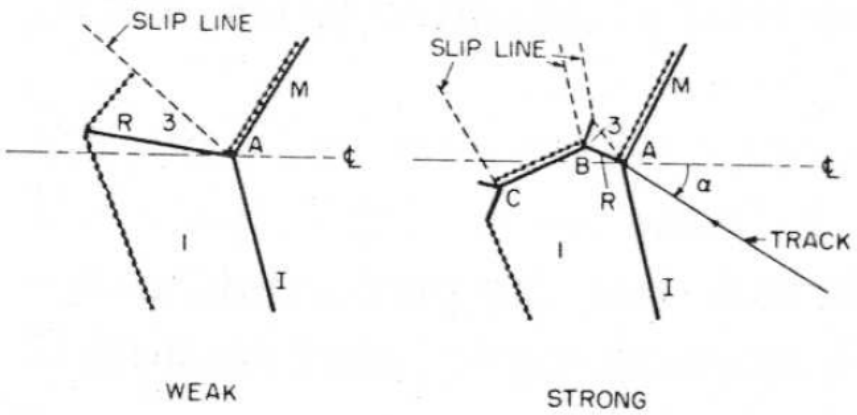
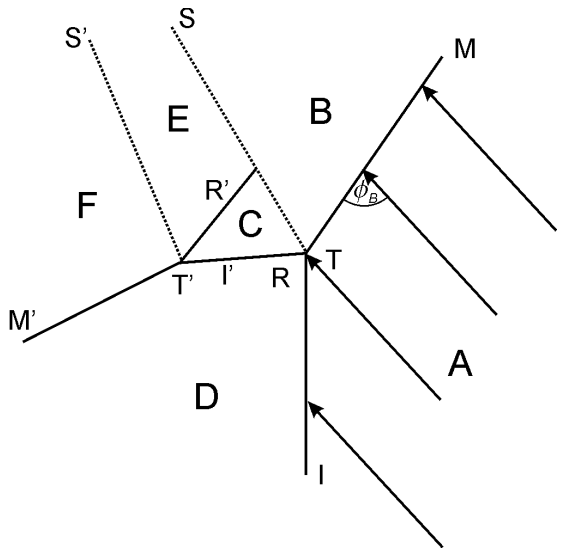
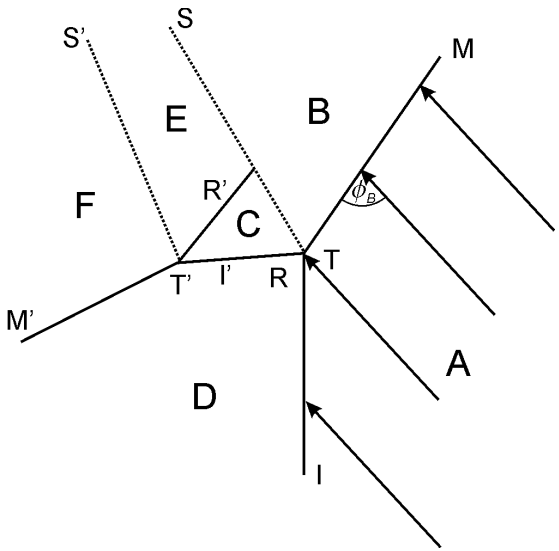


Shock polar analysis of triple points in detonations



Shock polar analysis of triple points in detonations

- Neglect reaction, but consider $c_{pi}(T)$
- Data extracted point-wise from simulation

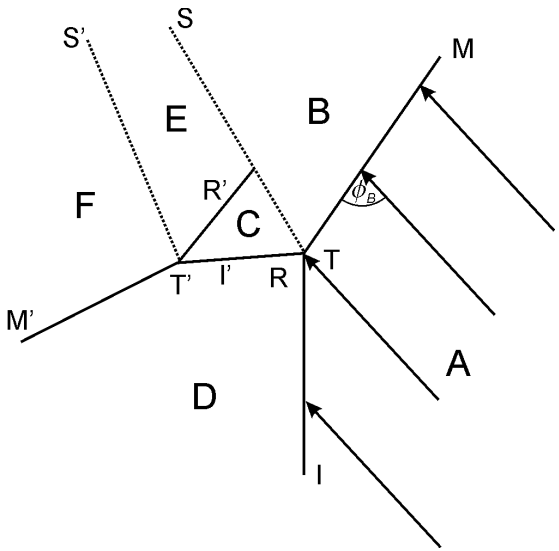


Shock polar analysis of triple points in detonations

- Neglect reaction, but consider $c_{pi}(T)$
- Data extracted point-wise from simulation
- Primary triple point T travels exactly at tip of Mach stem $\rightarrow$ use oblique shock relations between A and B

$$\begin{aligned} \rho_A u_A \sin(\phi_B) &= \rho_B u_B \sin(\phi_B - \theta_B)\,, \\ p_A + \rho_A u_A^2 \sin^2(\phi_B) &= p_B + \rho_B u_B^2 \sin^2(\phi_B - \theta_B) \end{aligned}$$

to evaluate inflow velocity as $u_A = \dfrac{1}{\sin\phi_B}\sqrt{\dfrac{\rho_B(p_B - p_A)}{\rho_A(\rho_B - \rho_A)}}$



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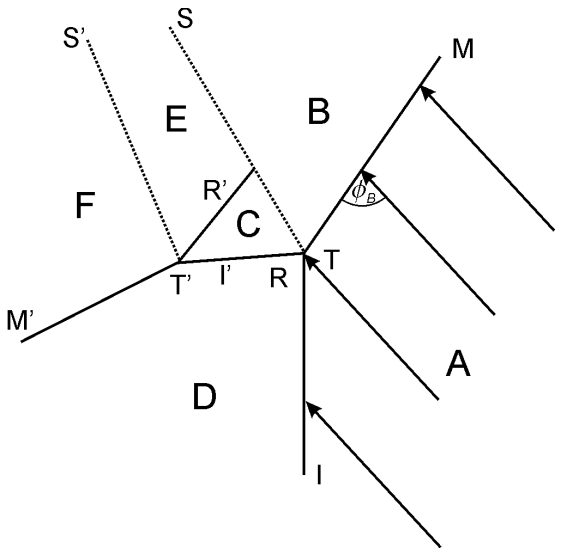

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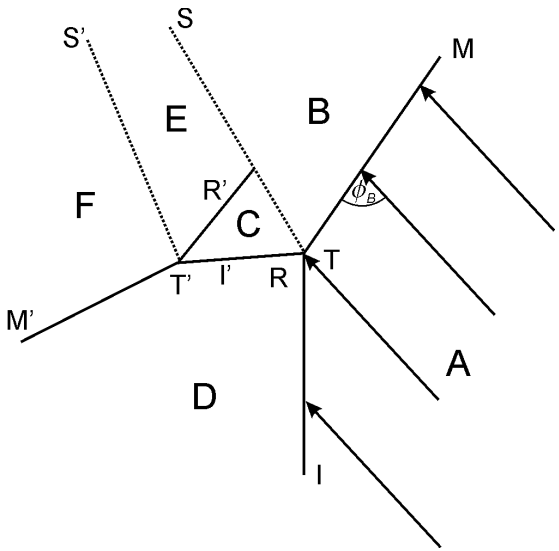

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- Velocity $\mathbf{a}$ of T' relative to T cannot be derived that easily: Oblique shock relations across C and D hold true both in frame of reference for T and T'

$$\begin{aligned} \rho_C u_{C,n} &= \rho_D u_{D,n} \\ p_C + \rho_C u_{C,n}^2 &= p_D + \rho_D u_{D,n}^2 \\ u_{C,t} &= u_{D,t} \\ h_C + \frac{1}{2} u_{C,n}^2 &= h_D + \frac{1}{2} u_{D,n}^2 \end{aligned}$$

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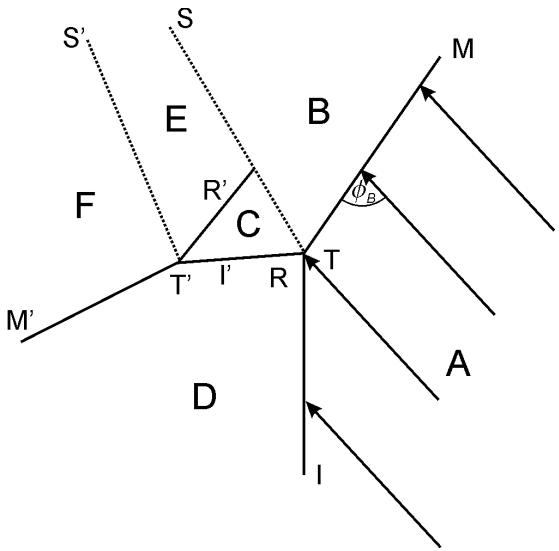

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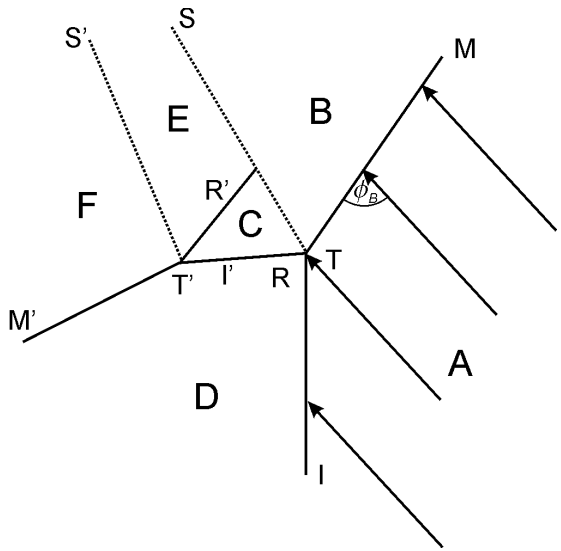

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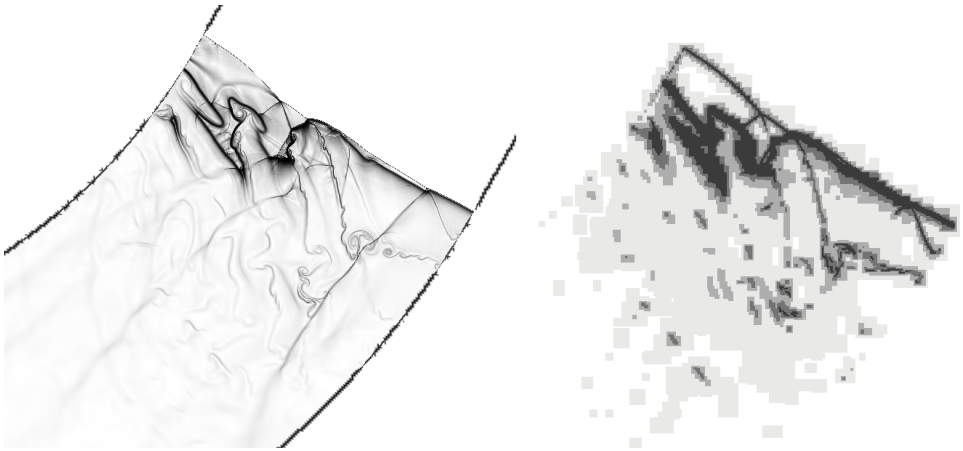
$\rightarrow a_n = 0$, a_t arbitrary

Estimate $a_t = \dfrac{L_R}{t_{\text{init}}}$

Detonation propagation through pipe bends

- 2D Simulation of CJ detonation for $\mathrm{H_2} : \mathrm{O_2} : \mathrm{Ar}/2 : 1 : 7$ at $T_0 = 298\,\mathrm{K}$ and $p_0 = 10\,\mathrm{kPa}$. Tube width of 5 detonation cells
- AMR base grid 1200×992. 4 additional refinement levels (2,2,2,4). $67.6\,\mathrm{Pts}/l_{ig}$
- Adaptive computations use up to $7.1 \cdot 10^6$ cells ($4.8 \cdot 10^6$ on highest level) instead of $1.22 \cdot 10^9$ cells (uniform grid)
- $\sim 70,000\,\mathrm{h}$ CPU on 128 CPUs Pentium-4 2.2GHz



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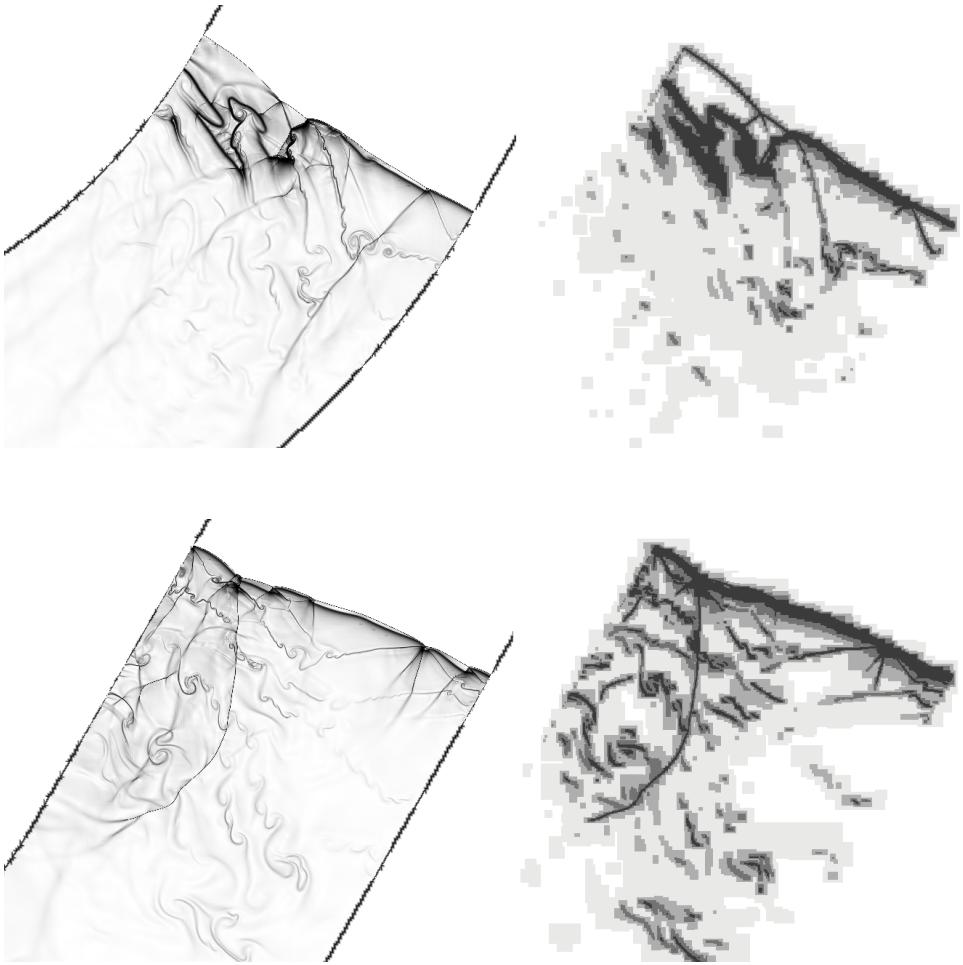

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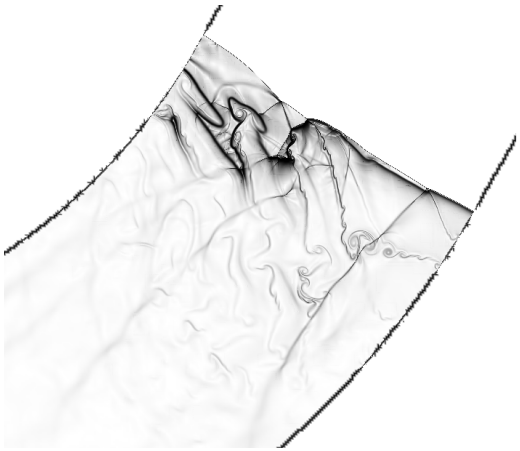
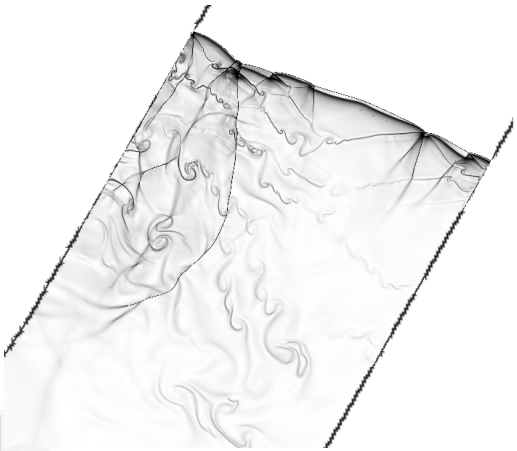
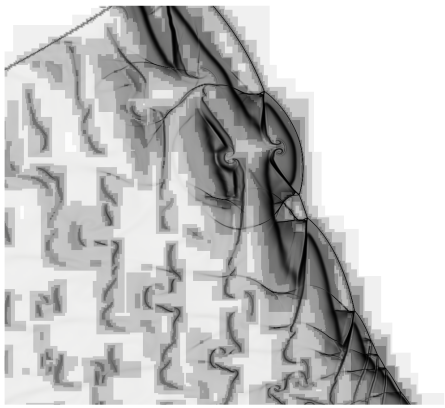
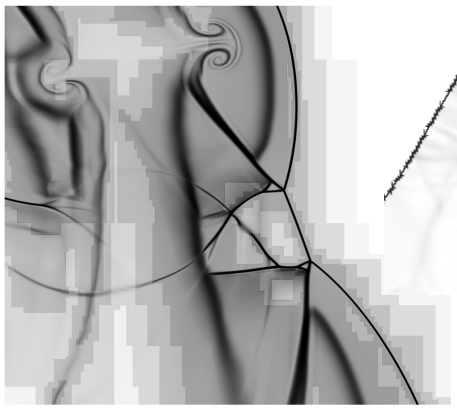
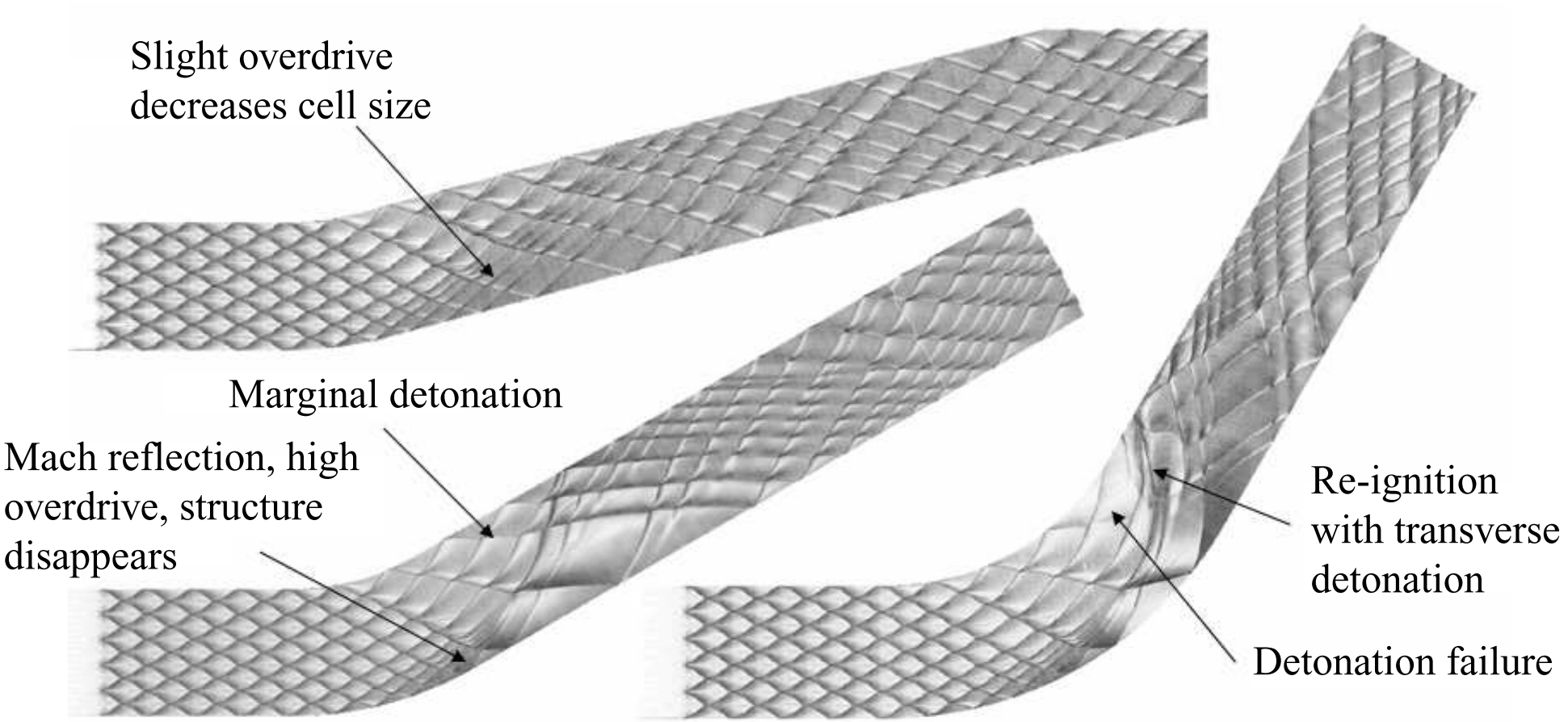




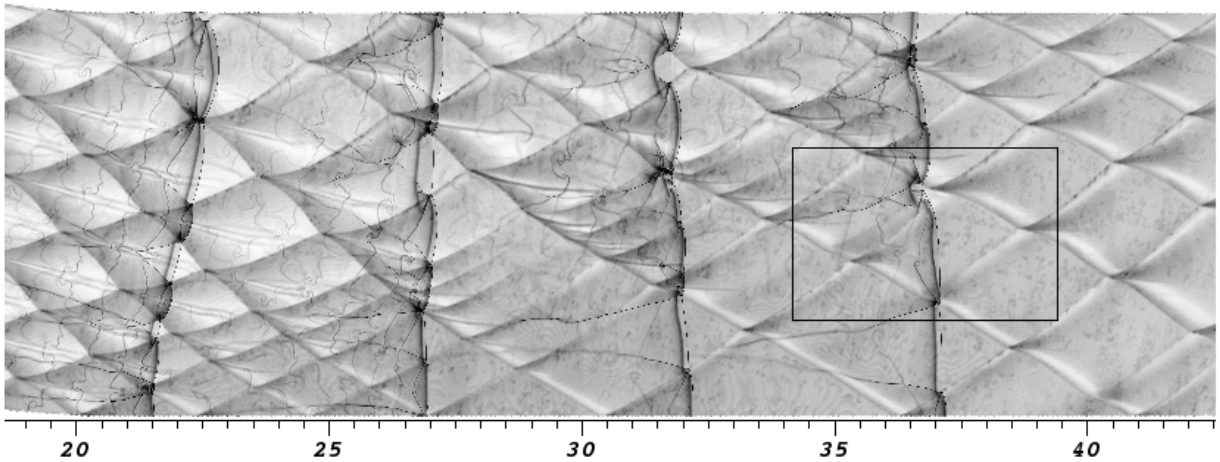
Triple point tracks



$\varphi = 15^{\circ}$ (left, top), $\varphi = 30^{\circ}$ (left, bottom), and $\varphi = 60^{\circ}$ (right)

`code/amroc/doc/html/apps/clawpack_2applications_2euler__chem_22d_2PipeBend_2src_2Problem_8h_source.html`

Triple point structures – $\varphi = 15^{\mathrm{o}}$



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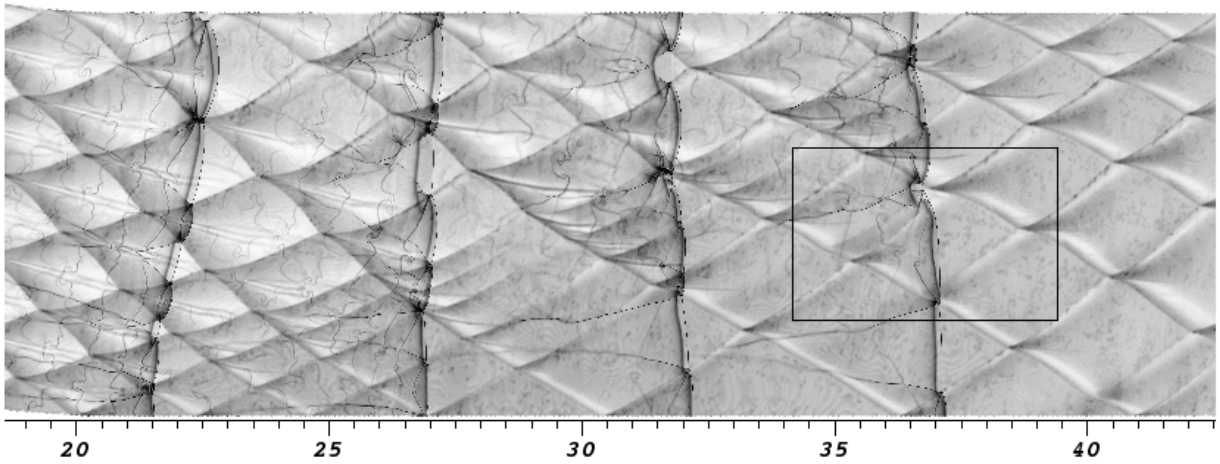
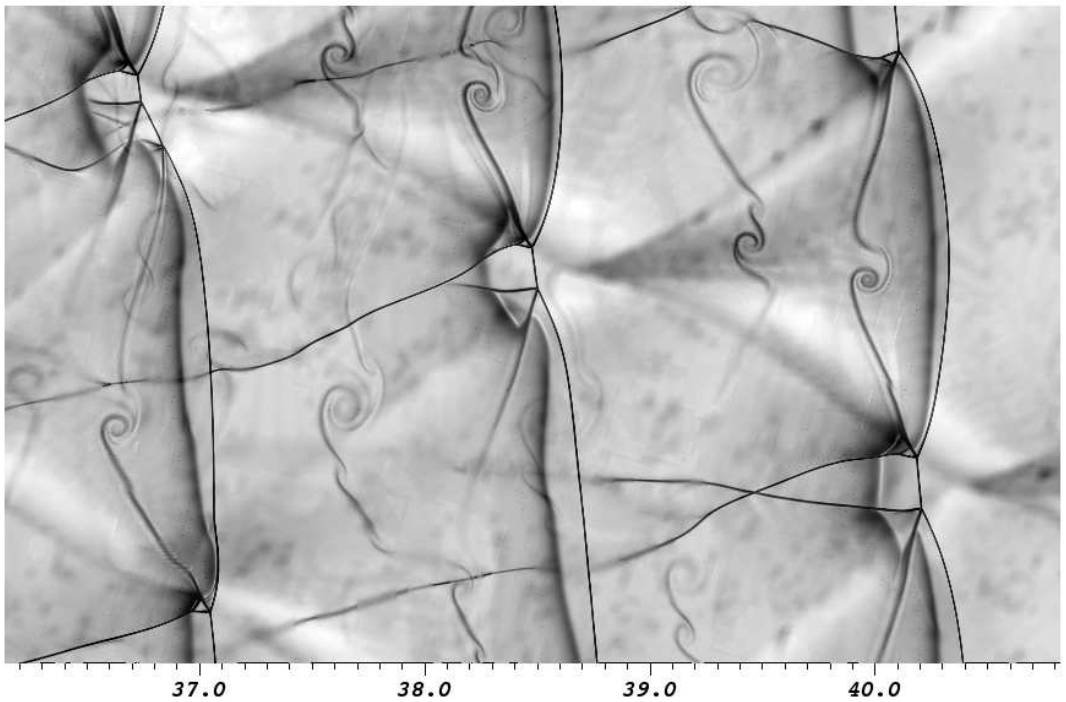
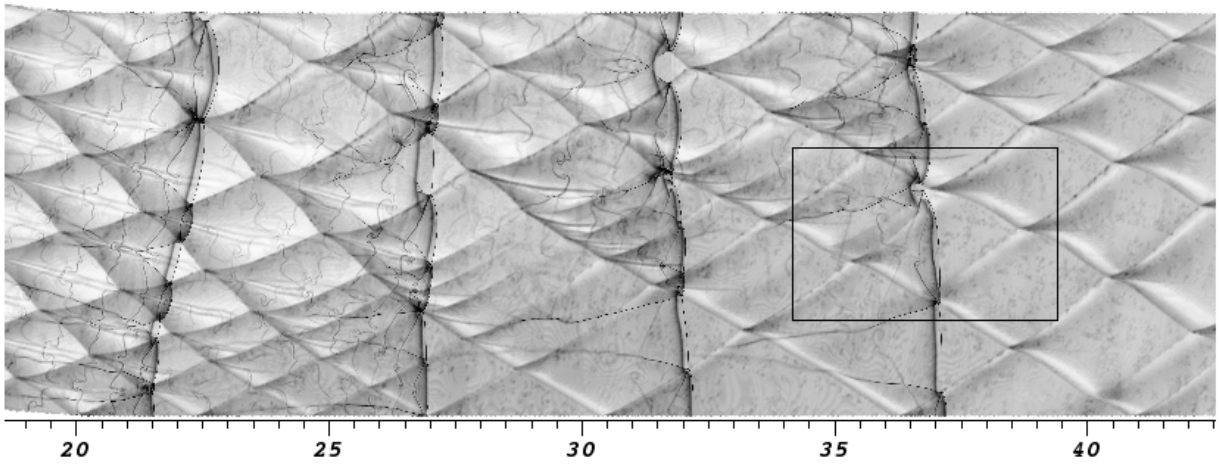
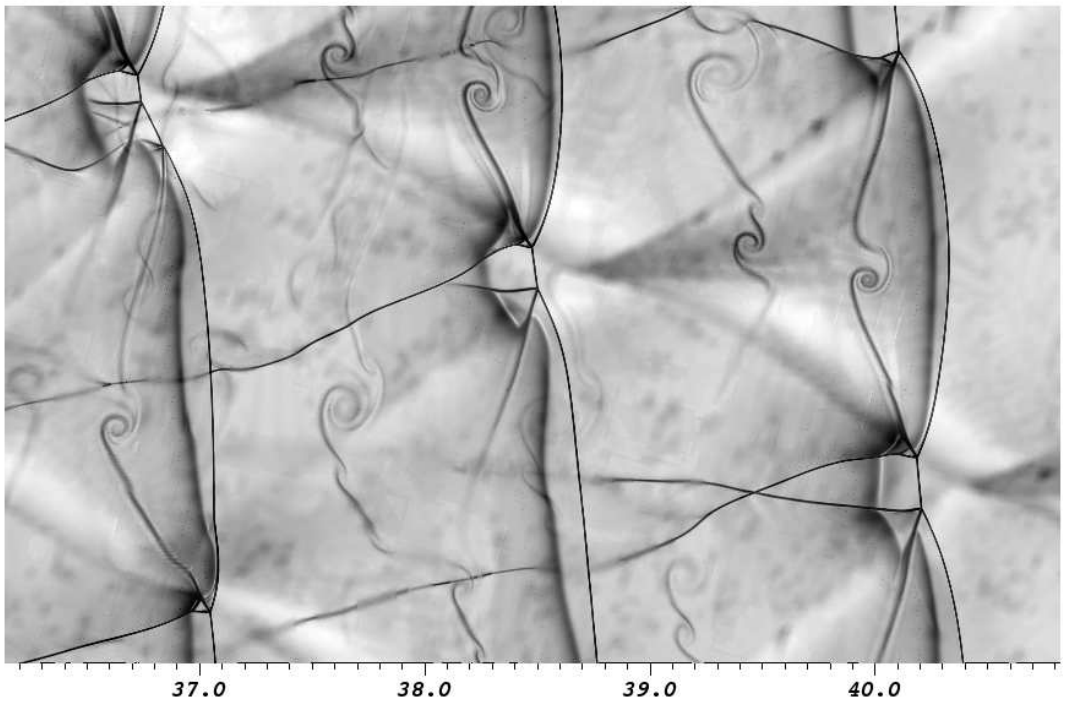




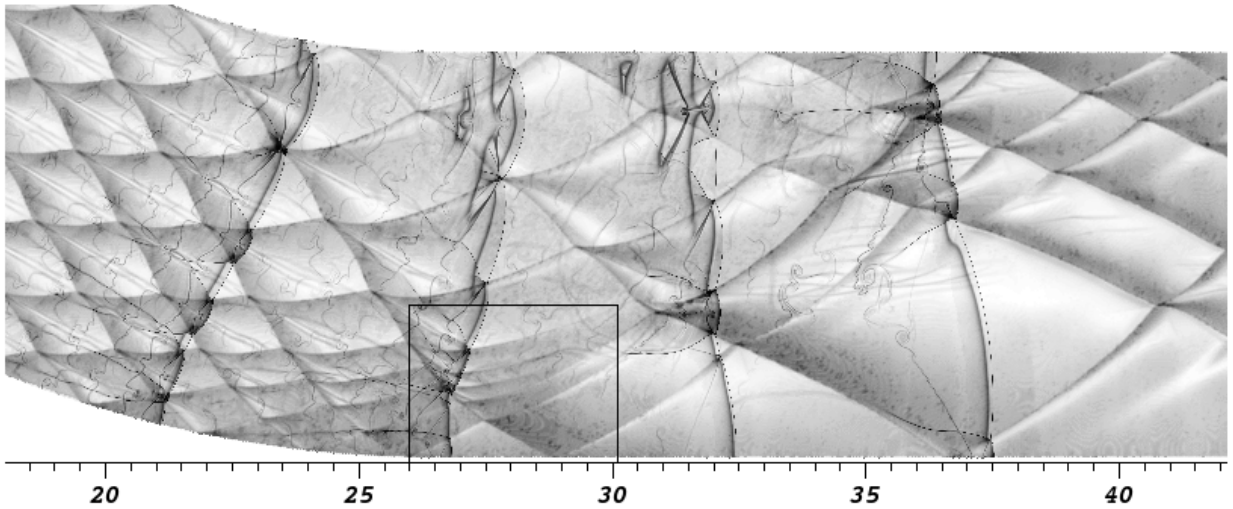
Triple point structures – $\varphi = 15^{\circ}$





- Triple point re-initiation after bend with change from transitional to Double Mach reflection

Triple point structures – $\varphi = 30^{\circ}$



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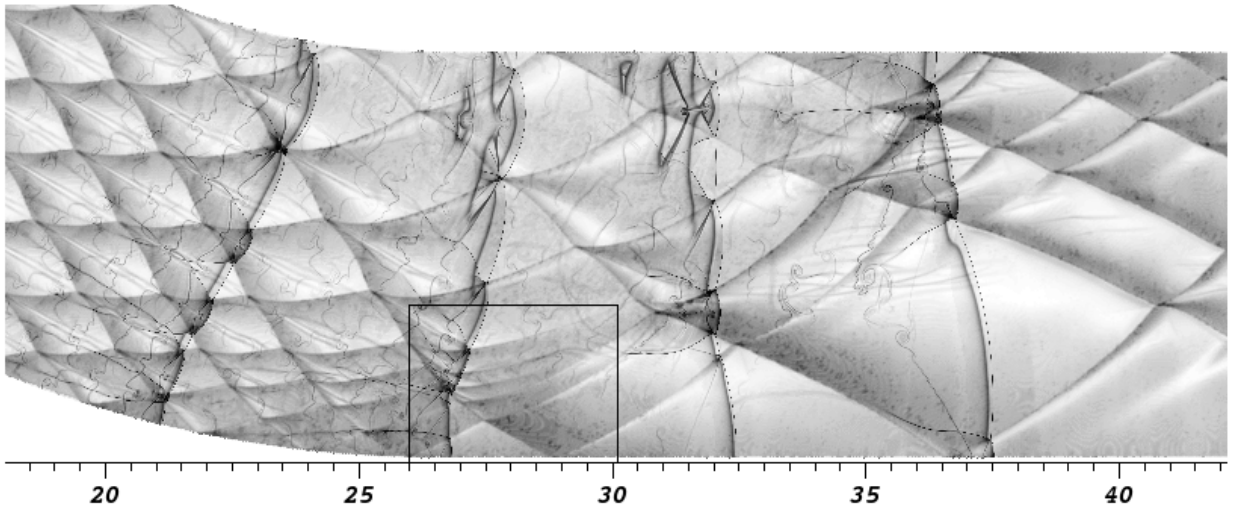

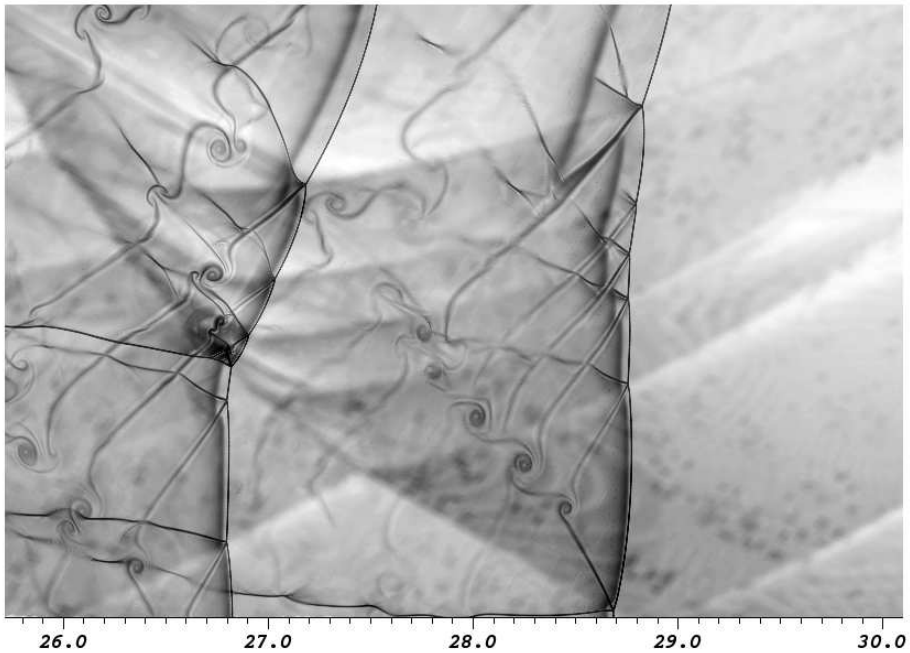

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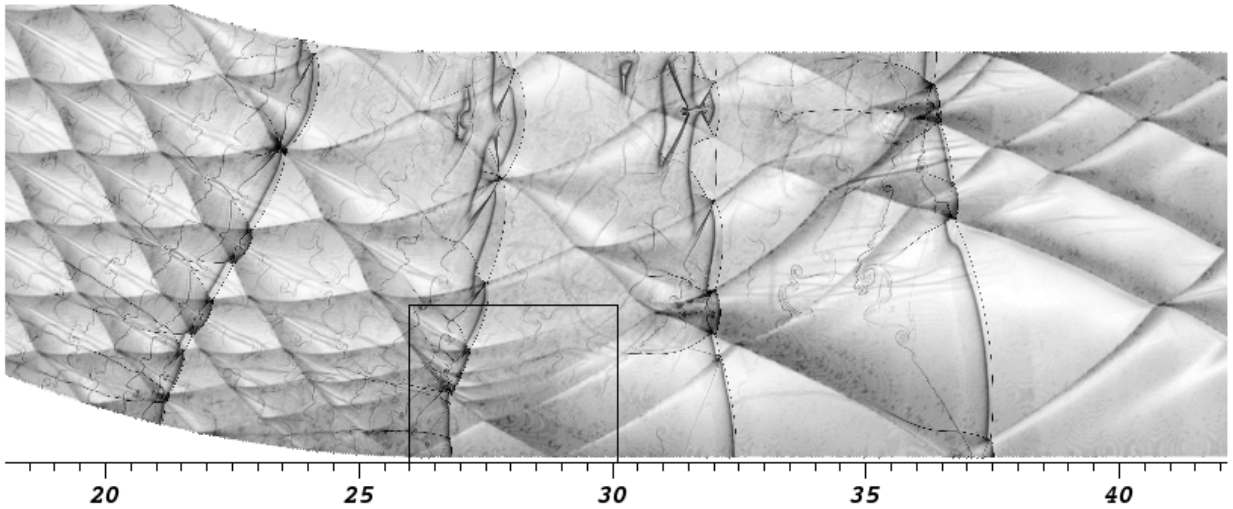

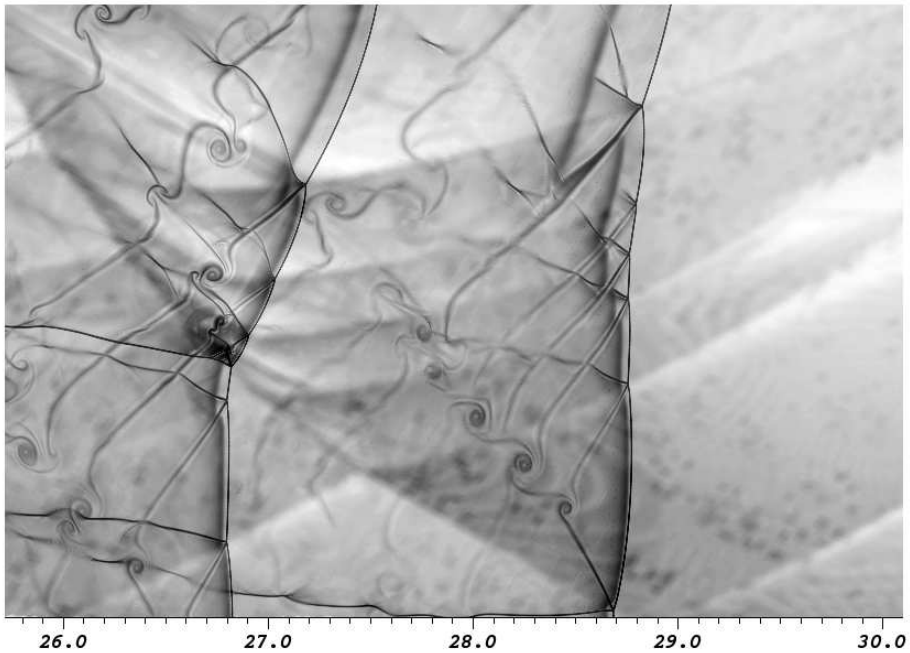

- Triple point quenching and failure as single Mach reflection

Transition criteria

Solve system of oblique shock relations numerically and determine transition boundaries [Ben-Dor, 2007].

- Regular reflection (RR): $M_B^T < 1$
- Single Mach reflection (SMR): $M_C^T < 1$ and $M_B^T > 1$
- Transitional Mach reflection: $M_C^{T'} < 1$ and $M_C^T > 1$
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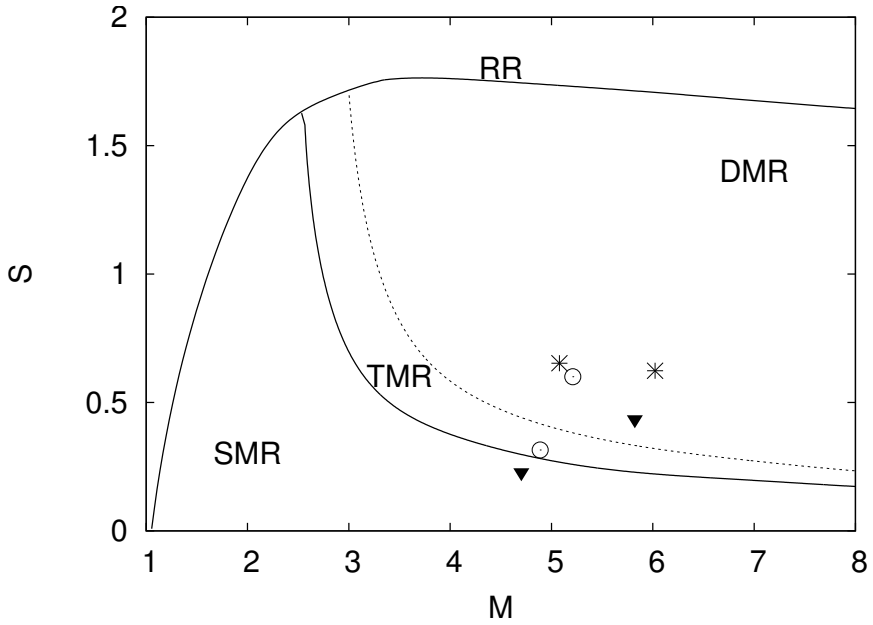
- Here: Nonreactive $\mathrm{H_2 : O_2 : Ar}$ mixture at initially $298\,\mathrm{K}$ and $10\,\mathrm{kPa}$

For detonations:

$$S := \frac{p_C - p_D}{p_D}$$



TMR/DMR transition for $a_t = 100\,\mathrm{m/s}$

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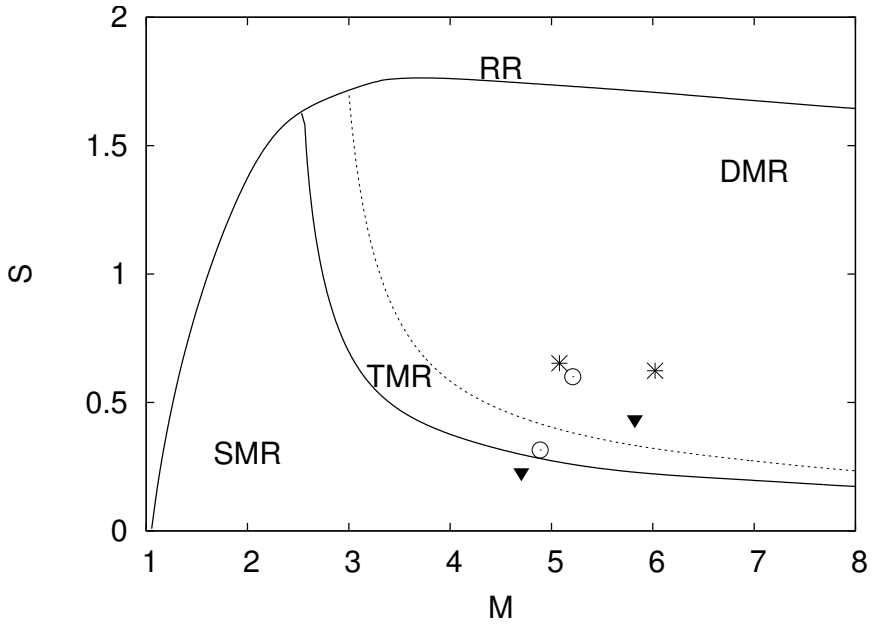
[Deiterding, 2011]

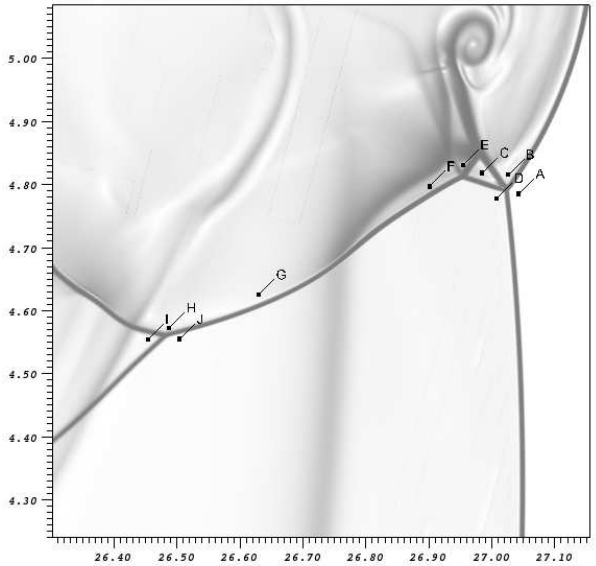


TMR/DMR transition for $a_t = 100\,\mathrm{m/s}$

- Non-reactive shock wave reflection theory seems applicable to predict local triple point structure and stability
- Triple point type is determined solely by S and M. Useful to determine type in underresolved situations.

Triple point structures, $\varphi = 15$

Strong DMR structure in diffraction region behind bend, $S = 1.062$



	p/p_A	r/r_A	T [K]	v[m/s]	M
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C	33.12	5.80	1701	1111	1.355
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E	66.90	9.10	2191	758	0.818
F	57.94	7.64	2259	668	0.710
G	35.28	3.41	3235	699	
H	38.98	3.41	3589	593	
I	23.66	2.37	3149	969	
J	13.58	1.67	2570	1347	

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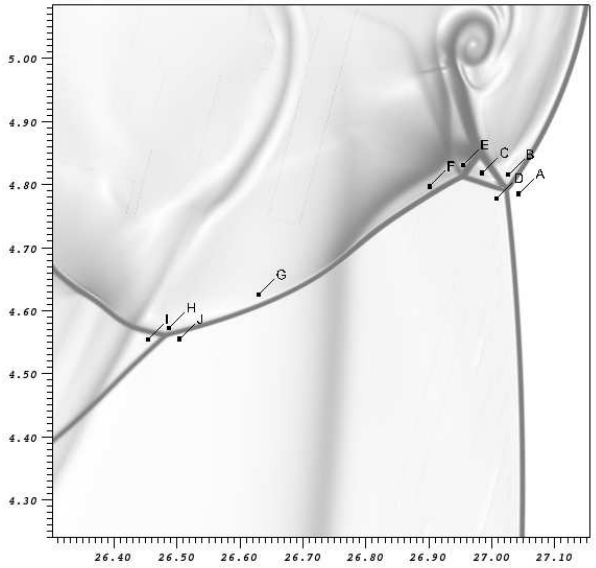
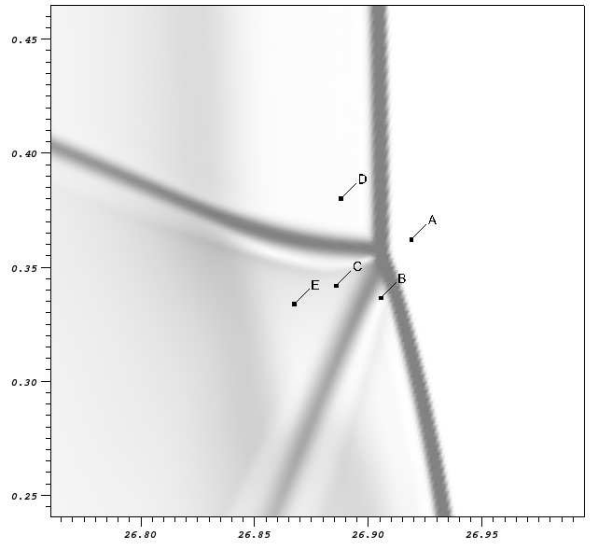
Strong DMR structure in diffraction region behind bend, $S = 1.062$



	p/p_A	r/r_A	T [K]	v[m/s]	M
A	1.00	1.00	298	1835	5.249
B	33.77	4.33	2326	447	0.469
C	33.12	5.80	1701	1111	1.355
D	16.06	3.67	1304	1363	1.889
E	66.90	9.10	2191	758	0.818
F	57.94	7.64	2259	668	0.710
G	35.28	3.41	3235	699	
H	38.98	3.41	3589	593	
I	23.66	2.37	3149	969	
J	13.58	1.67	2570	1347	

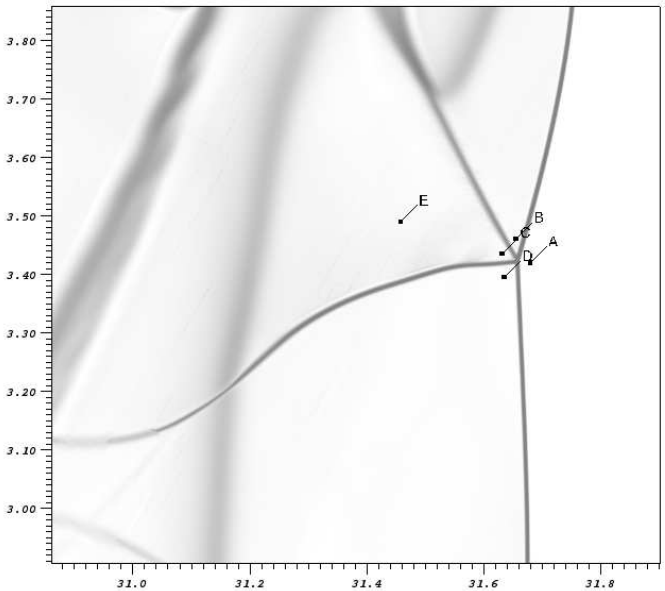
TMR structure in compression region shortly behind bend, $S = 0.338$



	p/p_A	r/r_A	T [K]	v[m/s]	M
A	1.00	1.00	298	1908	5.459
B	34.14	4.21	2418	647	0.666
C	35.49	4.95	2135	929	1.015
D	26.53	4.09	1934	1085	1.243
E	34.91	4.88	2134	938	1.025

Triple point structures

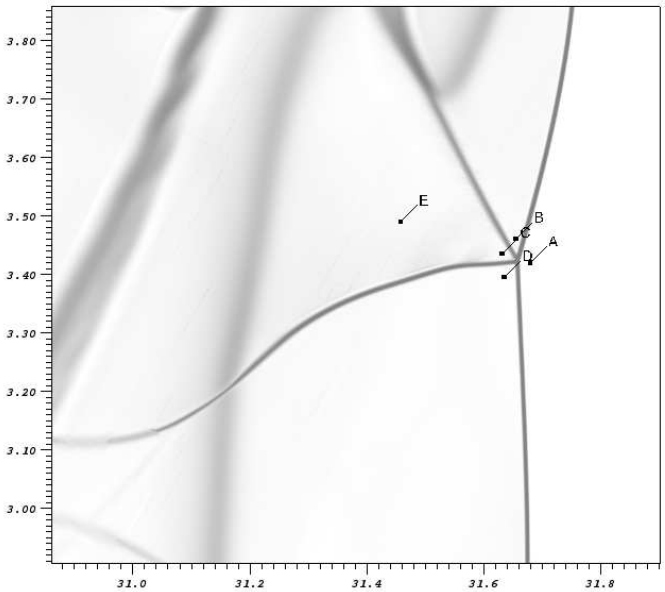
TMR structure in marginal region near limit of detonability, $\varphi = 30$, $S = 0.338$



	p/p_A	r/r_A	T [K]	v[m/s]	M
A	1.00	1.00	298	1424	4.073
B	18.97	3.83	1475	502	0.656
C	18.73	4.30	1297	726	1.009
D	14.00	3.58	1167	848	1.240
E	19.08	4.20	1352	744	1.014

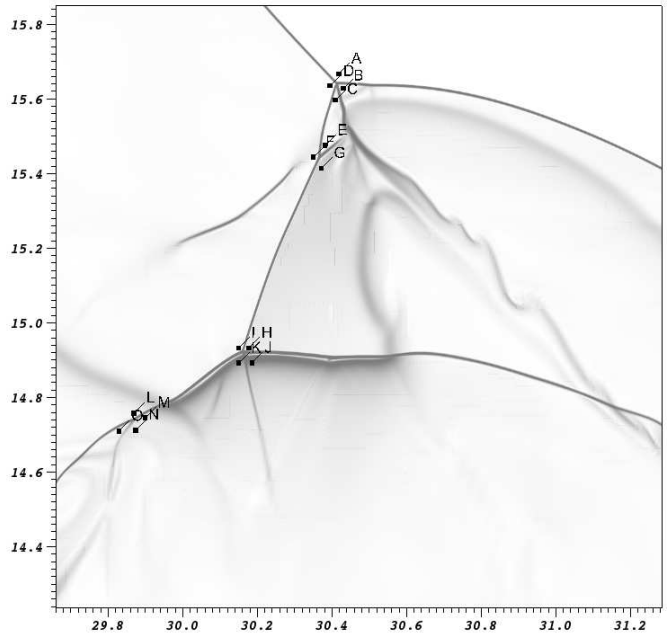
Triple point structures

TMR structure in marginal region near limit of detonability, $\varphi = 30$, $S = 0.338$



	p/p_A	r/r_A	T [K]	v[m/s]	M
A	1.00	1.00	298	1424	4.073
B	18.97	3.83	1475	502	0.656
C	18.73	4.30	1297	726	1.009
D	14.00	3.58	1167	848	1.240
E	19.08	4.20	1352	744	1.014

Re-ignition with strong DMR and transverse detonation, $\varphi = 45$, $S = 1.377$

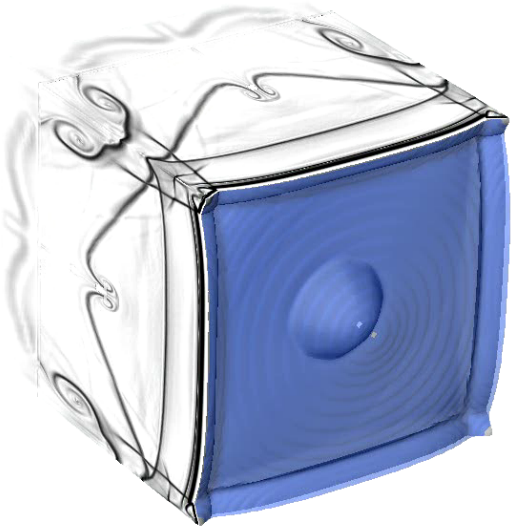


	p/p_A	r/r_A	T [K]	v[m/s]	M
A	1.00	1.00	298	1812	5.186
B	32.58	4.27	2272	456	0.483
C	33.23	6.21	1594	1156	1.454
D	13.98	3.58	1162	1446	2.119
E	31.54	6.30	1492	1208	1.569
F	16.13	4.14	1161	1393	2.042
G	41.63	7.45	1665	1034	1.274
H	30.57	6.31	1443	1180	1.557
I	14.11	3.85	1092	1431	2.161
J	77.31	9.08	2610	756	
K	78.85	8.59	2812	521	

Detonation cell structure in 3D

- Simulation of only one quadrant
- 44.8 Pts/l_{ig} for $\mathrm{H_2} : \mathrm{O_2} : \mathrm{Ar}$ CJ detonation
- SAMR base grid 400x24x24, 2 additional refinement levels (2, 4)
- Simulation uses $\sim 18\,\mathrm{M}$ cells instead of $\sim 118\,\mathrm{M}$ (unigrid)
- $\sim 51,000\,\mathrm{h}$ CPU on 128 CPU Compaq Alpha. $\mathcal{H}$: 37.6 %, $\mathcal{S}$: 25.1 %

Schlieren and isosurface of Y_{OH}



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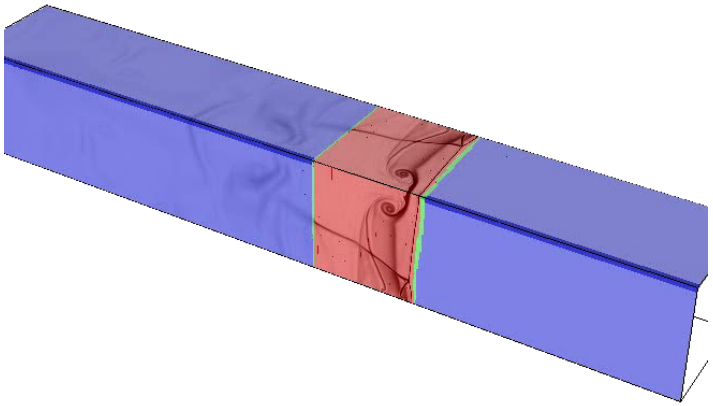
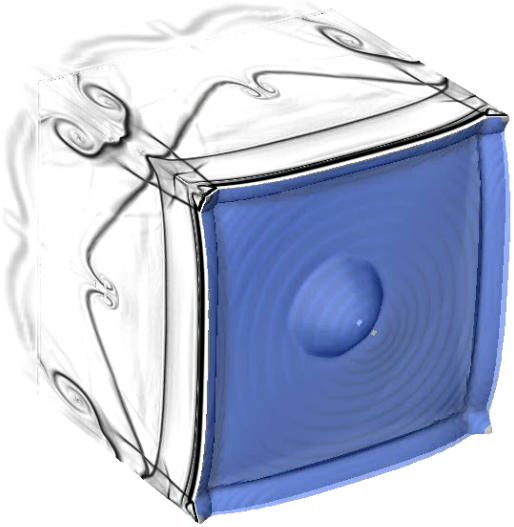
Schlieren on refinement levels



Schlieren and isosurface of Y_{OH}



Detonation cell structure in 3D

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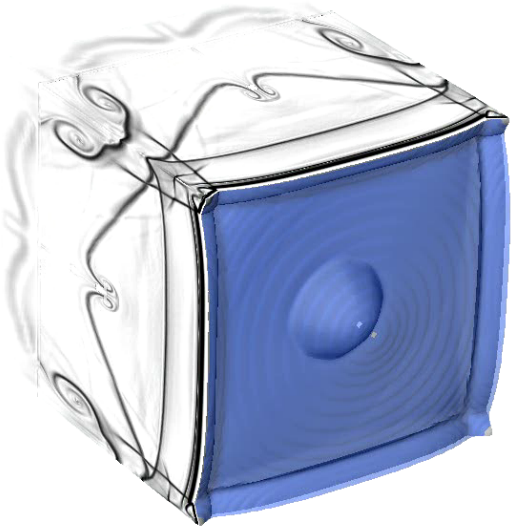
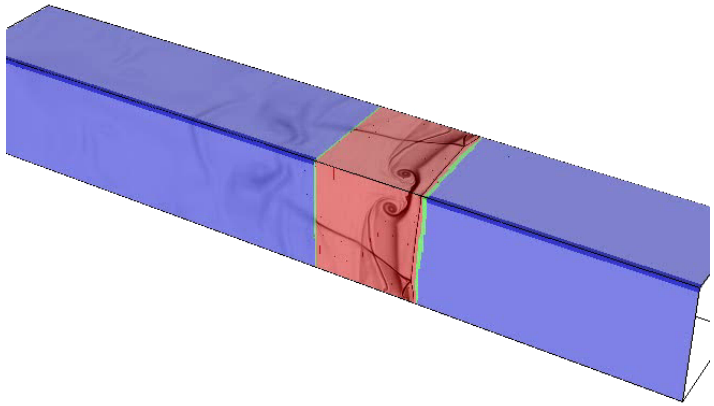
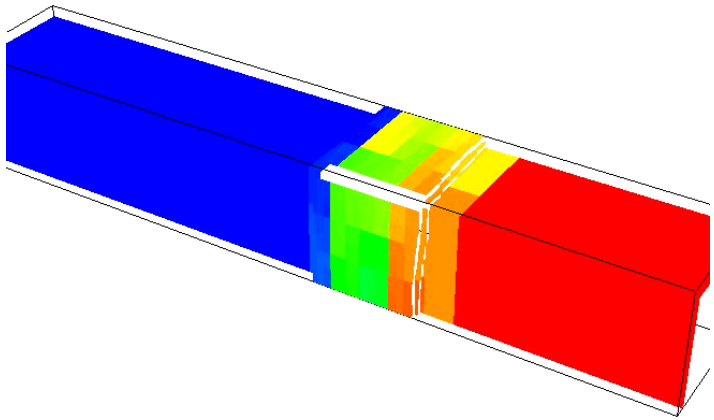
Schlieren and isosurface of Y_{OH}



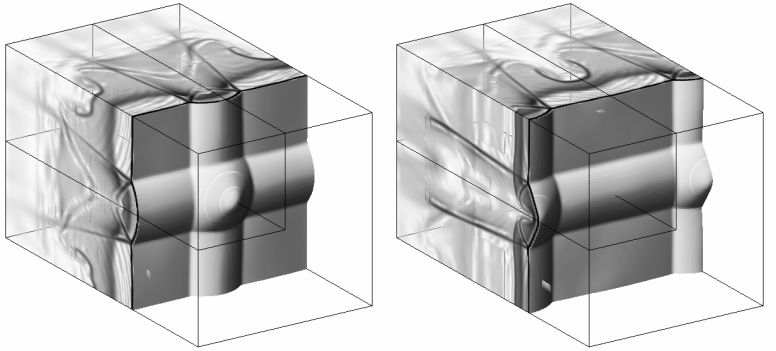
Schlieren on refinement levels



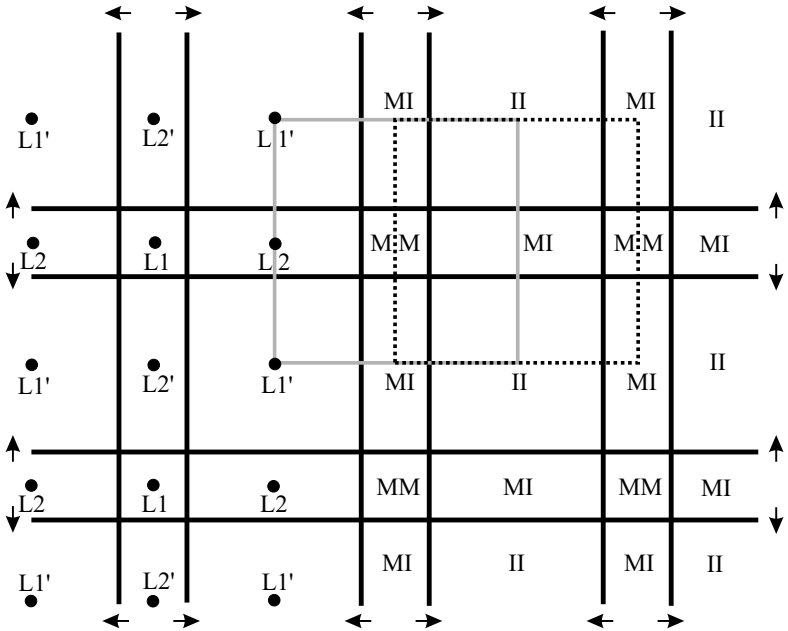
Distribution to 128 processors



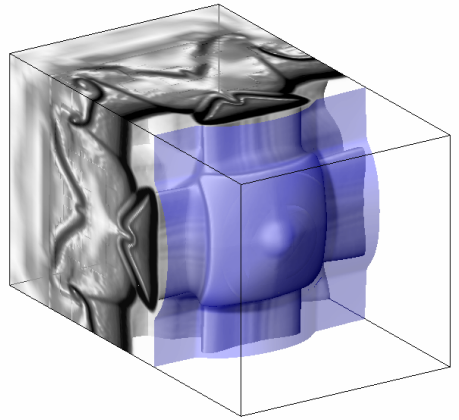
Detonation cell structure in 3D - II

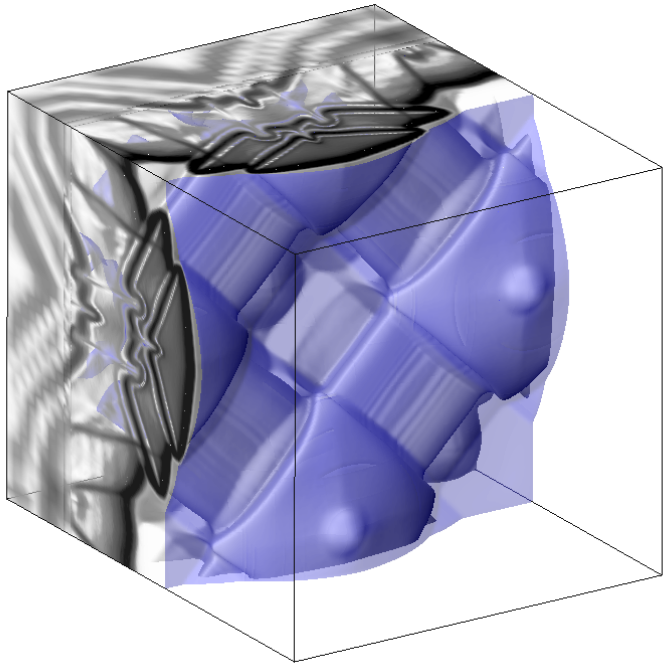


Schlieren plots of density, mirrored for visualization



Schematic front view of the periodic triple

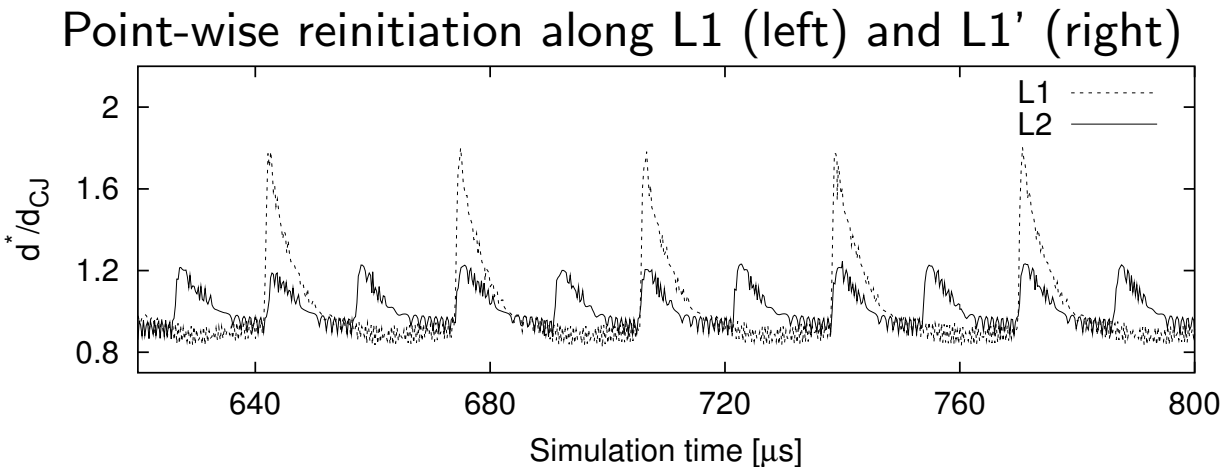




Schlieren plots of Y_{OH}

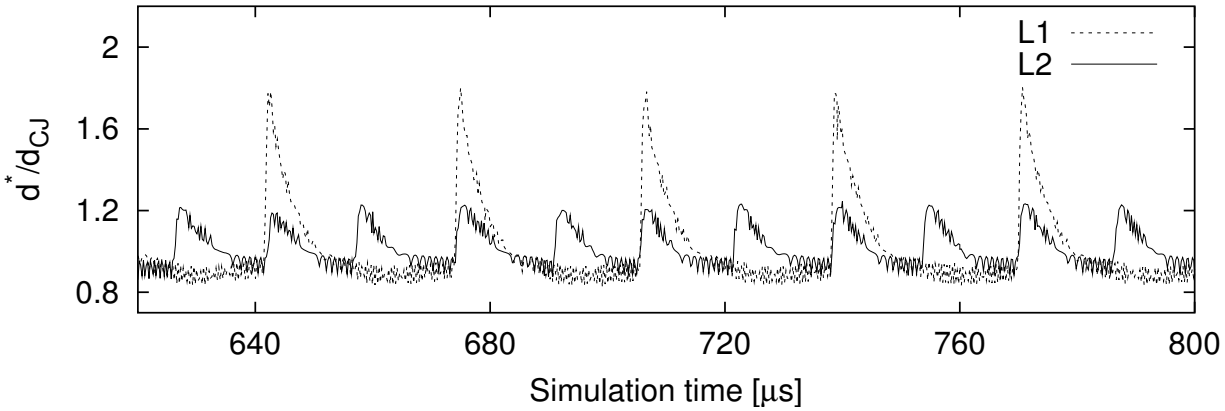
code/amroc/doc/html/apps/clawpack_2applications_2euler__chem_23d_2StrehlowH2O2_2StatDet_2src_2Problem_8h_source.html

Temporal Development of Detonation Velocity

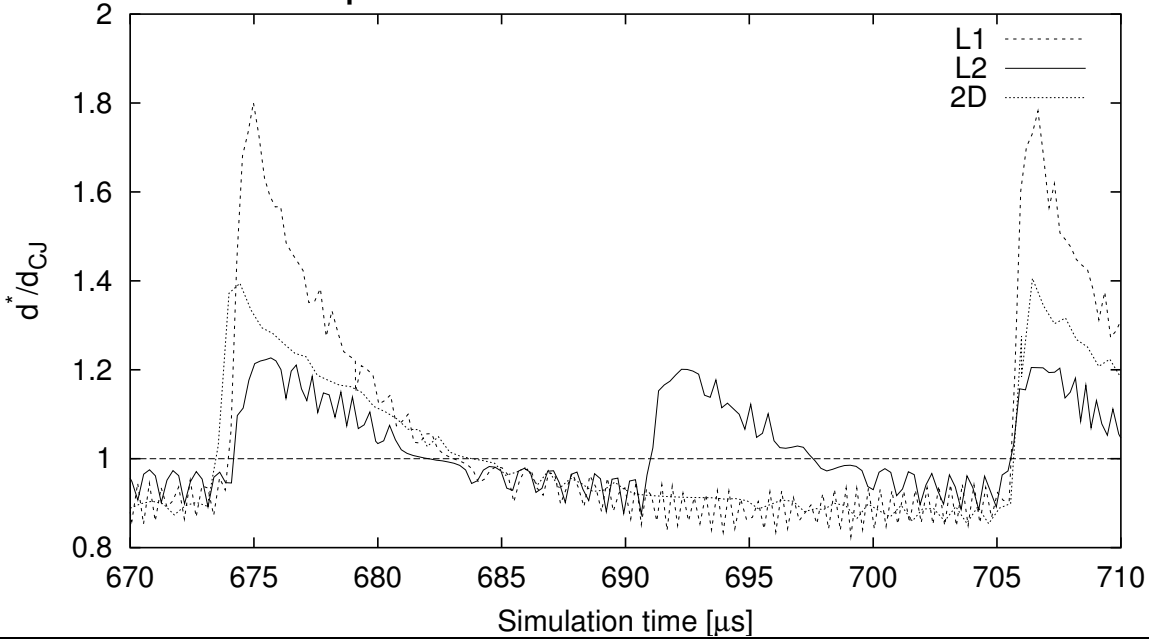


Temporal Development of Detonation Velocity

Point-wise reinitiation along L1 (left) and L1' (right)



Comparison with 2D Simulation



Axisymmetric Navier-Stokes equations with chemical reaction

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial (\mathbf{f} - \mathbf{f}_v)}{\partial x} + \frac{\partial (\mathbf{g} - \mathbf{g}_v)}{\partial y} = \frac{\alpha}{y}(\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s}$$

$$\mathbf{q} = \begin{bmatrix} \rho_i \\ \rho u \\ \rho v \\ \rho E \end{bmatrix}, \ \mathbf{f} = \begin{bmatrix} \rho_i u \\ \rho u^2 + p \\ \rho uv \\ u(\rho E + p) \end{bmatrix}, \ \mathbf{g} = \begin{bmatrix} \rho_i v \\ \rho uv \\ \rho v^2 + p \\ v(\rho E + p) \end{bmatrix}, \ \mathbf{c} = \begin{bmatrix} 0 \\ 0 \\ p - \tau_{\theta\theta} \\ 0 \end{bmatrix}, \ \mathbf{s} = \begin{bmatrix} \dot{\omega}_i \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Axisymmetric Navier-Stokes equations with chemical reaction

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$$\mathbf{f}_v = \begin{bmatrix} \rho D_i \dfrac{\partial Y_i}{\partial x} \\ \tau_{xx} \\ \tau_{xy} \\ k\dfrac{\partial T}{\partial x} + \rho \sum h_j D_j \dfrac{\partial Y_j}{\partial x} + u\tau_{xx} + v\tau_{xy} \end{bmatrix}$$

$$\mathbf{g}_v = \begin{bmatrix} \rho D_i \dfrac{\partial Y_i}{\partial y} \\ \tau_{xy} \\ \tau_{yy} \\ k\dfrac{\partial T}{\partial y} + \rho \sum h_j D_j \dfrac{\partial Y_j}{\partial y} + u\tau_{xy} + v\tau_{yy} \end{bmatrix}$$

$$\tau_{xx} = -\frac{2}{3}\mu(\nabla \cdot \mathbf{v}) + 2\mu\frac{\partial u}{\partial x}$$

$$\tau_{yy} = -\frac{2}{3}\mu(\nabla \cdot \mathbf{v}) + 2\mu\frac{\partial v}{\partial y}$$

$$\tau_{\theta\theta} = -\frac{2}{3}\mu(\nabla \cdot \mathbf{v}) + 2\mu\frac{v}{y}$$

$$\tau_{xy} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

$$\nabla \cdot \mathbf{v} = \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \alpha\frac{v}{y}\right)$$

Chemistry and transport properties

Arrhenius-kinetics:

$$\dot{\omega}_i = \sum_{j=1}^{M} (\nu_{ji}^r - \nu_{ji}^f) \left[k_j^f \prod_{n=1}^{K} \left(\frac{\rho_n}{W_n} \right)^{\nu_{jn}^f} - k_j^r \prod_{n=1}^{K} \left(\frac{\rho_n}{W_n} \right)^{\nu_{jn}^r} \right] \quad i = 1, \ldots, K$$

Chemistry and transport properties

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- Parsing of mechanisms and evaluation of $\dot{\omega}_i$ with Chemkin-II
- $c_{pi}(T)$ and $h_i(T)$ tabulated, linear interpolation between values

Chemistry and transport properties

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Mixture viscosity $\mu = \mu(T, Y_i)$ with Wilke formula

$$\mu = \sum_{i=1}^{K} \frac{Y_i \mu_i}{W_i \sum_{m=1}^{K} Y_m \Phi_{im} / W_m} \text{ with } \Phi_{im} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_i}{W_m} \right)^{-\frac{1}{2}} \left(1 + \left(\frac{\mu_i}{\mu_m} \right)^{\frac{1}{2}} \left(\frac{W_m}{W_j} \right)^{\frac{1}{4}} \right)^2$$

Chemistry and transport properties

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Mixture thermal conductivity $k = k(T, Y_i)$ following Mathur

$$k = \frac{1}{2} \left(W \sum_{i=1}^{K} \frac{Y_i k_i}{W_i} + \frac{1}{W \sum_{i=1}^{K} Y_i / (W_i k_i)} \right)$$

Chemistry and transport properties

Arrhenius-kinetics:

$$\dot{\omega}_i = \sum_{j=1}^{M} (\nu_{ji}^r - \nu_{ji}^f) \left[k_j^f \prod_{n=1}^{K} \left(\frac{\rho_n}{W_n} \right)^{\nu_{jn}^f} - k_j^r \prod_{n=1}^{K} \left(\frac{\rho_n}{W_n} \right)^{\nu_{jn}^r} \right] \quad i = 1, \ldots, K$$

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Mixture diffusion coefficients $D_i = D_i(T, p, Y_i)$ from binary diffusion $D_{mi}(T, p)$ as

$$D_i = \frac{1 - Y_i}{W \sum_{m \neq i} Y_m / (W_m D_{mi})}$$

- Evaluation with Chemkin-II Transport library

Splitting method

$$\partial_t \mathbf{q} + \partial_x(\mathbf{f} - \mathbf{f}_v) + \partial_y(\mathbf{g} - \mathbf{g}_v) = \frac{\alpha}{y}(\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s}$$

Splitting method

$$\partial_t \mathbf{q} + \partial_x(\mathbf{f} - \mathbf{f}_v) + \partial_y(\mathbf{g} - \mathbf{g}_v) = \frac{\alpha}{y}(\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s}$$

Dimensional splitting for PDE

$$\mathcal{X}^{(\Delta t)}: \quad \partial_t \mathbf{q} + \partial_x(\mathbf{f}(\mathbf{q}) - \mathbf{f}_v(\mathbf{q})) = 0\,, \qquad \text{IC: } \mathbf{Q}(t_m) \overset{\Delta t}{\Longrightarrow} \tilde{\mathbf{Q}}^{1/2}$$

$$\mathcal{Y}^{(\Delta t)}: \quad \partial_t \mathbf{q} + \partial_y(\mathbf{g}(\mathbf{q}) - \mathbf{g}_v(\mathbf{q})) = 0\,, \qquad \text{IC: } \tilde{\mathbf{Q}}^{1/2} \overset{\Delta t}{\Longrightarrow} \tilde{\mathbf{Q}}$$

Splitting method

$$\partial_t \mathbf{q} + \partial_x(\mathbf{f} - \mathbf{f}_v) + \partial_y(\mathbf{g} - \mathbf{g}_v) = \frac{\alpha}{y}(\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s}$$

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$$\mathcal{Y}^{(\Delta t)}: \quad \partial_t \mathbf{q} + \partial_y(\mathbf{g}(\mathbf{q}) - \mathbf{g}_v(\mathbf{q})) = 0\,, \qquad \text{IC: } \tilde{\mathbf{Q}}^{1/2} \overset{\Delta t}{\Longrightarrow} \tilde{\mathbf{Q}}$$

Treat right-hand side as source term

$$\mathcal{C}^{(\Delta t)}: \quad \partial_t \mathbf{q} = \tfrac{\alpha}{y}(\mathbf{c}(\mathbf{q}) - \mathbf{g}(\mathbf{q}) + \mathbf{g}_v(\mathbf{q}))\,, \qquad \text{IC: } \tilde{\mathbf{Q}} \overset{\Delta t}{\Longrightarrow} \bar{\mathbf{Q}}$$

Splitting method

$$\partial_t \mathbf{q} + \partial_x(\mathbf{f} - \mathbf{f}_v) + \partial_y(\mathbf{g} - \mathbf{g}_v) = \frac{\alpha}{y}(\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s}$$

Dimensional splitting for PDE

$$\mathcal{X}^{(\Delta t)}: \quad \partial_t \mathbf{q} + \partial_x(\mathbf{f}(\mathbf{q}) - \mathbf{f}_v(\mathbf{q})) = 0\,, \qquad \text{IC: } \mathbf{Q}(t_m) \overset{\Delta t}{\Longrightarrow} \tilde{\mathbf{Q}}^{1/2}$$

$$\mathcal{Y}^{(\Delta t)}: \quad \partial_t \mathbf{q} + \partial_y(\mathbf{g}(\mathbf{q}) - \mathbf{g}_v(\mathbf{q})) = 0\,, \qquad \text{IC: } \tilde{\mathbf{Q}}^{1/2} \overset{\Delta t}{\Longrightarrow} \tilde{\mathbf{Q}}$$

Treat right-hand side as source term

$$\mathcal{C}^{(\Delta t)}: \quad \partial_t \mathbf{q} = \tfrac{\alpha}{y}(\mathbf{c}(\mathbf{q}) - \mathbf{g}(\mathbf{q}) + \mathbf{g}_v(\mathbf{q}))\,, \qquad \text{IC: } \tilde{\mathbf{Q}} \overset{\Delta t}{\Longrightarrow} \bar{\mathbf{Q}}$$

Chemical source term

$$\mathcal{S}^{(\Delta t)}: \quad \partial_t \mathbf{q} = \mathbf{s}(\mathbf{q})\,, \qquad \text{IC: } \bar{\mathbf{Q}} \overset{\Delta t}{\Longrightarrow} \mathbf{Q}(t_m + \Delta t)$$

Splitting method

$$\partial_t \mathbf{q} + \partial_x(\mathbf{f} - \mathbf{f}_v) + \partial_y(\mathbf{g} - \mathbf{g}_v) = \frac{\alpha}{y}(\mathbf{c} - \mathbf{g} + \mathbf{g}_v) + \mathbf{s}$$

Dimensional splitting for PDE

$$\mathcal{X}^{(\Delta t)}: \quad \partial_t \mathbf{q} + \partial_x(\mathbf{f}(\mathbf{q}) - \mathbf{f}_v(\mathbf{q})) = 0\,, \qquad \text{IC: } \mathbf{Q}(t_m) \overset{\Delta t}{\Longrightarrow} \tilde{\mathbf{Q}}^{1/2}$$

$$\mathcal{Y}^{(\Delta t)}: \quad \partial_t \mathbf{q} + \partial_y(\mathbf{g}(\mathbf{q}) - \mathbf{g}_v(\mathbf{q})) = 0\,, \qquad \text{IC: } \tilde{\mathbf{Q}}^{1/2} \overset{\Delta t}{\Longrightarrow} \tilde{\mathbf{Q}}$$

Treat right-hand side as source term

$$\mathcal{C}^{(\Delta t)}: \quad \partial_t \mathbf{q} = \tfrac{\alpha}{y}(\mathbf{c}(\mathbf{q}) - \mathbf{g}(\mathbf{q}) + \mathbf{g}_v(\mathbf{q}))\,, \qquad \text{IC: } \tilde{\mathbf{Q}} \overset{\Delta t}{\Longrightarrow} \bar{\mathbf{Q}}$$

Chemical source term

$$\mathcal{S}^{(\Delta t)}: \quad \partial_t \mathbf{q} = \mathbf{s}(\mathbf{q})\,, \qquad \text{IC: } \bar{\mathbf{Q}} \overset{\Delta t}{\Longrightarrow} \mathbf{Q}(t_m + \Delta t)$$

Formally 1st-order algorithm

$$\mathbf{Q}(t_m + \Delta t) = \mathcal{S}^{(\Delta t)}\mathcal{C}^{(\Delta t)}\mathcal{Y}^{(\Delta t)}\mathcal{X}^{(\Delta t)}(\mathbf{Q}(t_m))$$

but all sub-operators 2nd-order accurate or higher.

Finite volume discretization

Time discretization $t_n = n\Delta t$, discrete volumes $I_{jk} = [x_j - \frac{1}{2}\Delta x, x_j + \frac{1}{2}\Delta x[\times[y_k - \frac{1}{2}\Delta y, y_k + \frac{1}{2}\Delta y[\times =: [x_{j-1/2}, x_{j+1/2}[\times[y_{k-1/2}, y_{k+1/2}[$

Approximation $\mathbf{Q}_{jk}(t) \approx \frac{1}{|I_{jk}|} \int_{I_{jk}} \mathbf{q}(\mathbf{x}, t)\, dx$ and numerical fluxes

$$\mathbf{F}\left(\mathbf{Q}_{jk}(t), \mathbf{Q}_{j+1,k}(t)\right) \approx \mathbf{f}(\mathbf{q}(x_{j+1/2}, y_k, t)),$$

$$\mathbf{F}_v\left(\mathbf{Q}_{jk}(t), \mathbf{Q}_{j+1,k}(t)\right) \approx \mathbf{f}_v(\mathbf{q}(x_{j+1/2}, y_k, t), \nabla\mathbf{q}(x_{j+1/2}, y_k, t))$$

yield (for simplicity)

$$\mathbf{Q}_{jk}^{n+1} = \mathbf{Q}_{kj}^{n} - \frac{\Delta t}{\Delta x}\left[\mathbf{F}\left(\mathbf{Q}_{jk}^{n}, \mathbf{Q}_{j+1,k}^{n}\right) - \mathbf{F}\left(\mathbf{Q}_{j-1,k}^{n}, \mathbf{Q}_{jk}^{n}\right)\right] + \frac{\Delta t}{\Delta x}\left[\mathbf{F}_v\left(\mathbf{Q}_{jk}^{n}, \mathbf{Q}_{j+1,k}^{n}\right) - \mathbf{F}_v\left(\mathbf{Q}_{j-1,k}^{n}, \mathbf{Q}_{jk}^{n}\right)\right]$$

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Stability condition used:

$$\max_{i,j,k}\left\{\frac{\Delta t}{\Delta x}(|u_{jk}| + c_{jk}) + \frac{8}{3}\frac{\mu_{jk}\Delta t}{\rho_{jk}\Delta x^2}, \frac{\Delta t}{\Delta x}(|u_{jk}| + c_{jk}) + \frac{2k_j\Delta t}{c_{v,jk}\rho_j\Delta x^2}, \frac{\Delta t}{\Delta x}(|u_{jk}| + c_{jk}) + D_{i,jk}\frac{\Delta t}{\Delta x^2}\right\} \leq 1$$

Finite volume discretization – cont.

Symmetry source term $\mathcal{C}^{(\Delta t)}$: Use

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within explicit 2nd-order accurate Runge-Kutta method

- Gives 2nd-order central difference approximation of $\mathbf{G}_v$

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Chemical source term $\mathcal{S}^{(\cdot)}$:

- 4th-order accurate semi-implicit ODE-solver subcycles within each cell
- ρ, e, u, v remain unchanged!

$$\partial_t \rho_i = W_i \dot{\omega}_i(\rho_1, \ldots, \rho_K, T) \qquad i = 1, \ldots, K$$

Lehr's ballistic range experiments

- Spherical-nosed projectile of radius $1.5\,\mathrm{mm}$ travels with constant velocity through stoichiometric $\mathrm{H_2} : \mathrm{O_2} : \mathrm{N_2}$ mixture (molar ratios 2:1:3.76) at $42.663\,\mathrm{kPa}$ and $T = 293\,\mathrm{K}$ [Lehr, 1972]
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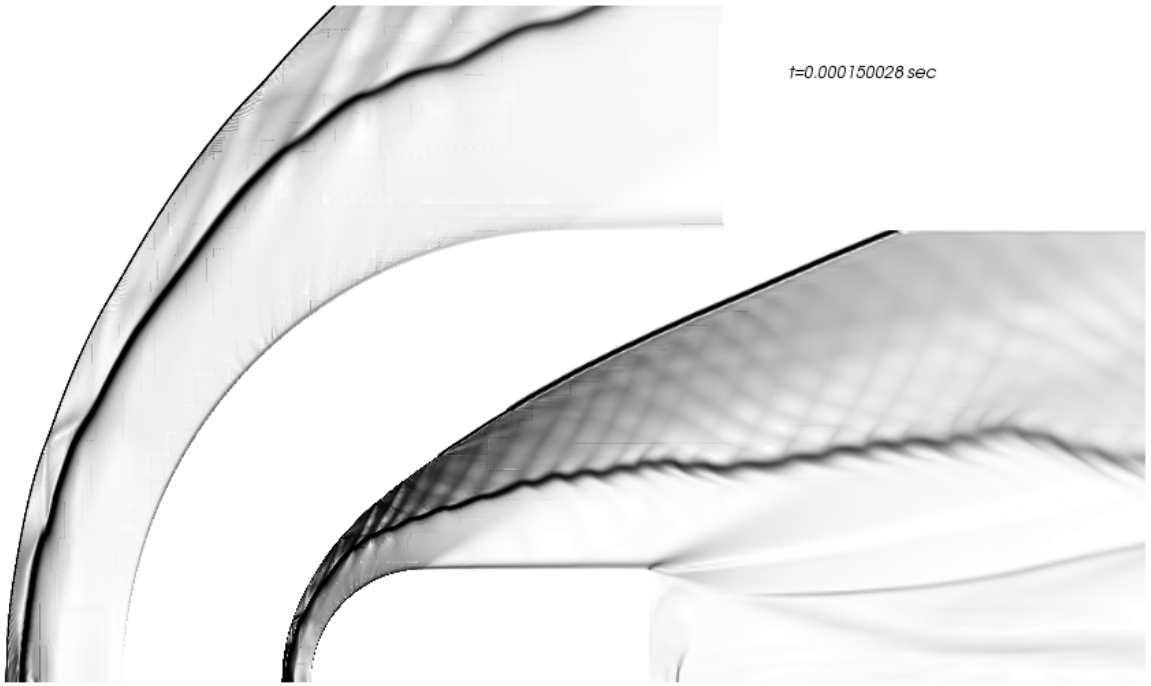
`code/amroc/doc/html/apps/clawpack_2applications_2euler__chem_22d_2SphereLehr_2src_2Problem_8h_source.html`

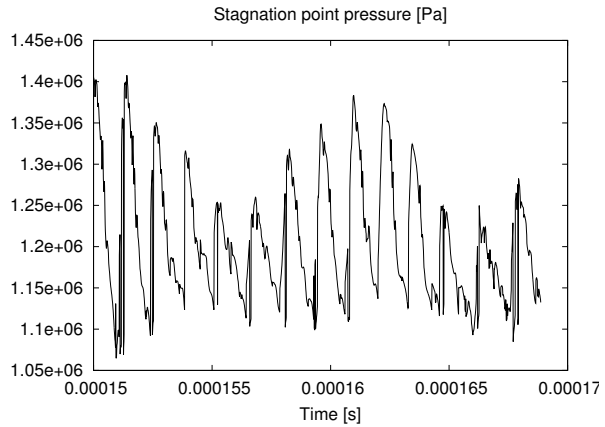
`code/amroc/doc/html/apps/clawpack_2applications_2euler__chem_22d_2SphereLehrNav_2src_2Problem_8h_source.html`

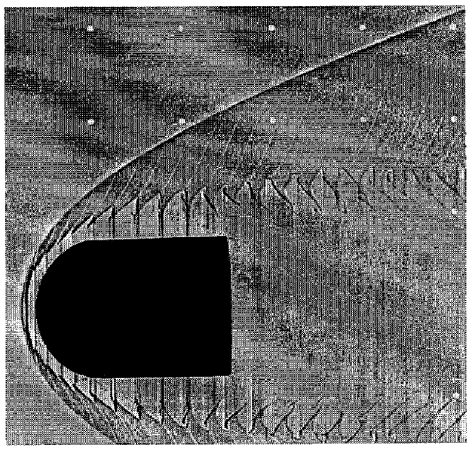
Viscous case – $M = 4.79$

- 5619 iterations with CFL=0.9 to $t = 170\,\mu\mathrm{s}$
- Oscillation frequency in last $20\,\mu\mathrm{s}$: $\sim 722\,\mathrm{kHz}$ (viscous), $\sim 737\,\mathrm{kHz}$ (inviscid)
- Experimental value: $\sim 720\,\mathrm{kHz}$

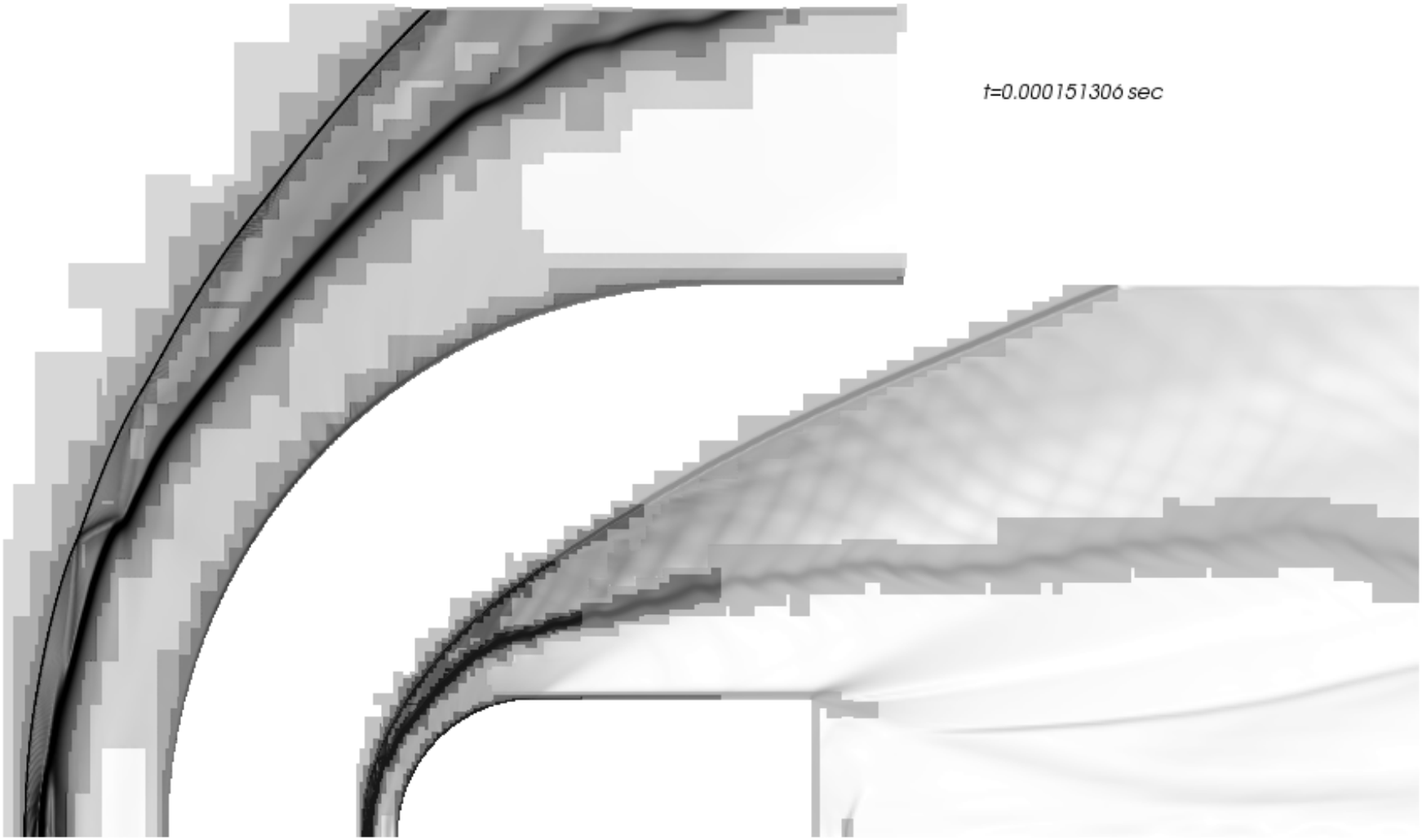


Schlieren plot of density

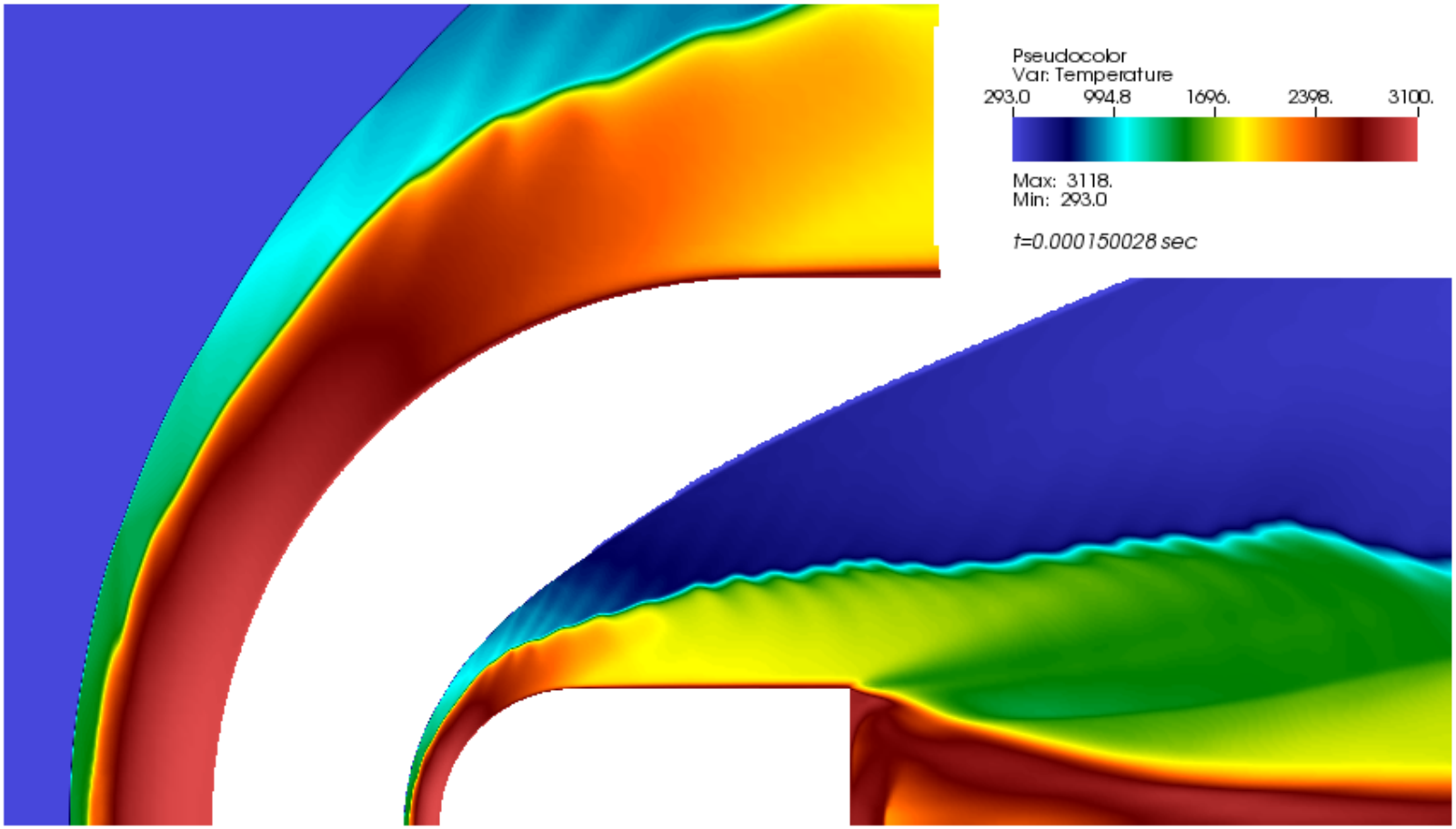




Viscous case – $M = 4.79$ – mesh adaptation



Comparison of temperature field



Viscous

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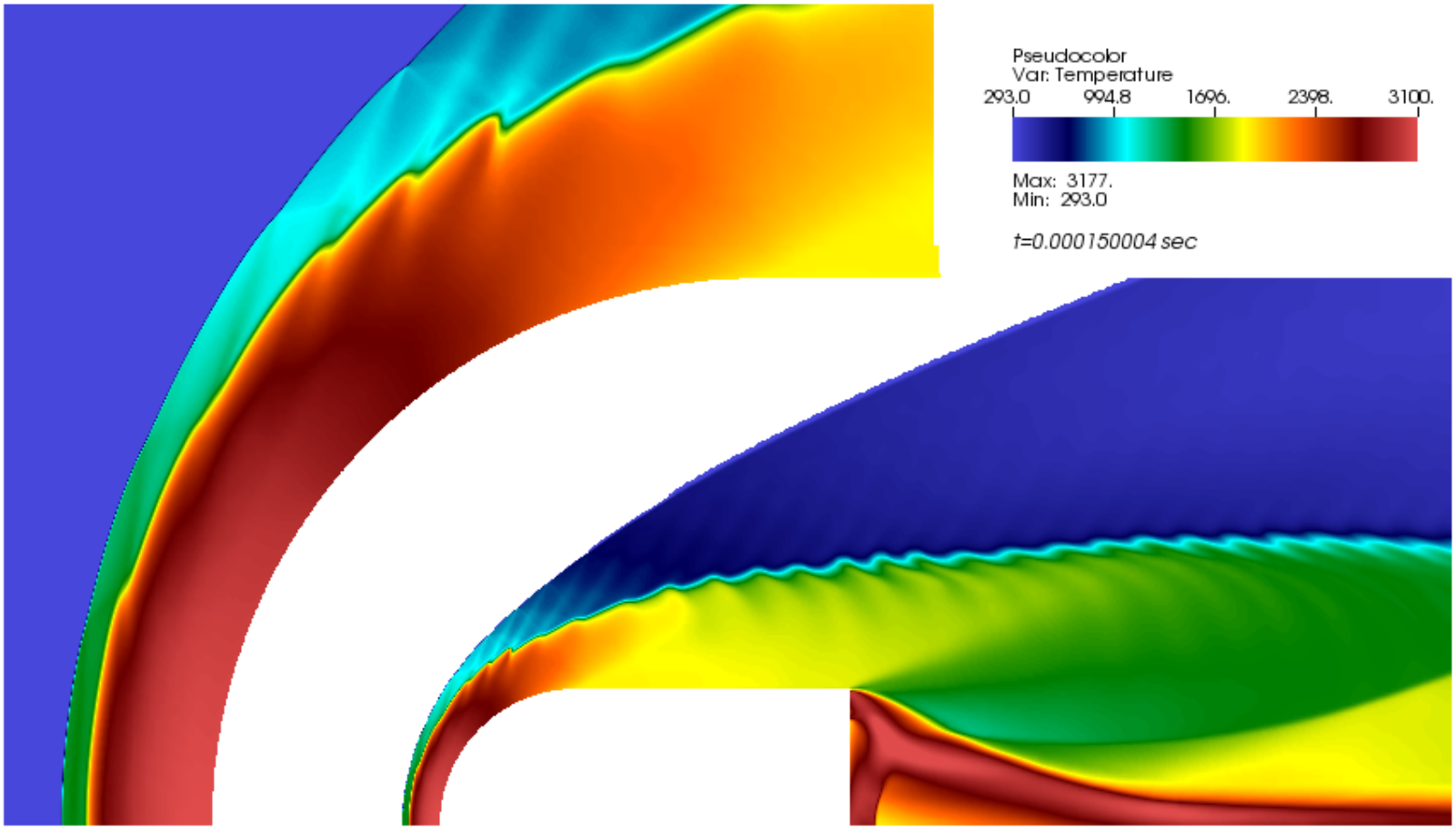
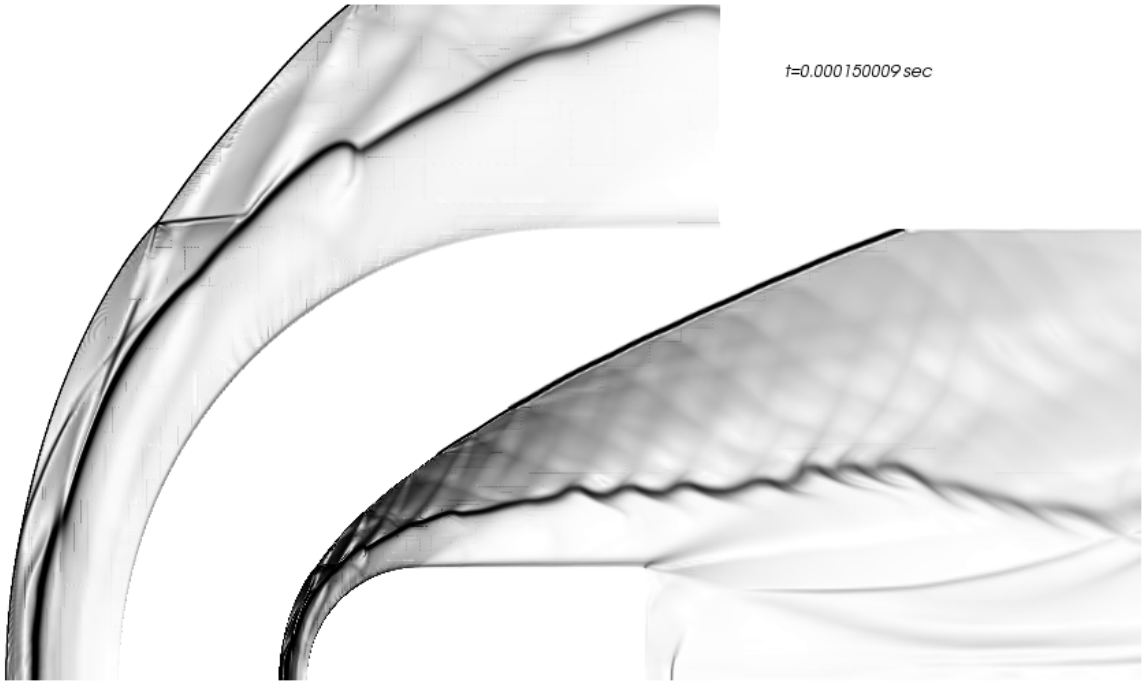


Inviscid

Viscous case – $M = 4.48$

- 5432 iterations with CFL=0.9 to $t = 170\,\mu\mathrm{s}$
- Oscillation frequency in last $20\,\mu\mathrm{s}$: $\sim 417\,\mathrm{kHz}$
- Experimental value: $\sim 425\,\mathrm{kHz}$



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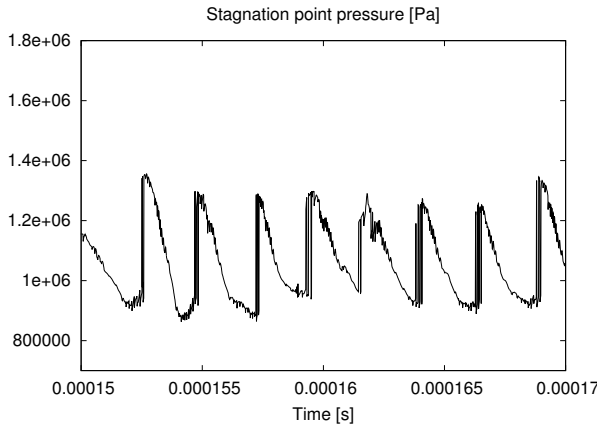
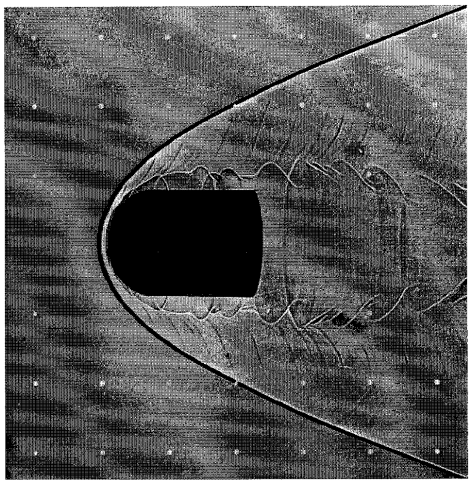
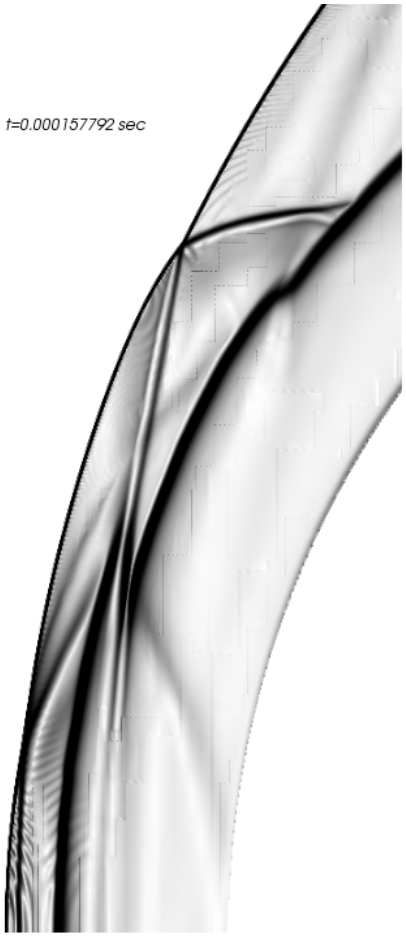


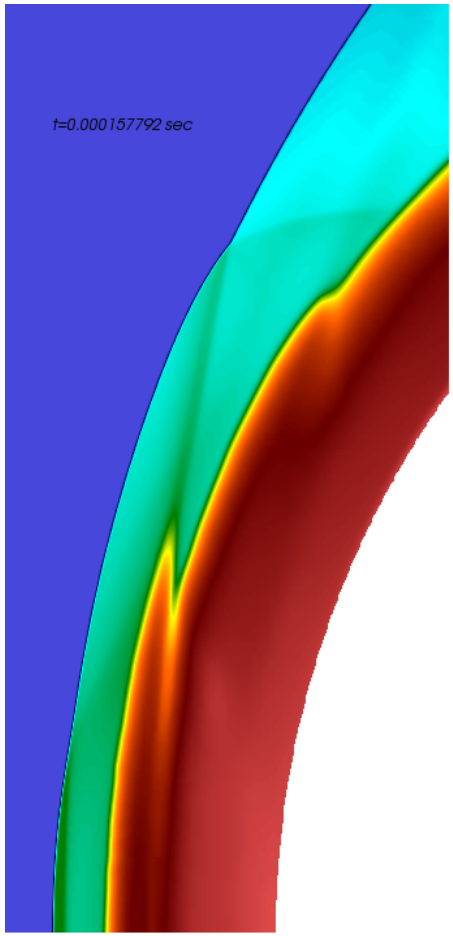


Oscillation mechanism

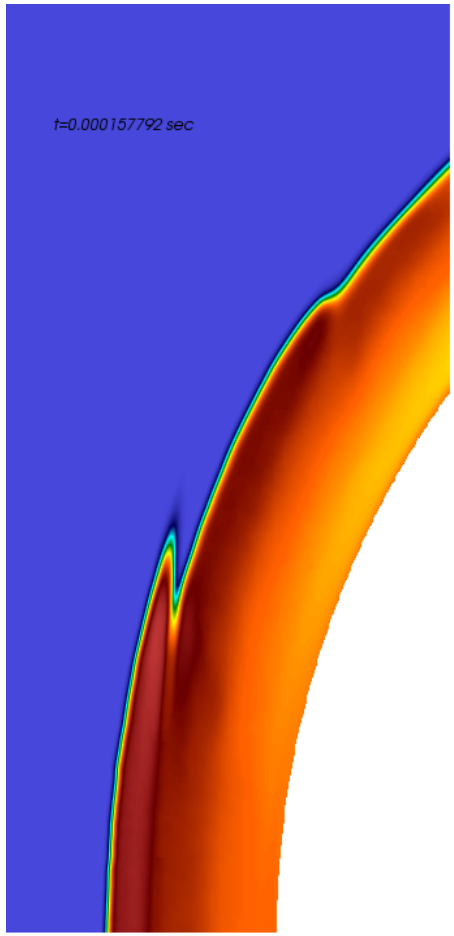
Schlieren of density



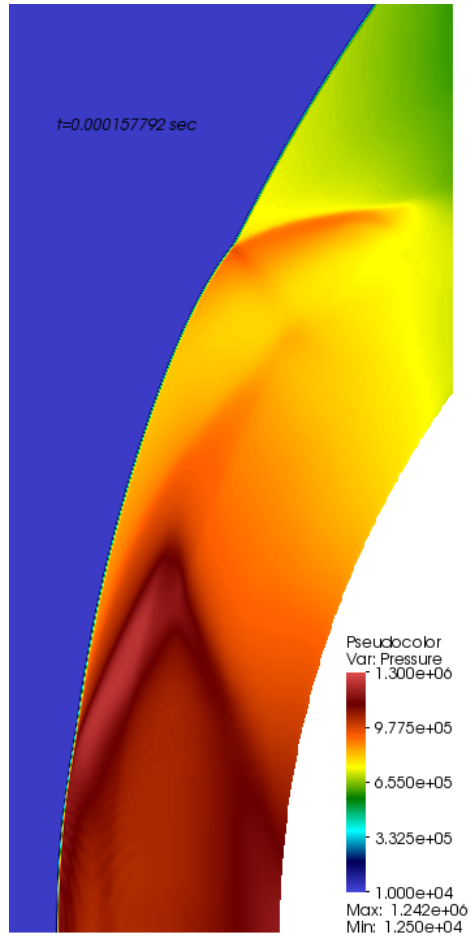
Temperature



Mass fraction OH



Pressure



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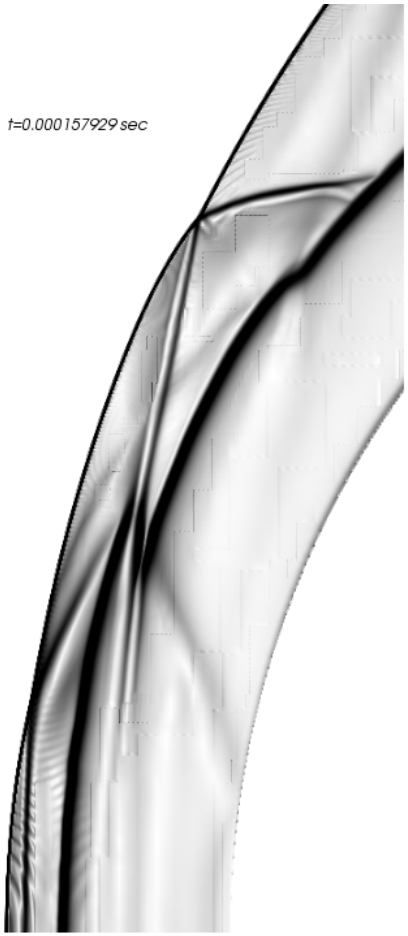

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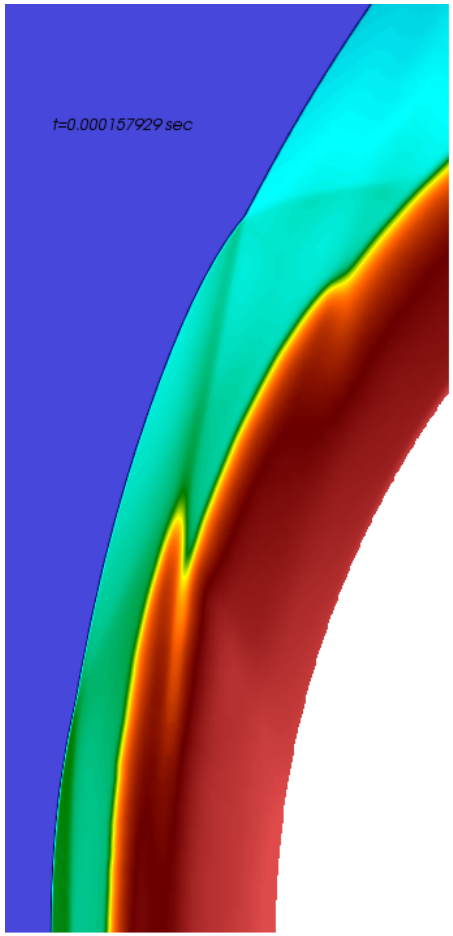

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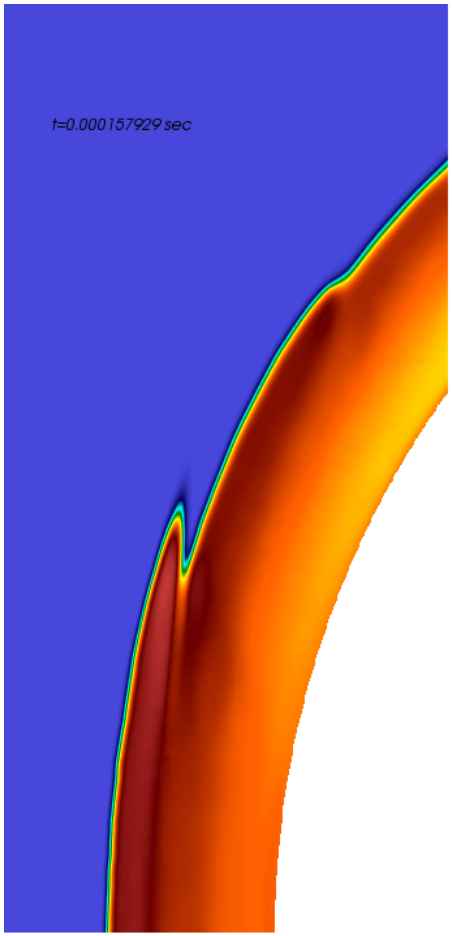

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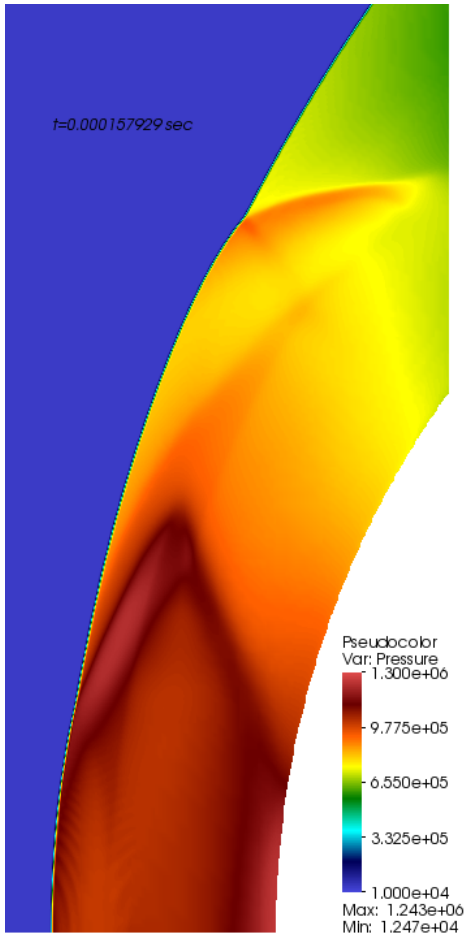

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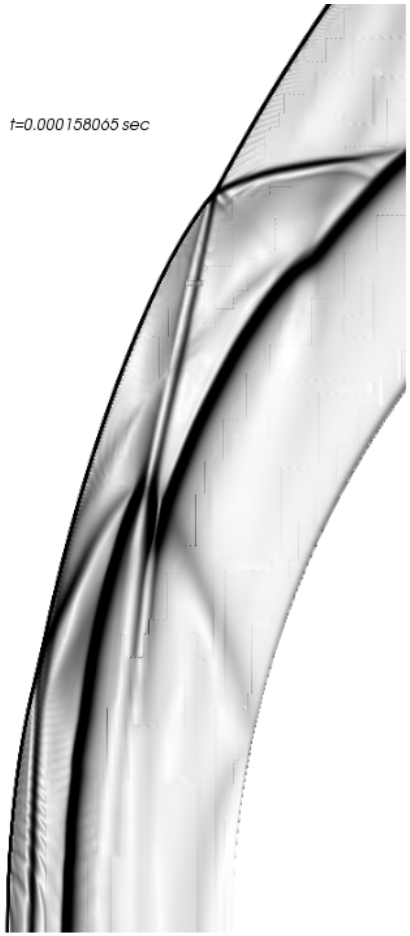

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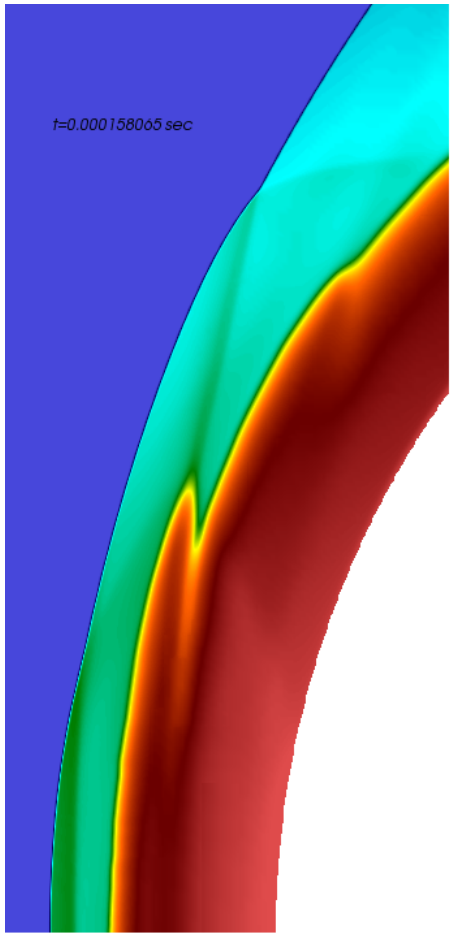
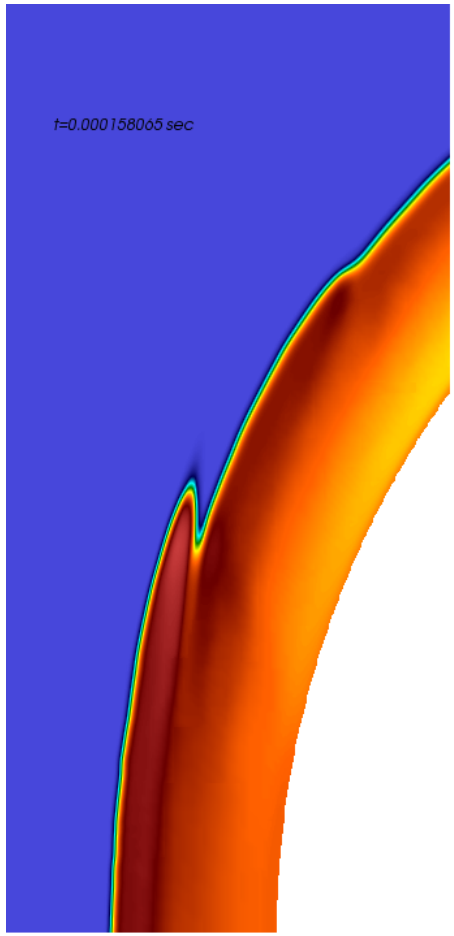
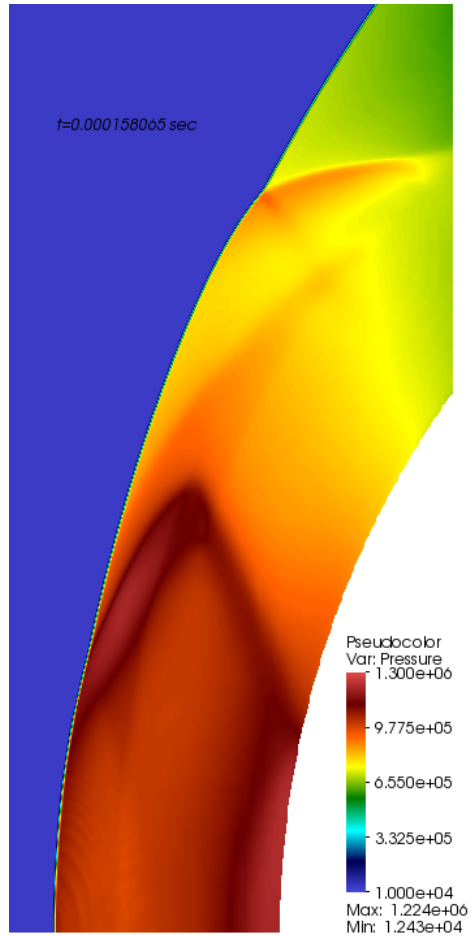


Mass fraction OH

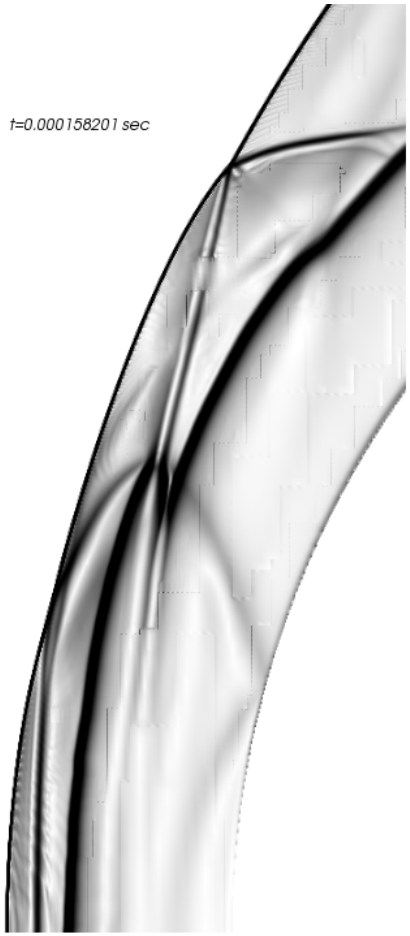


Pressure

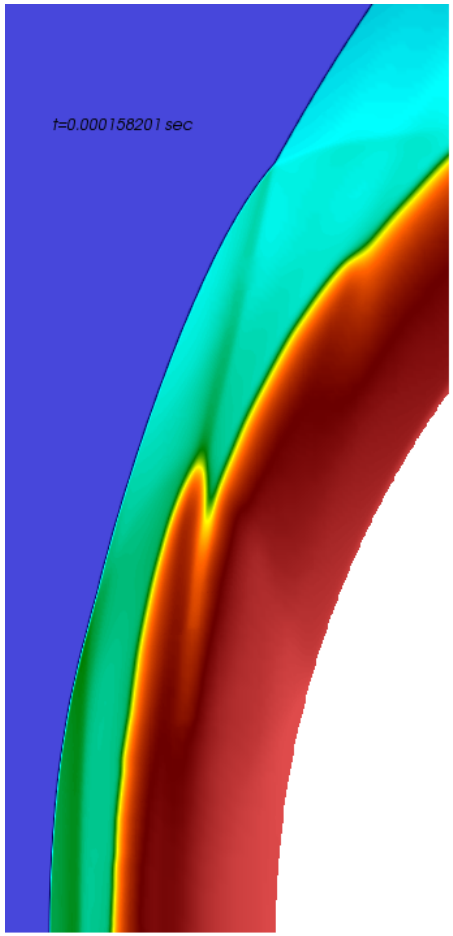


Oscillation mechanism

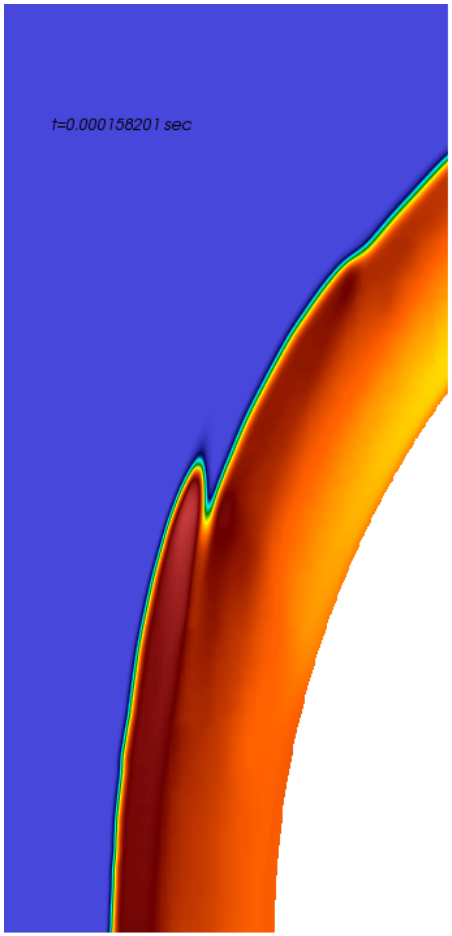
Schlieren of density



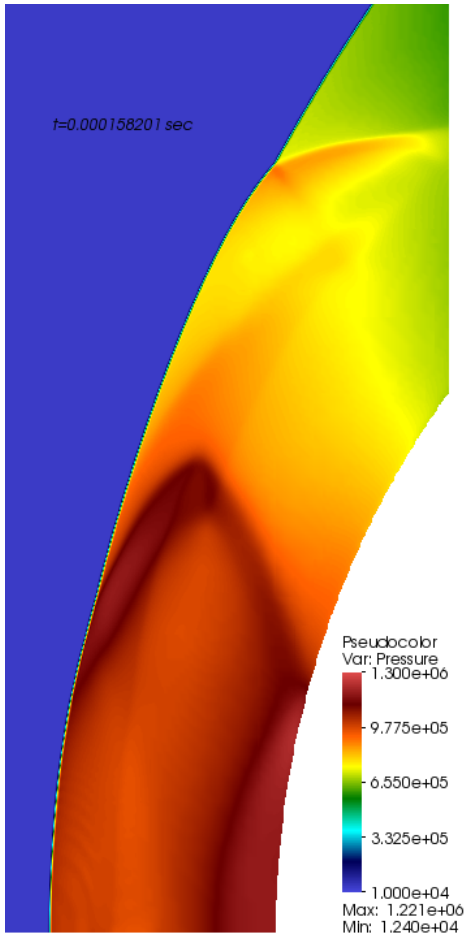
Temperature



Mass fraction OH

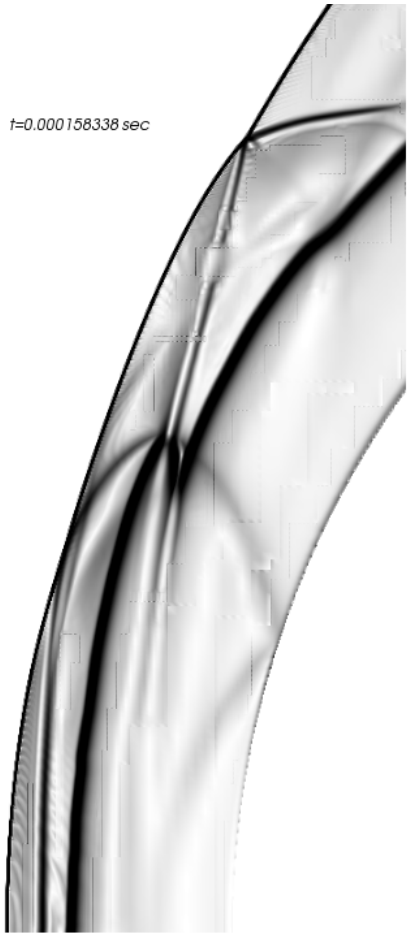


Pressure

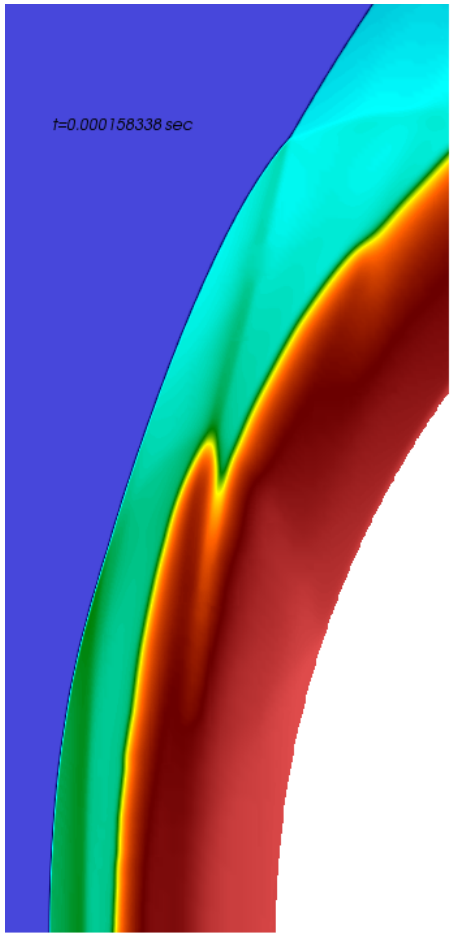


Oscillation mechanism

Schlieren of density



Temperature



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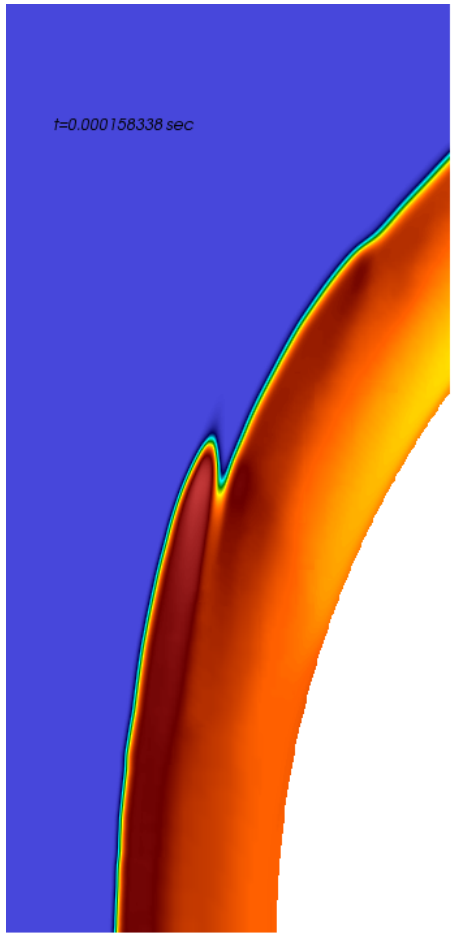
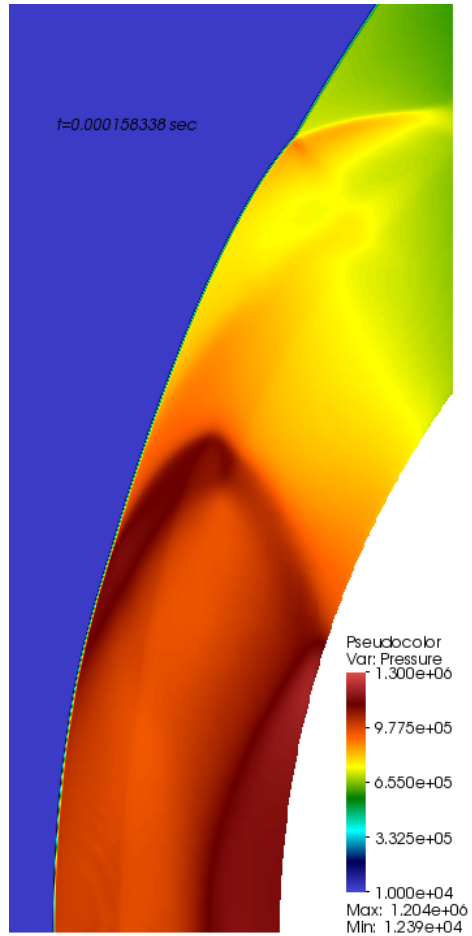
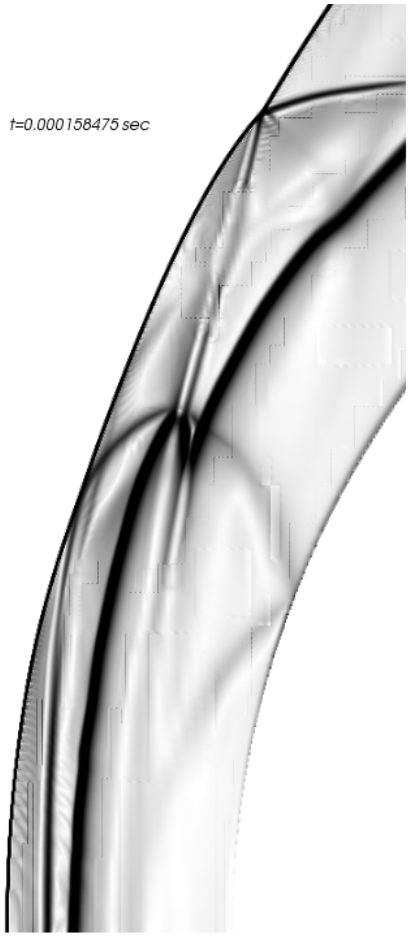


Pressure

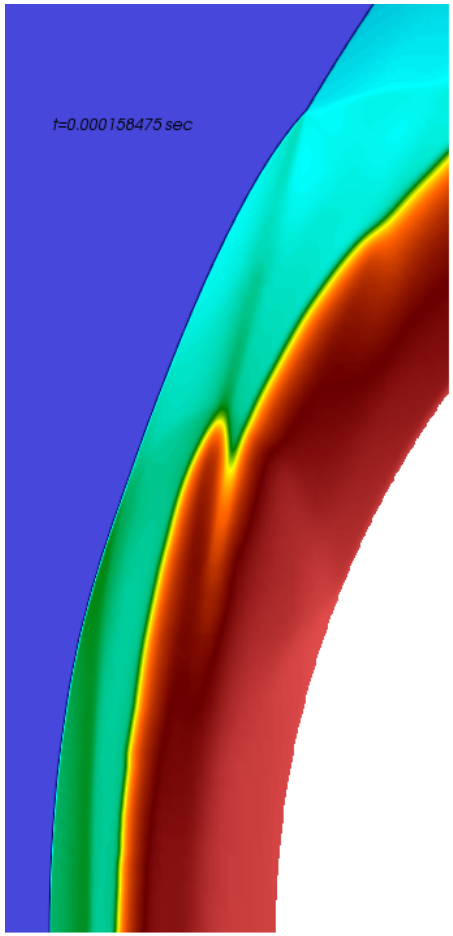


Oscillation mechanism

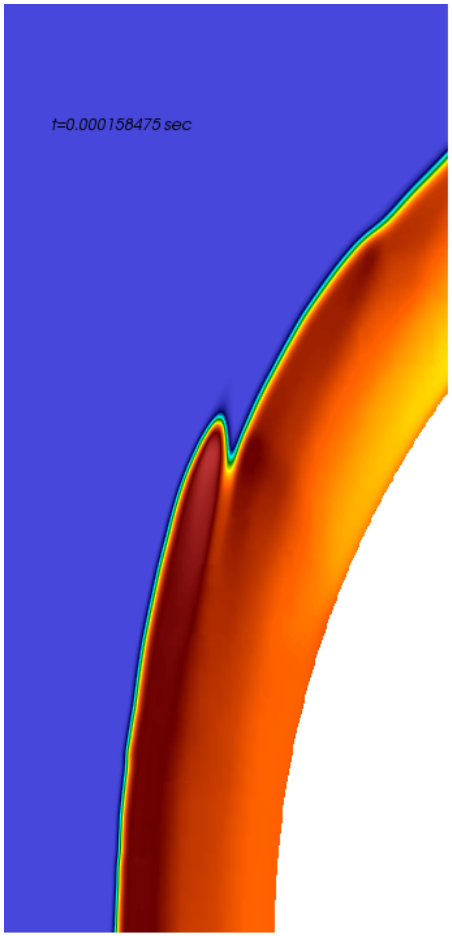
Schlieren of density



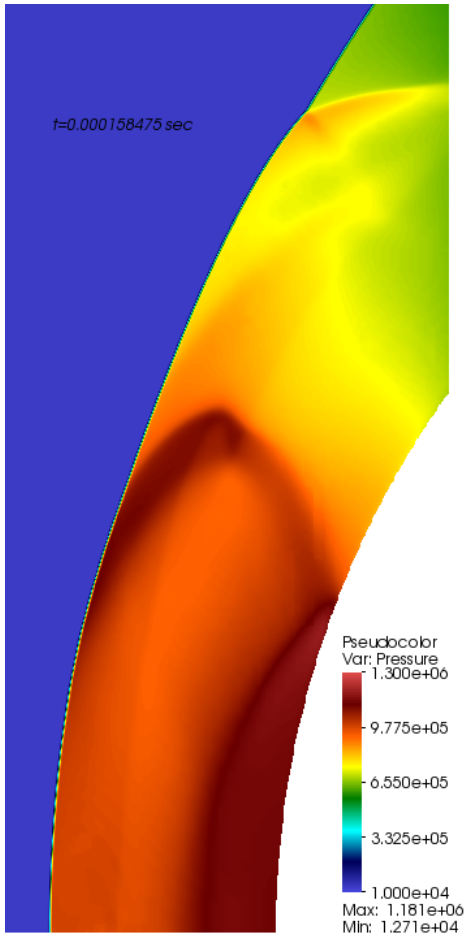
Temperature



Mass fraction OH

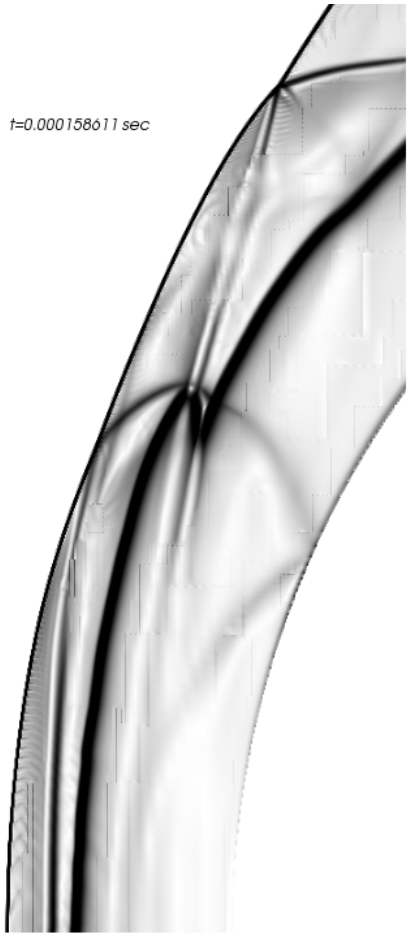


Pressure

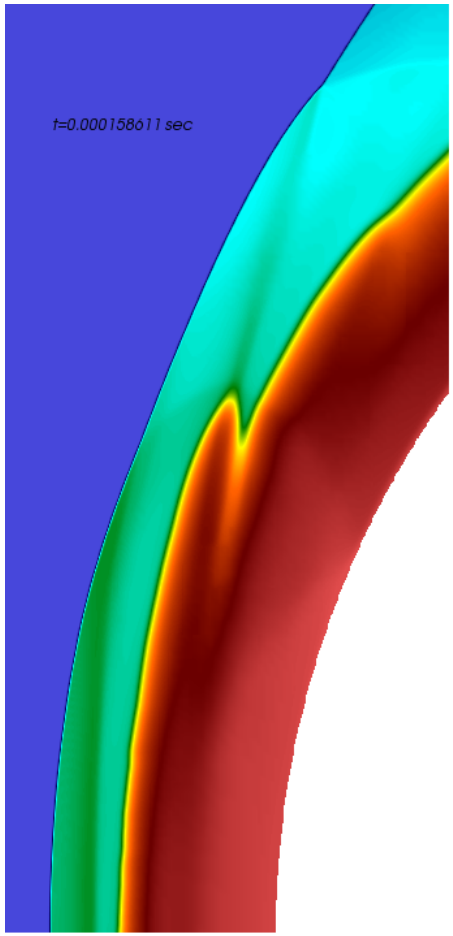


Oscillation mechanism

Schlieren of density



Temperature



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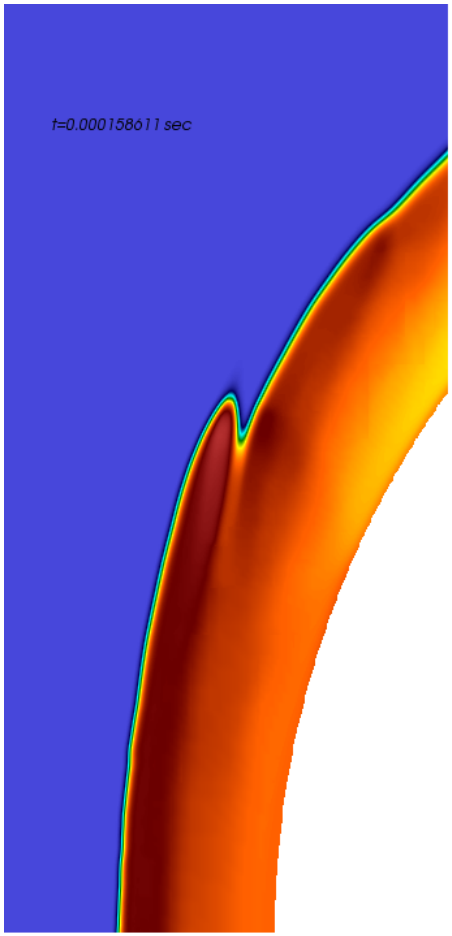
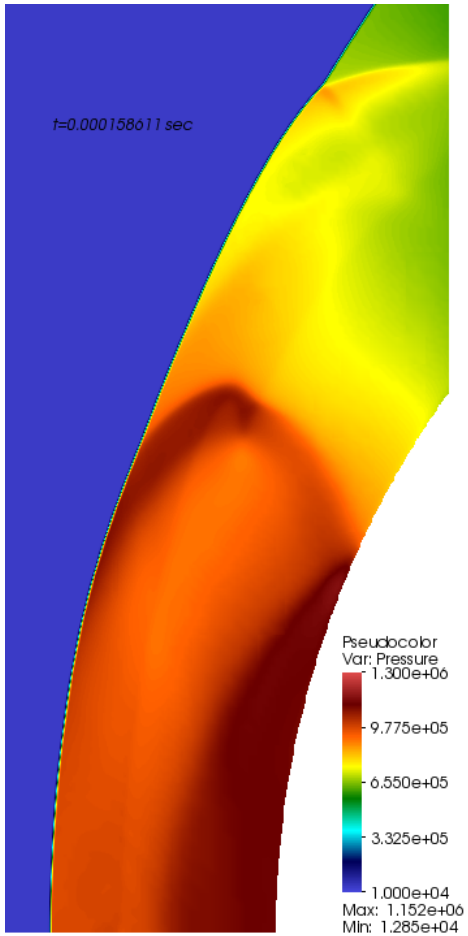
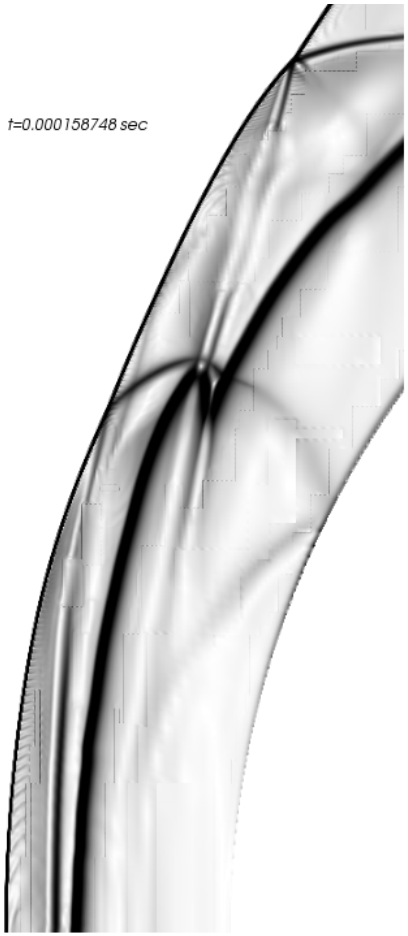


Pressure

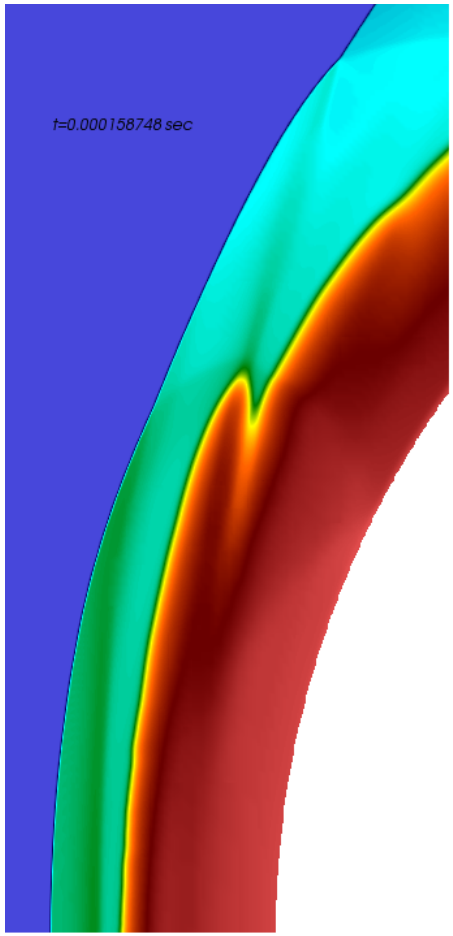


Oscillation mechanism

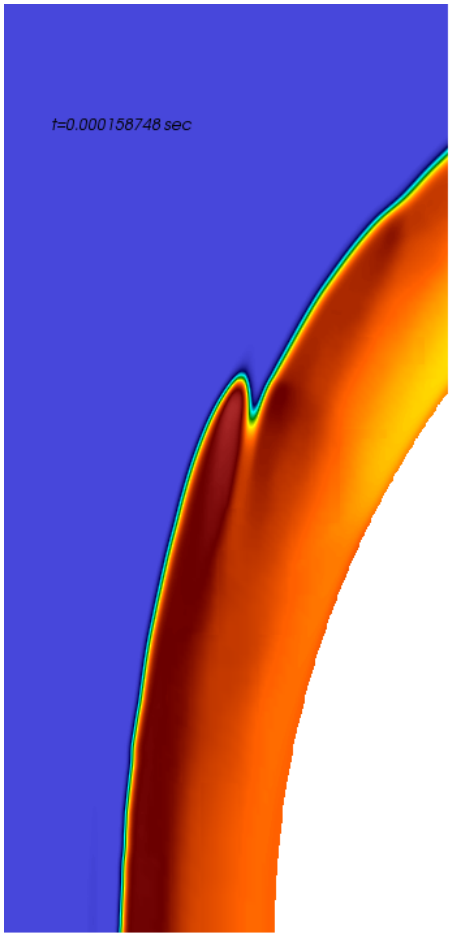
Schlieren of density



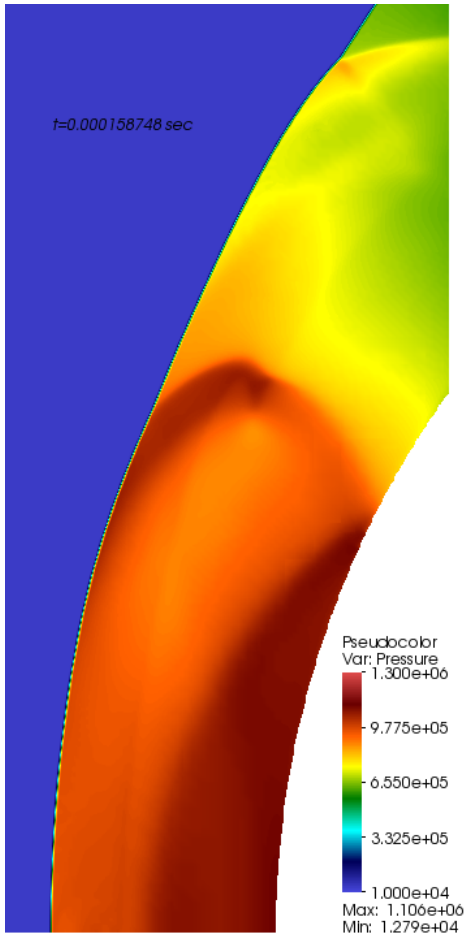
Temperature



Mass fraction OH

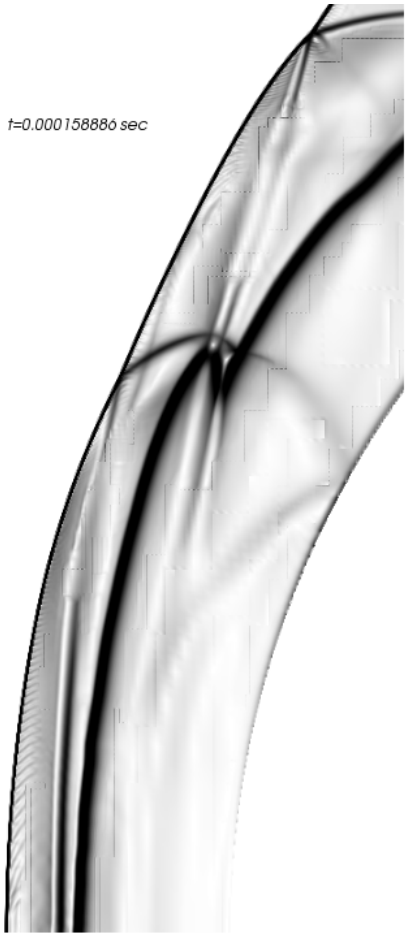


Pressure

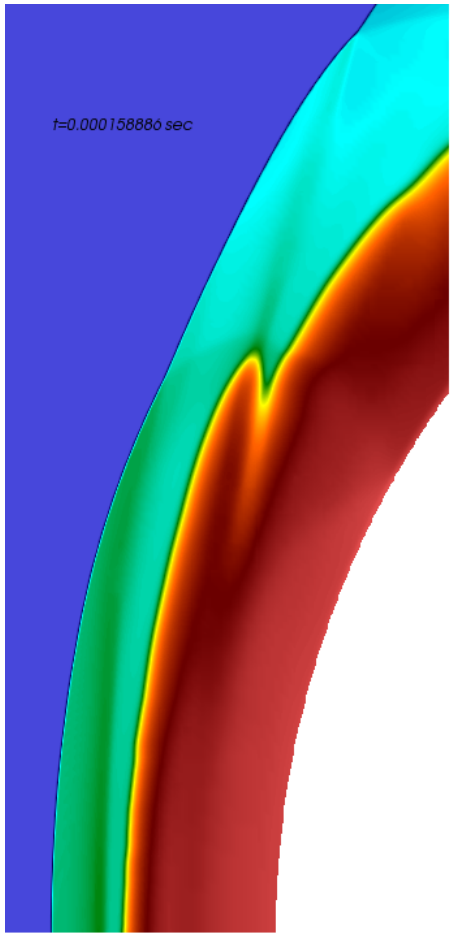


Oscillation mechanism

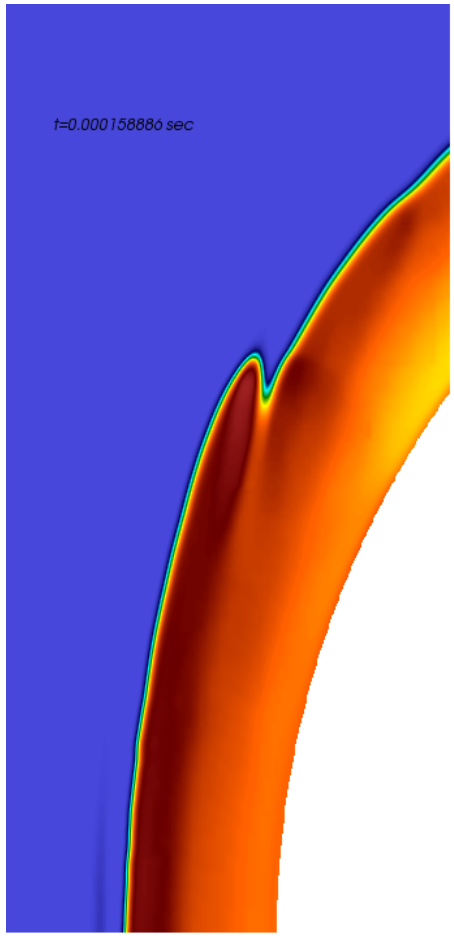
Schlieren of density



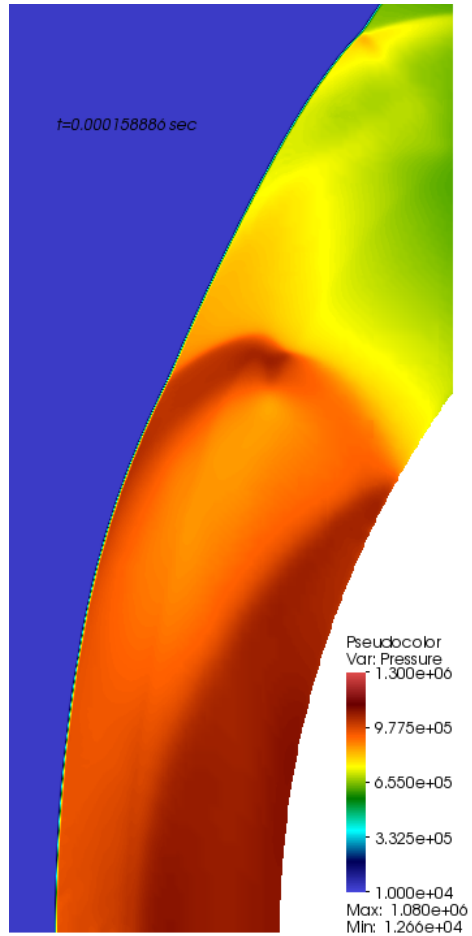
Temperature



Mass fraction OH

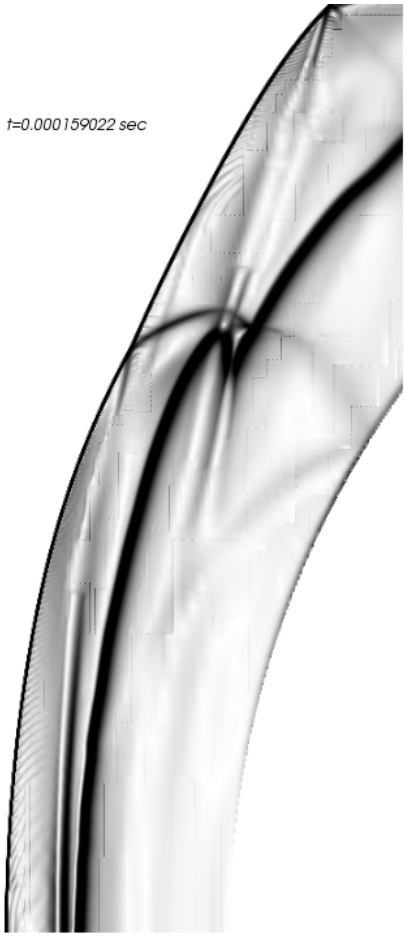


Pressure

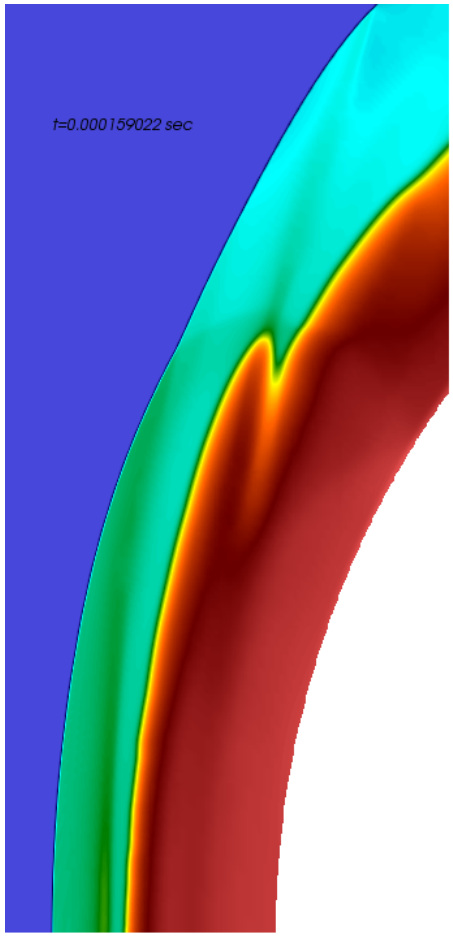


Oscillation mechanism

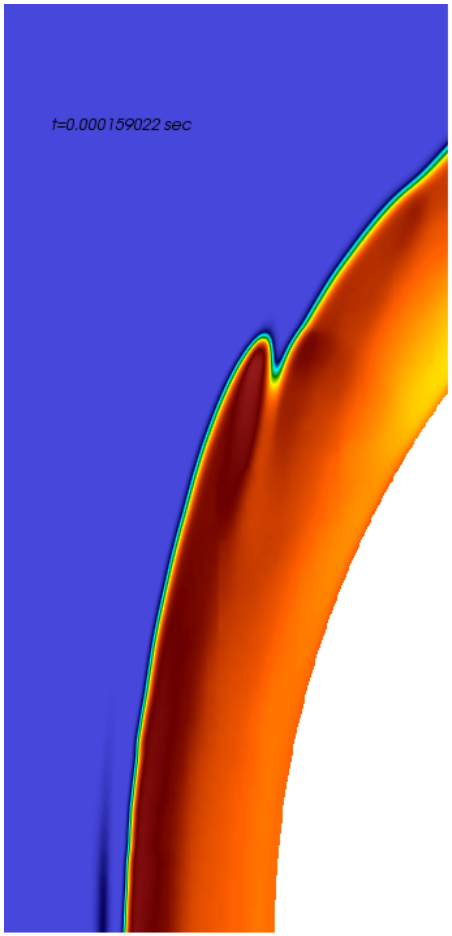
Schlieren of density



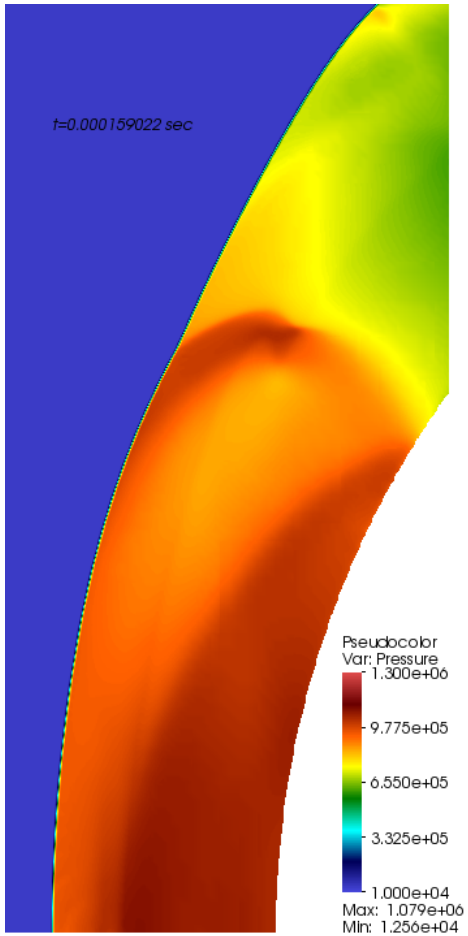
Temperature



Mass fraction OH

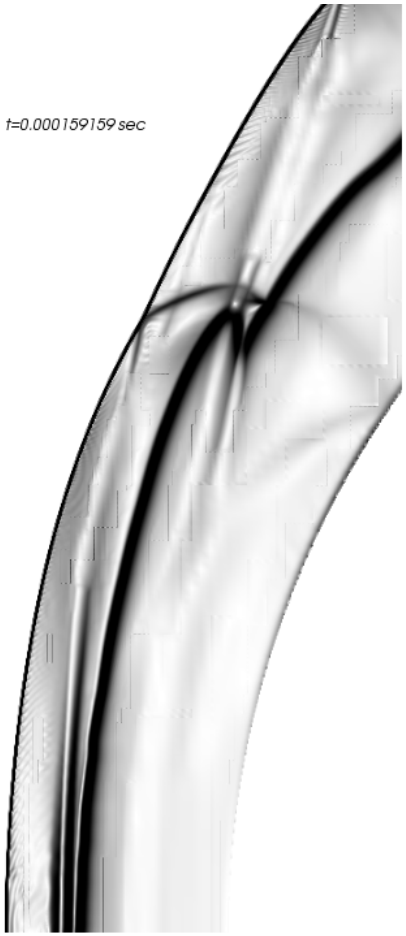


Pressure

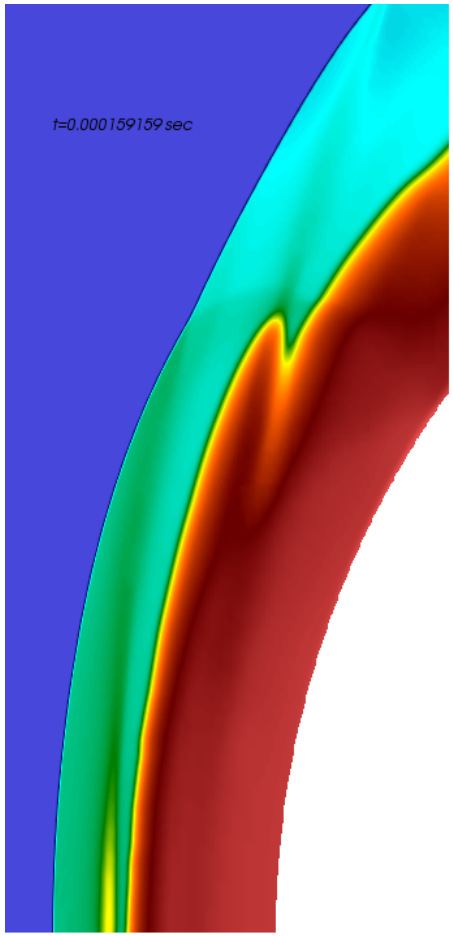


Oscillation mechanism

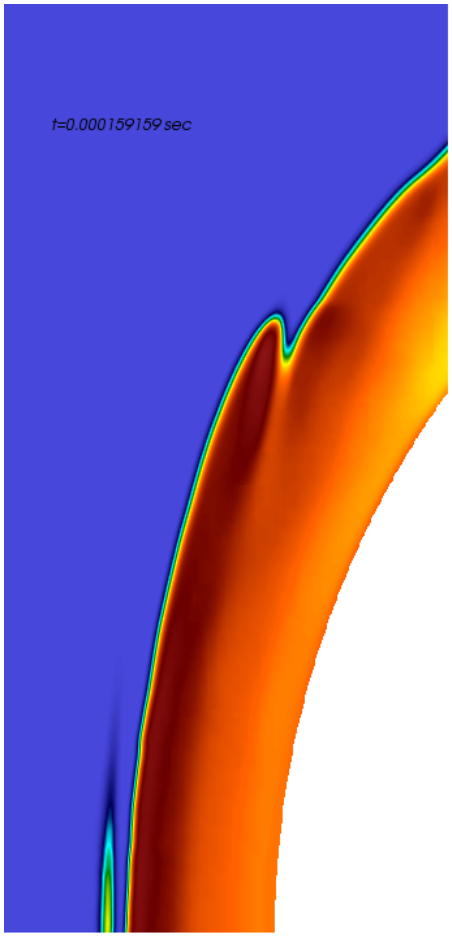
Schlieren of density



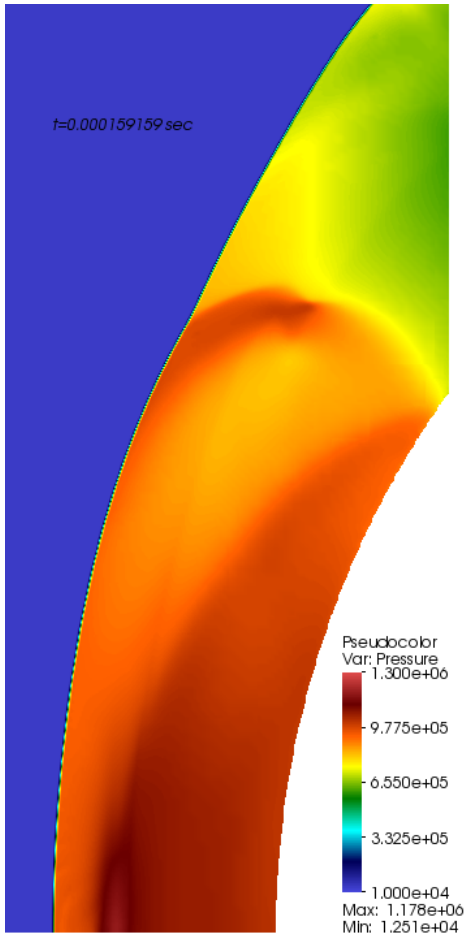
Temperature



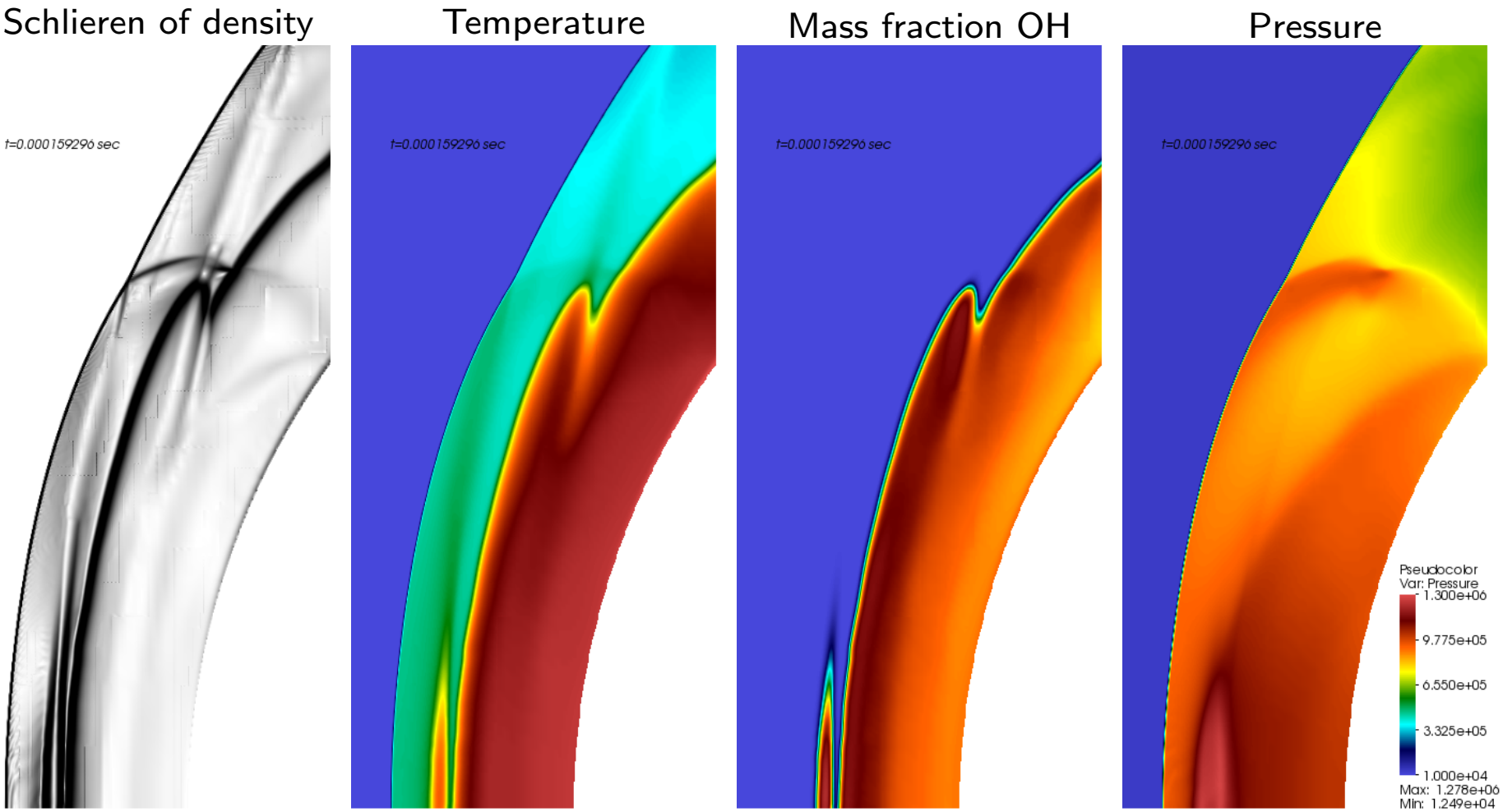
Mass fraction OH



Pressure

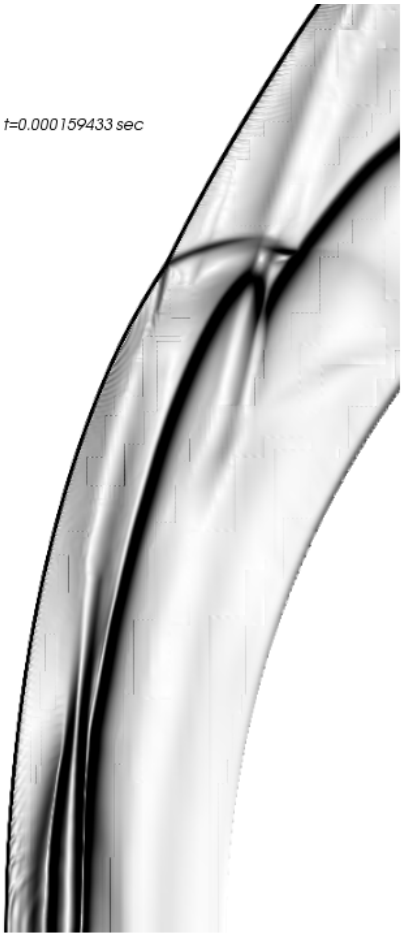


Oscillation mechanism

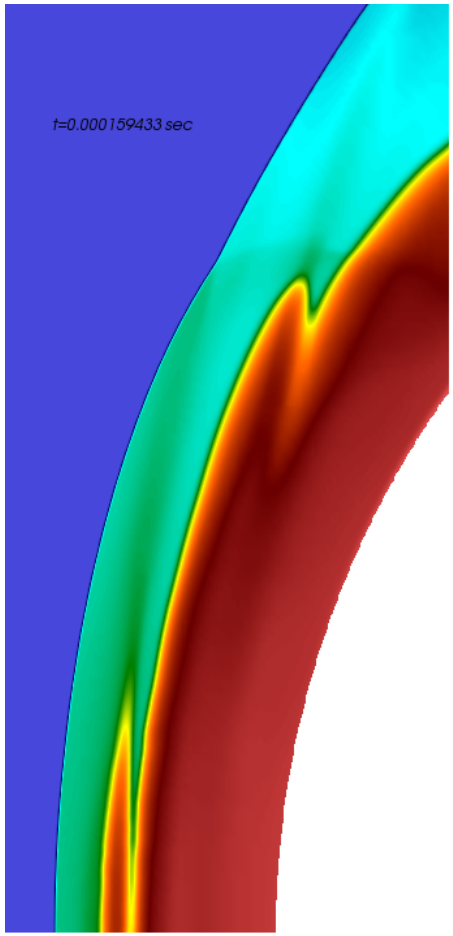


Oscillation mechanism

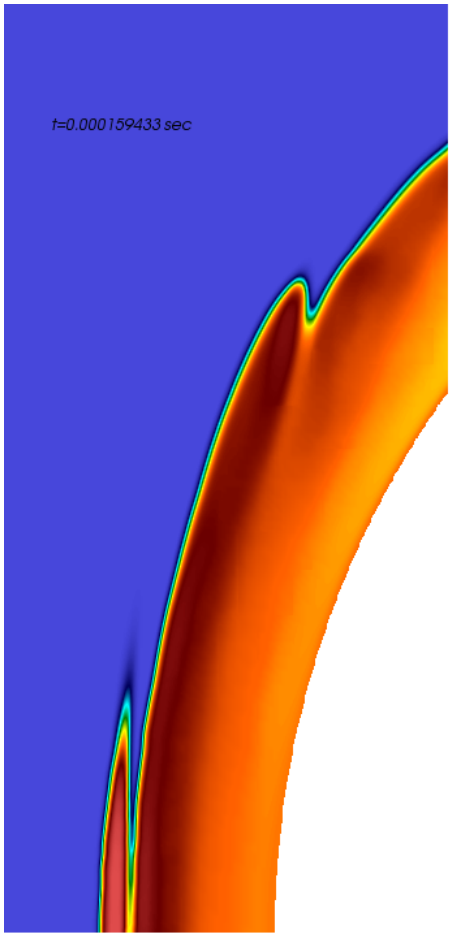
Schlieren of density



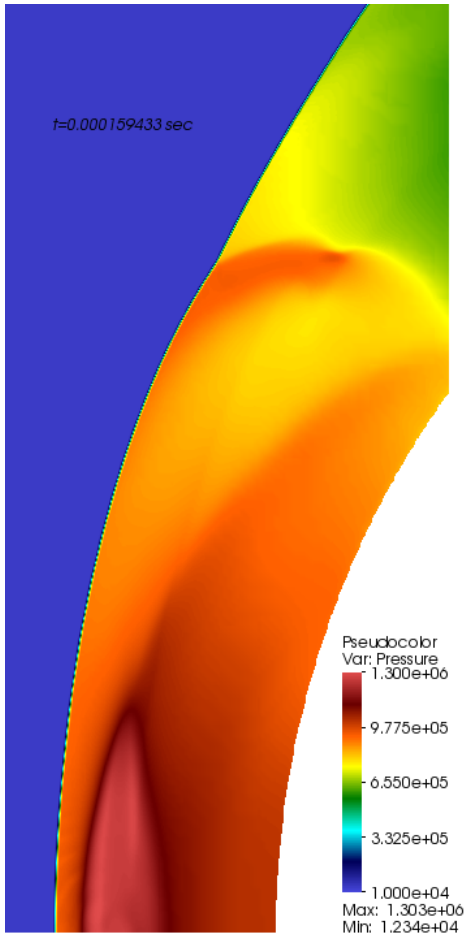
Temperature



Mass fraction OH

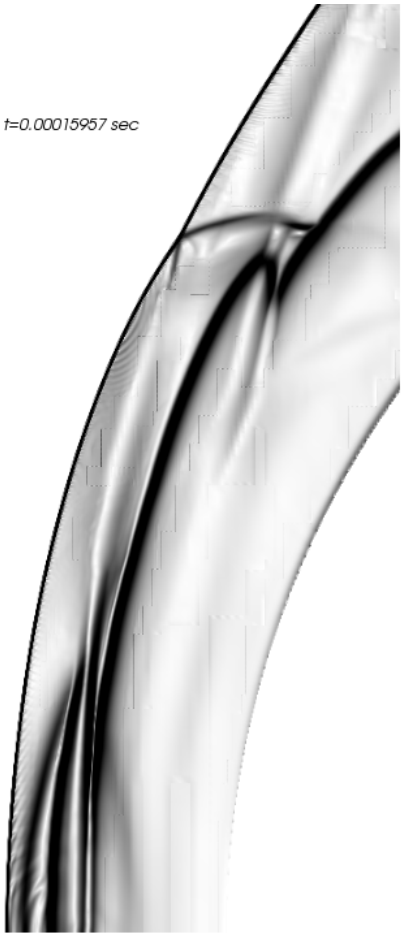


Pressure

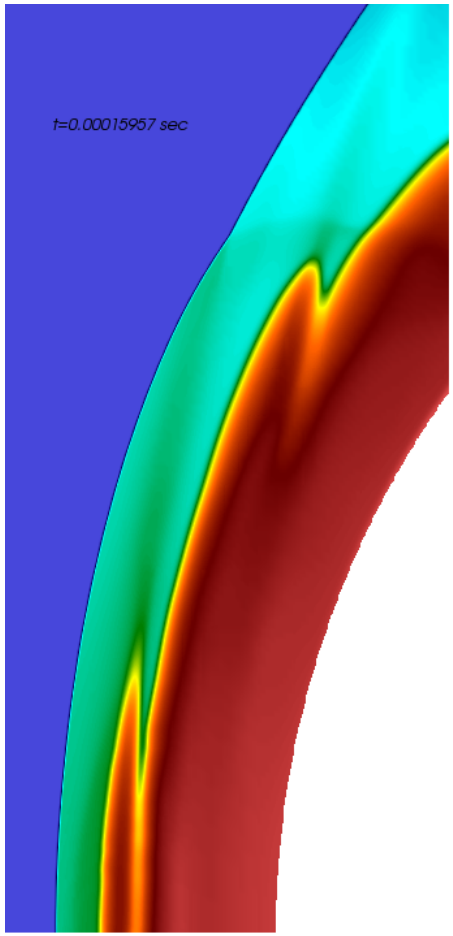


Oscillation mechanism

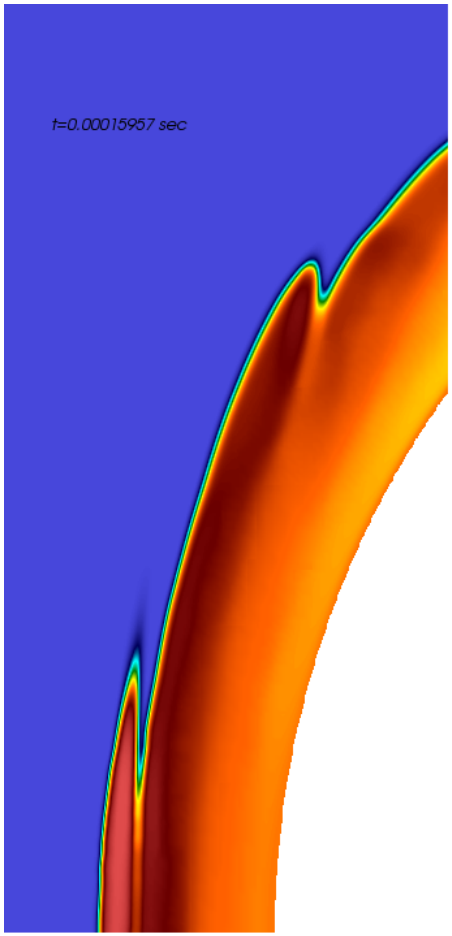
Schlieren of density



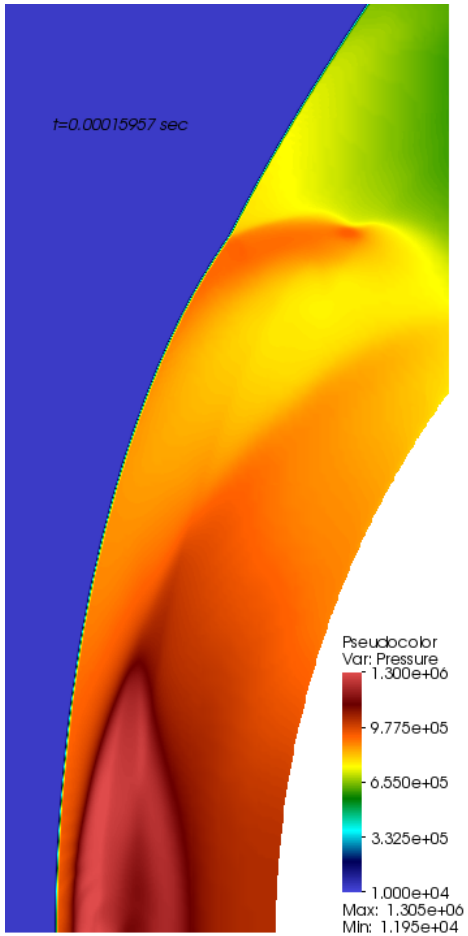
Temperature



Mass fraction OH

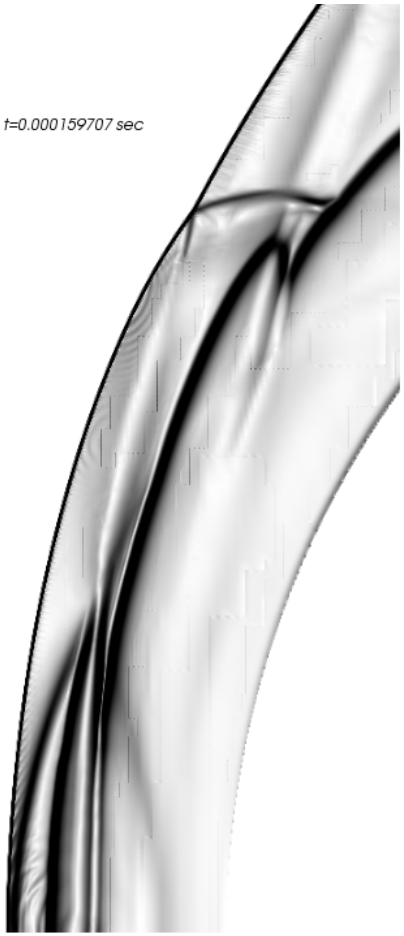


Pressure

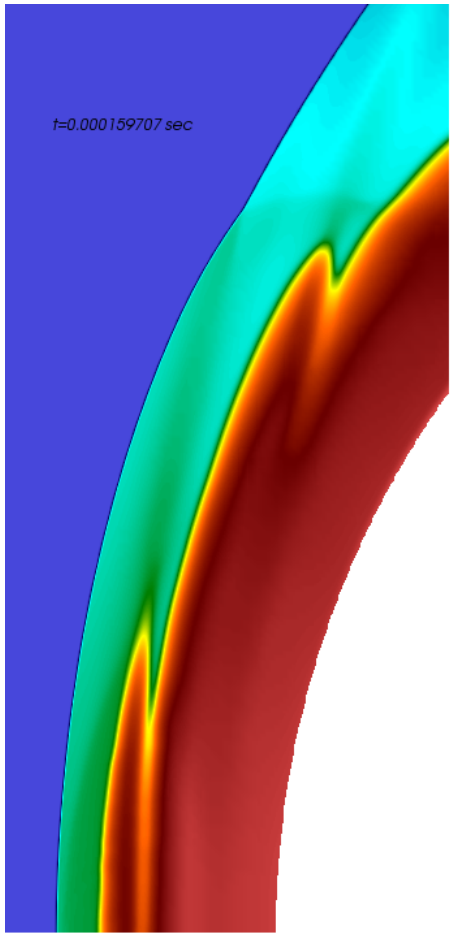


Oscillation mechanism

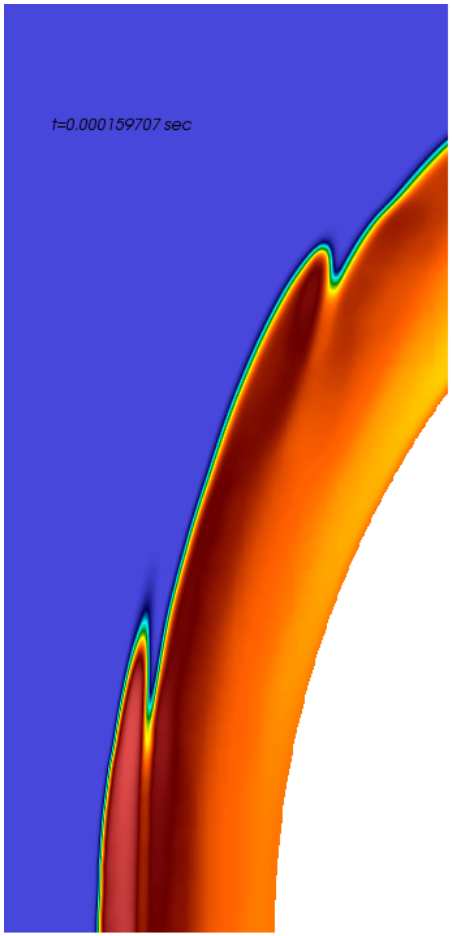
Schlieren of density



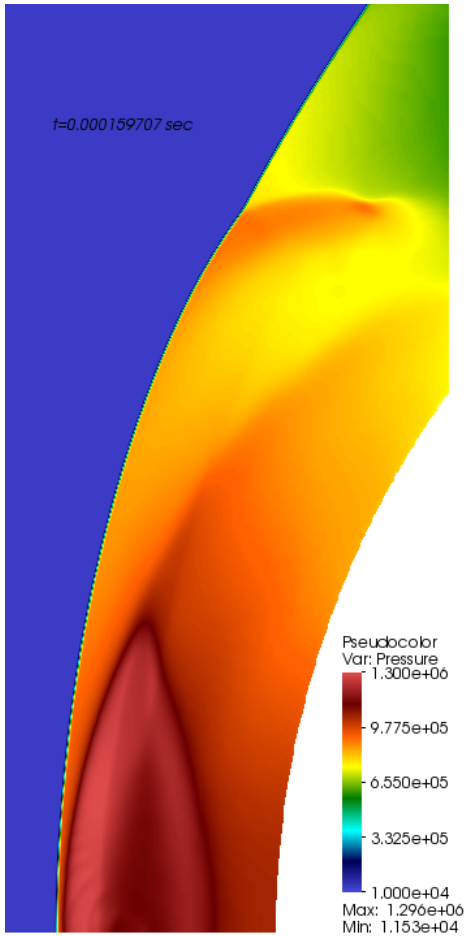
Temperature



Mass fraction OH

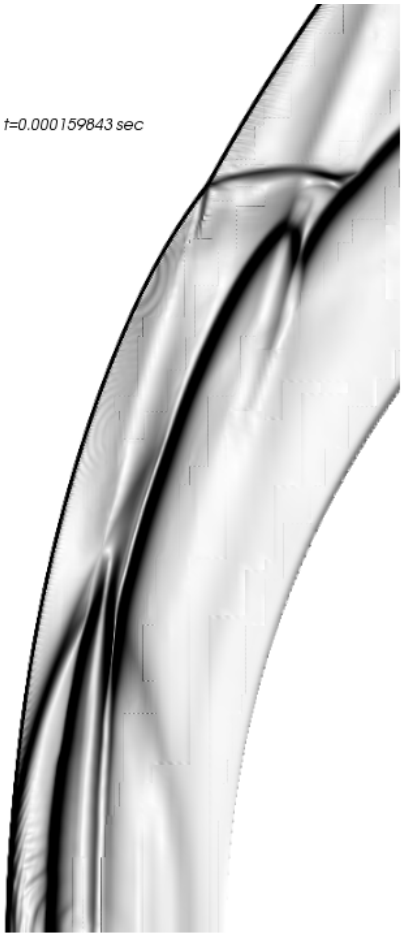


Pressure

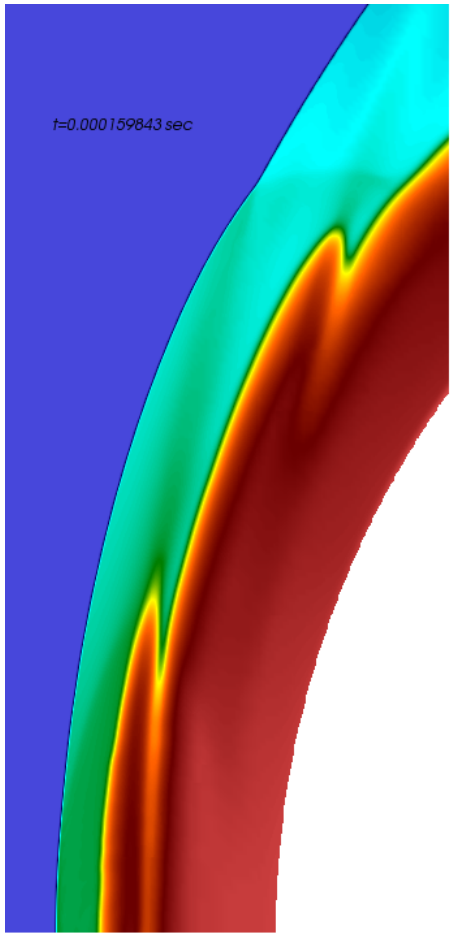


Oscillation mechanism

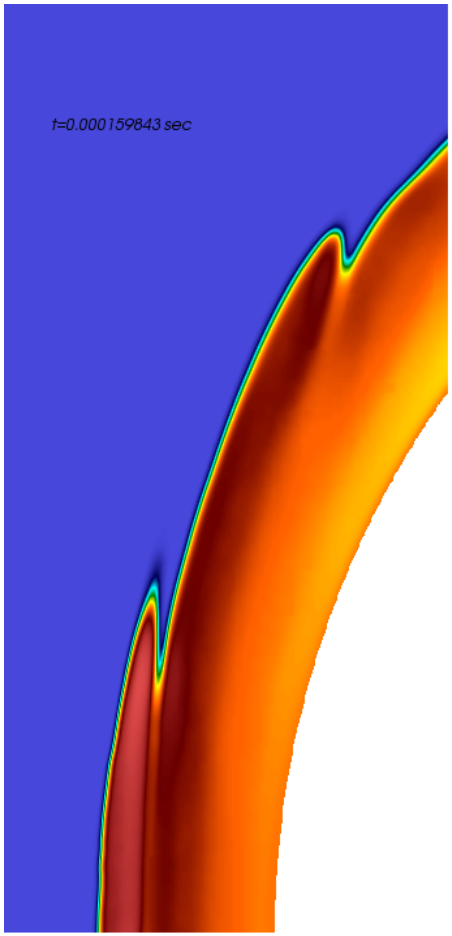
Schlieren of density



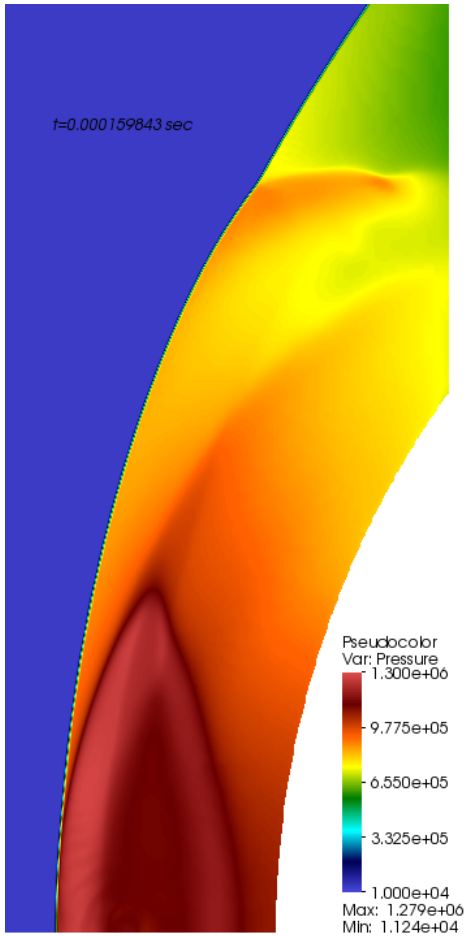
Temperature



Mass fraction OH

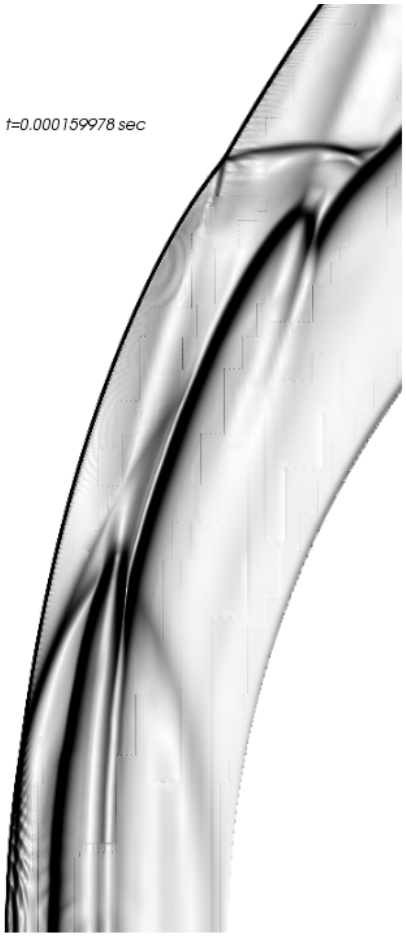


Pressure

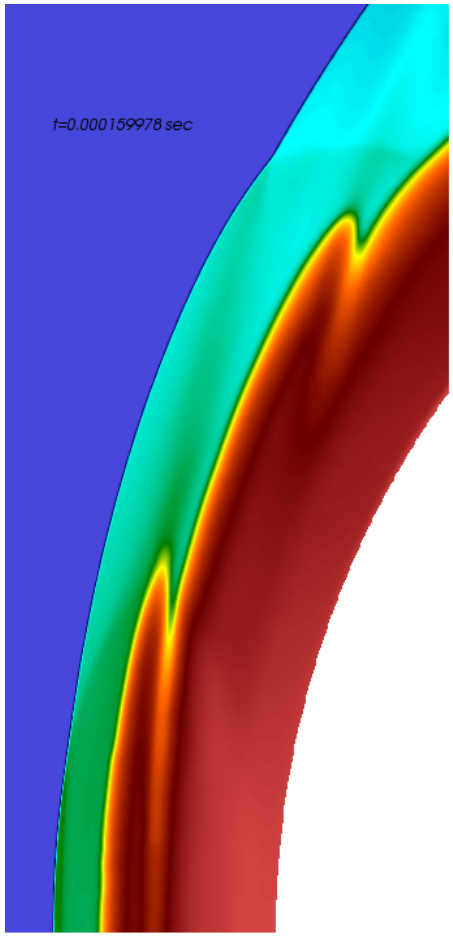


Oscillation mechanism

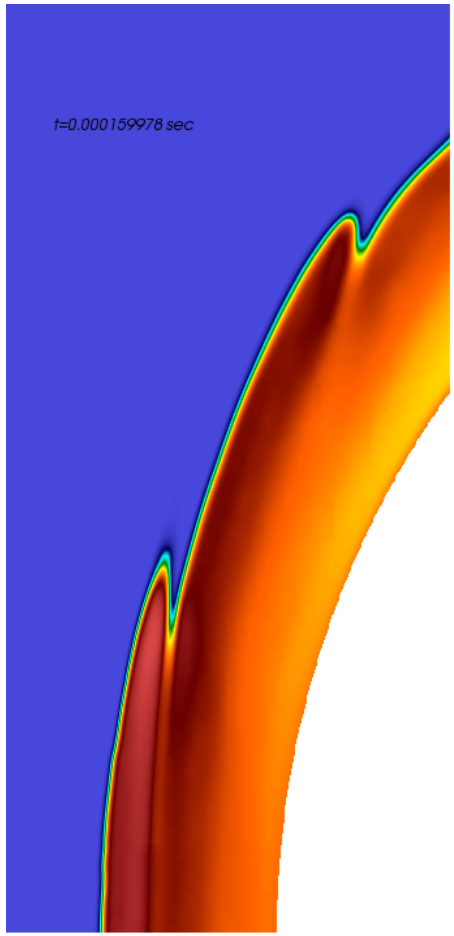
Schlieren of density



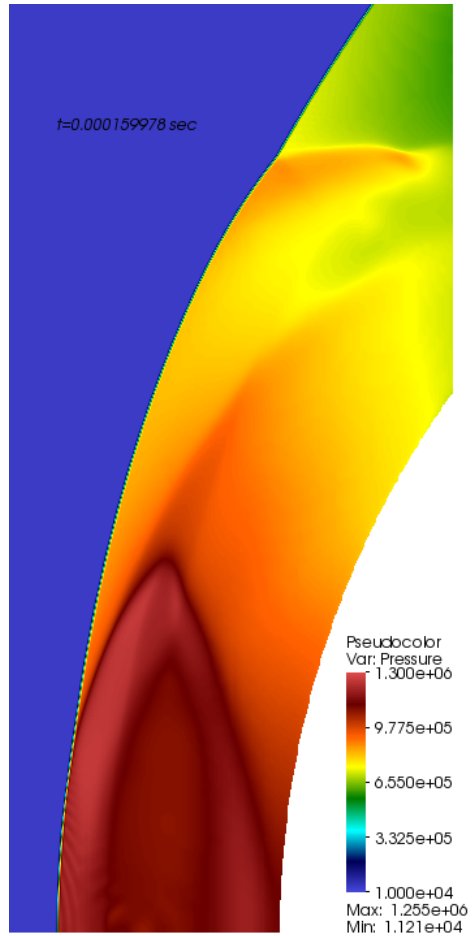
Temperature



Mass fraction OH

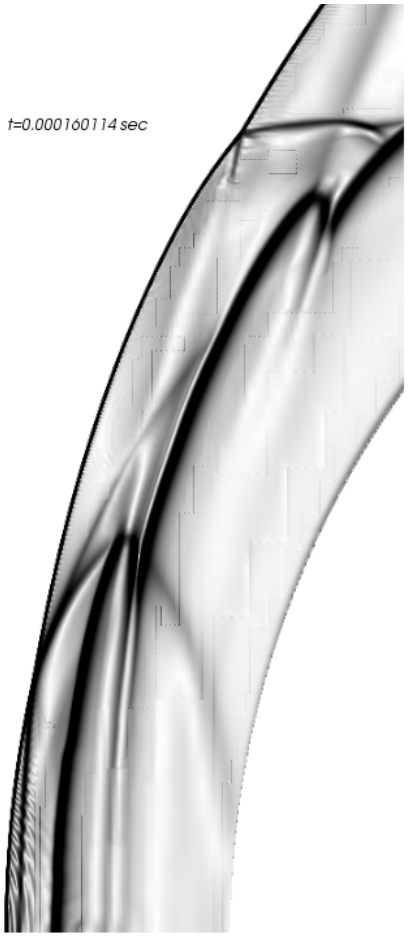


Pressure

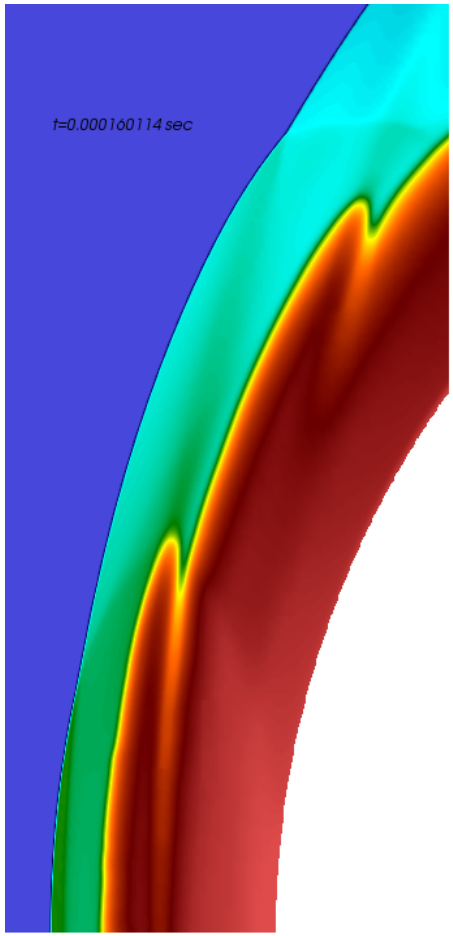


Oscillation mechanism

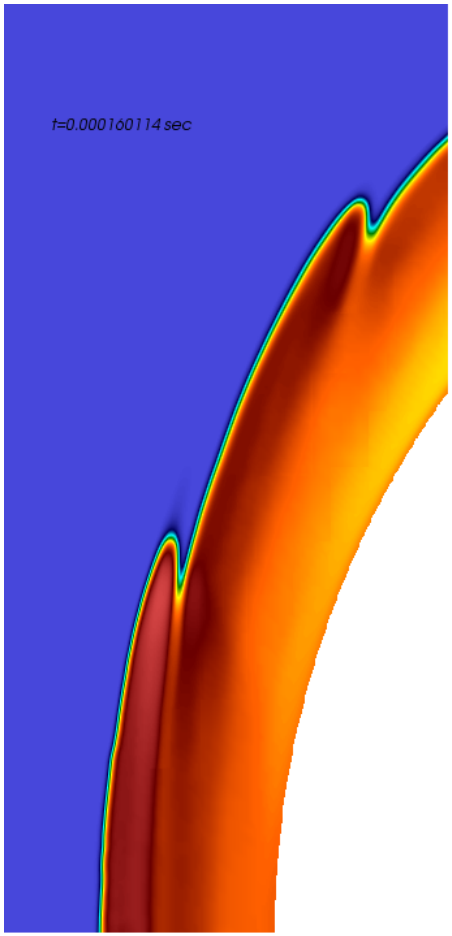
Schlieren of density



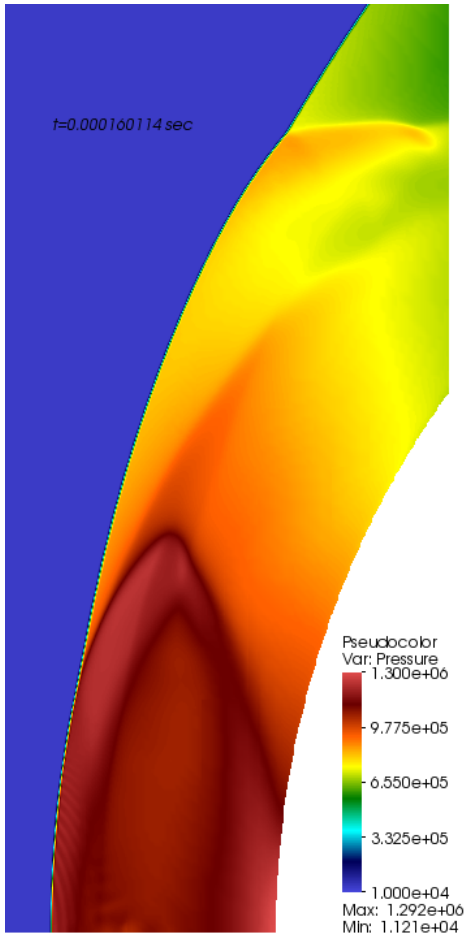
Temperature



Mass fraction OH

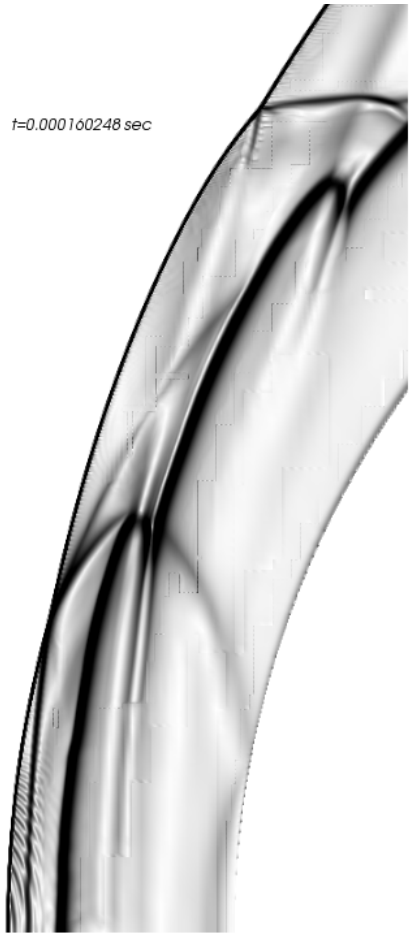


Pressure

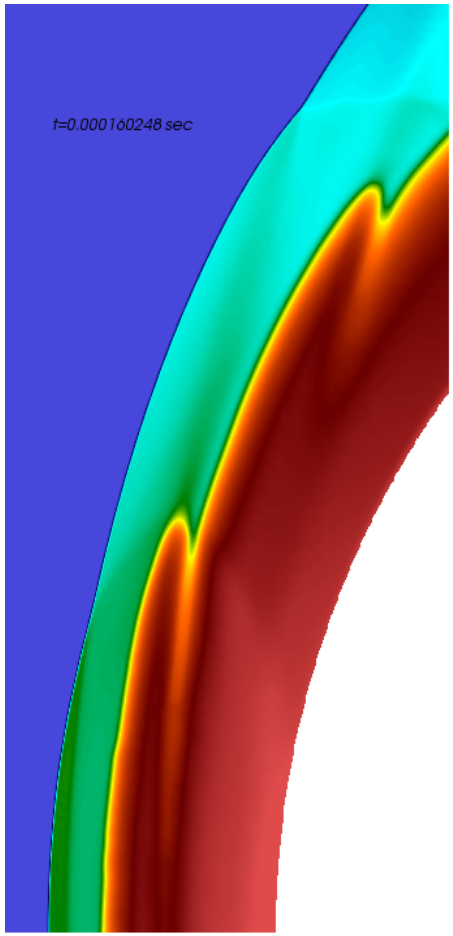


Oscillation mechanism

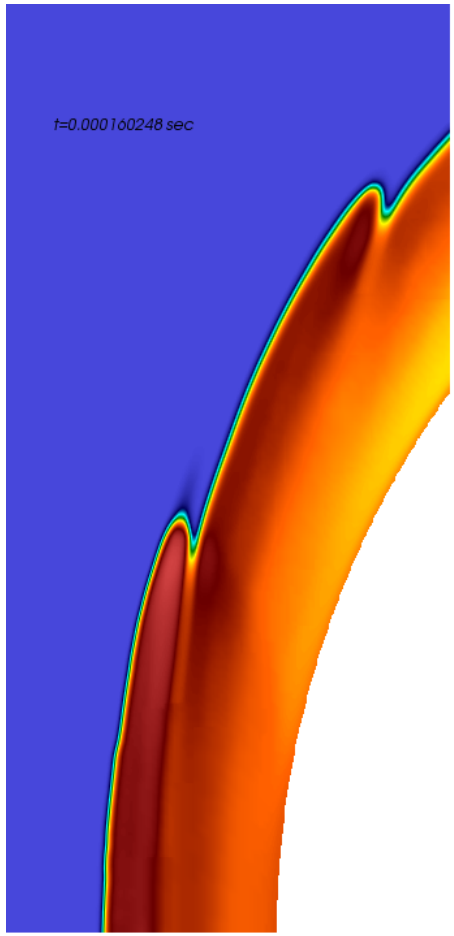
Schlieren of density



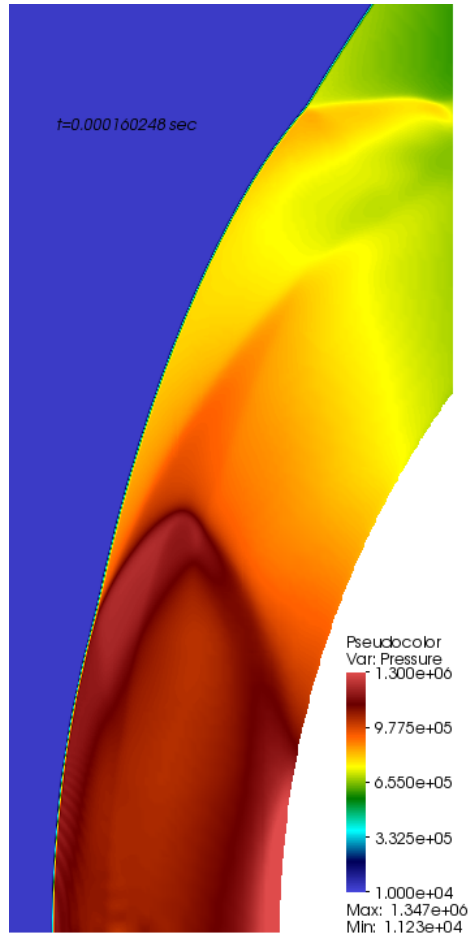
Temperature



Mass fraction OH

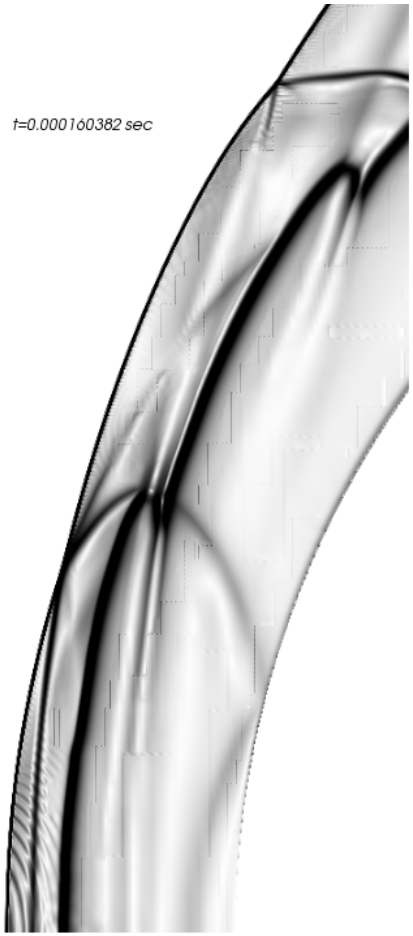


Pressure

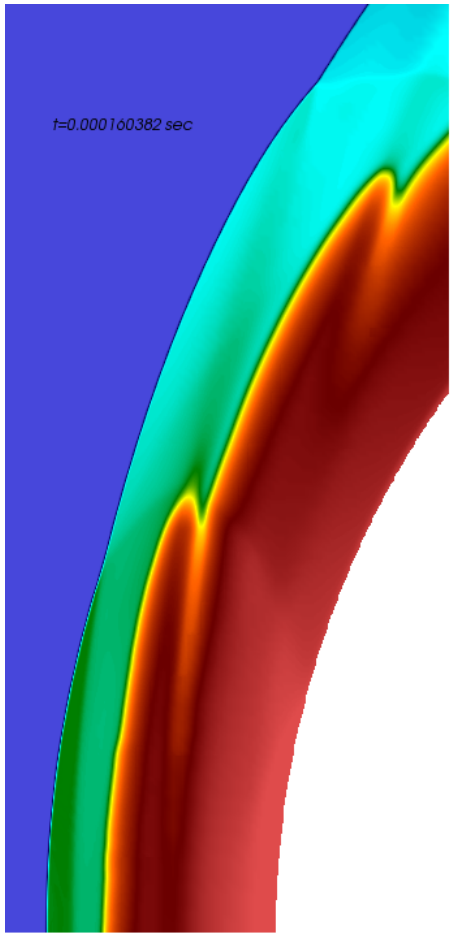


Oscillation mechanism

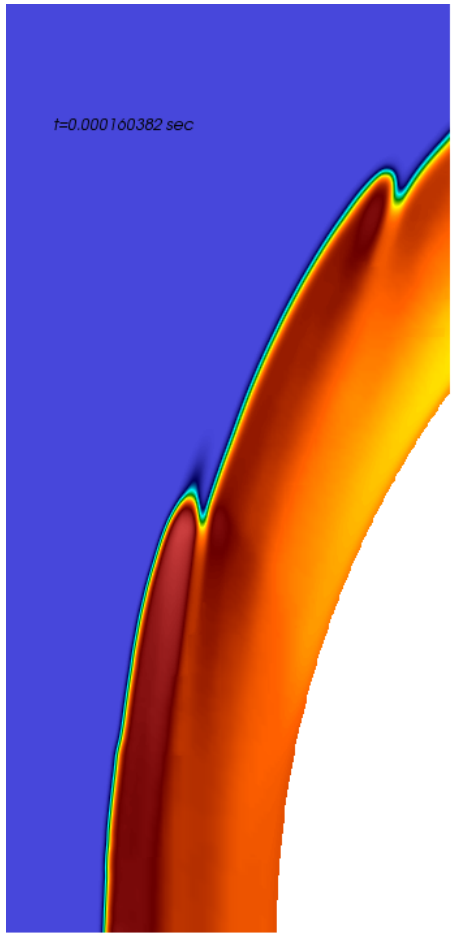
Schlieren of density



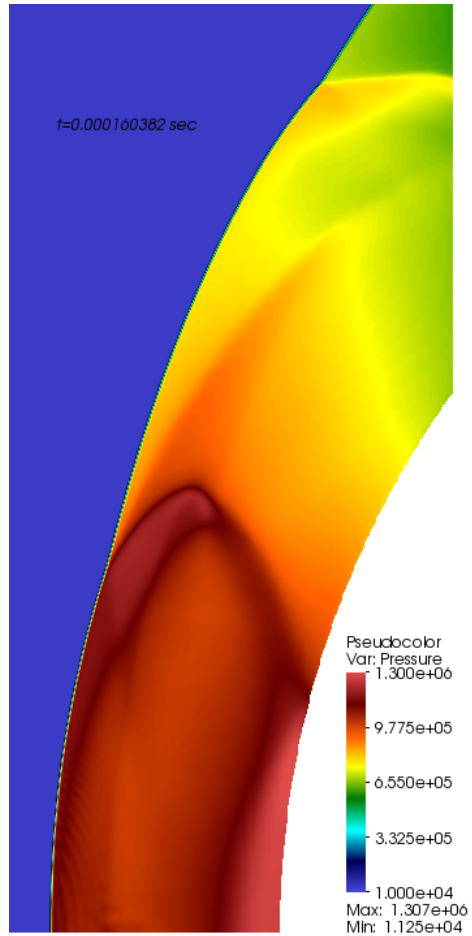
Temperature



Mass fraction OH

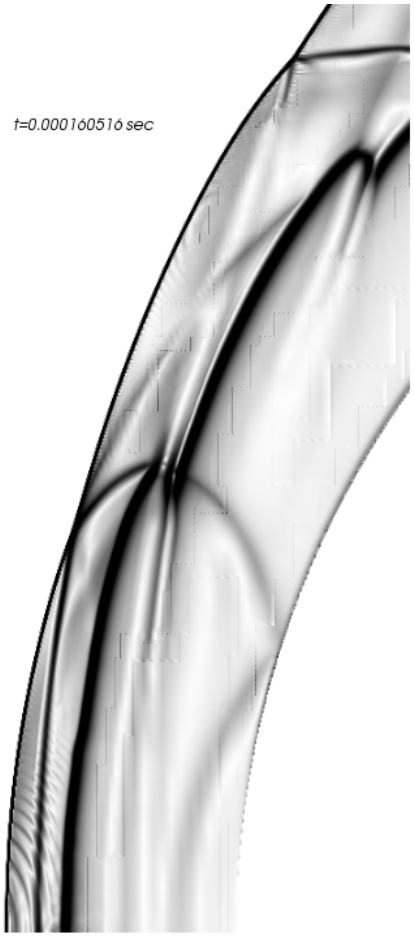


Pressure

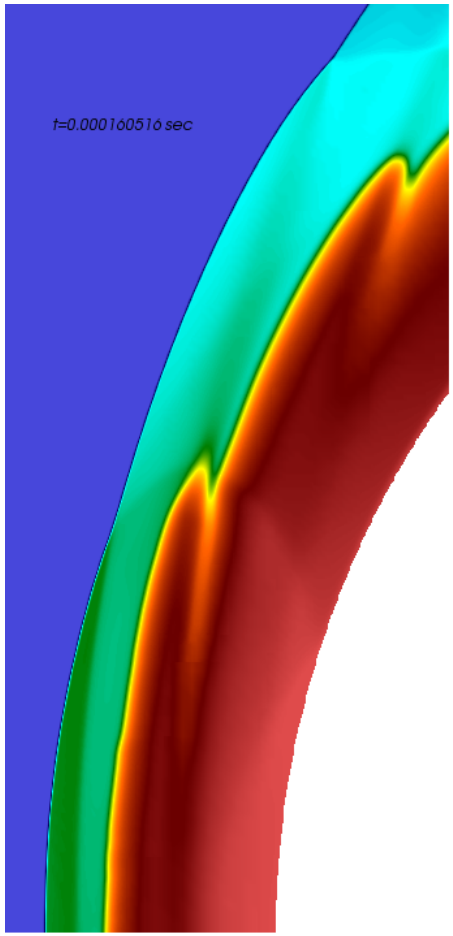


Oscillation mechanism

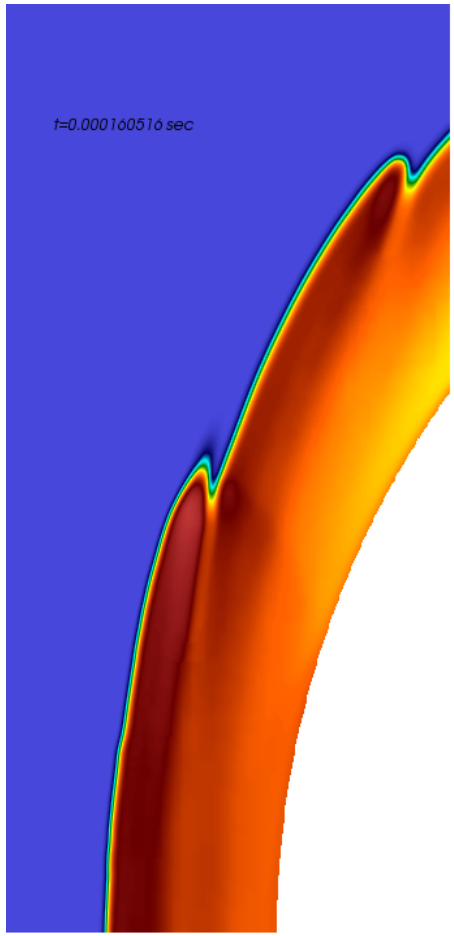
Schlieren of density



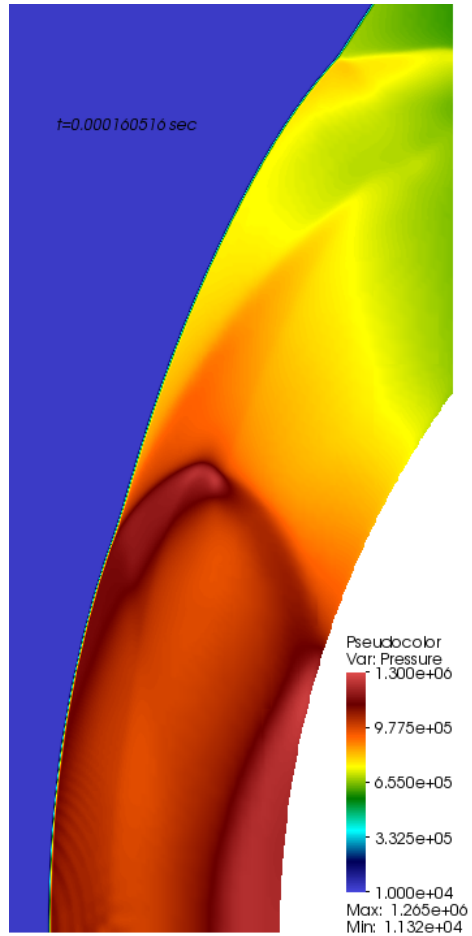
Temperature



Mass fraction OH

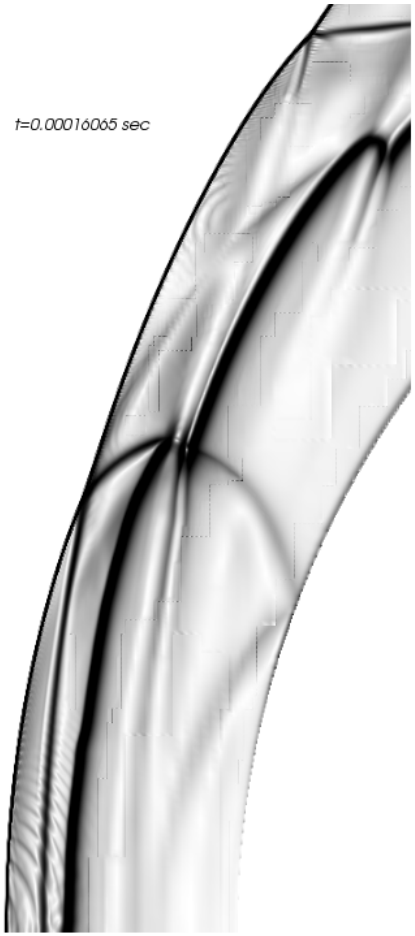


Pressure

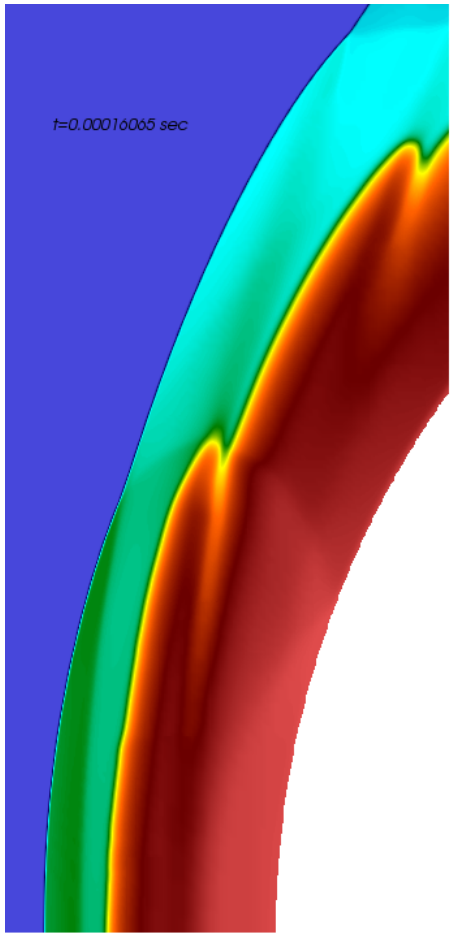


Oscillation mechanism

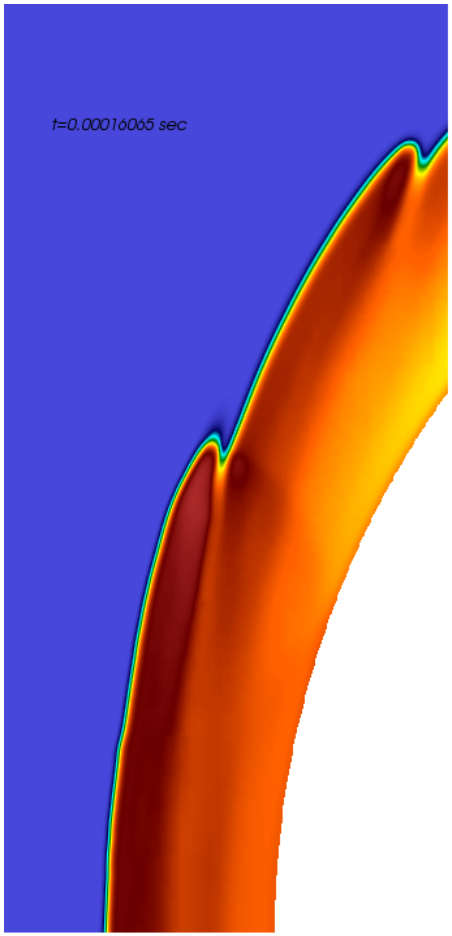
Schlieren of density



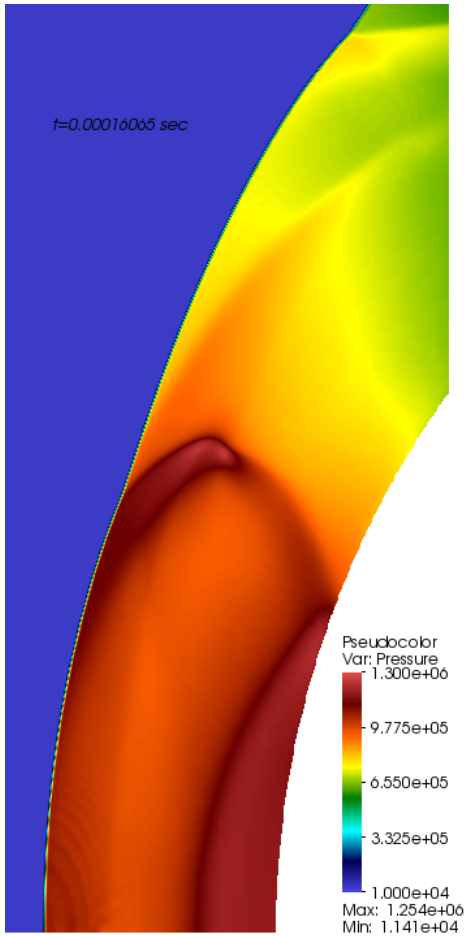
Temperature



Mass fraction OH

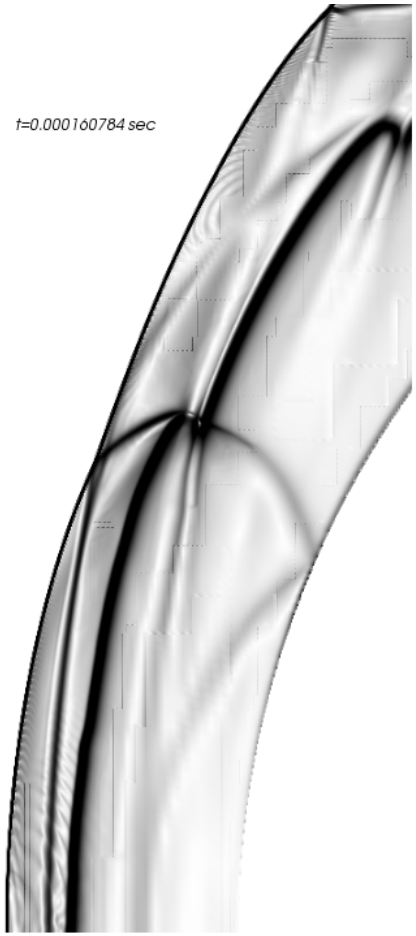


Pressure

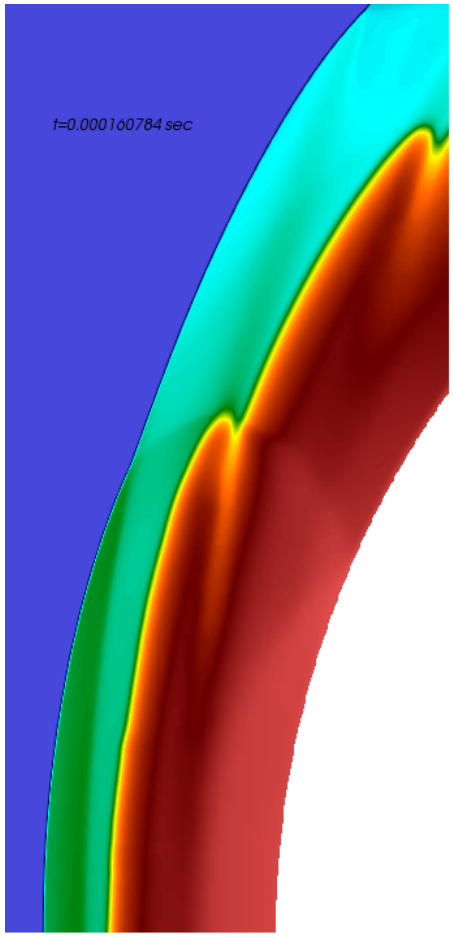


Oscillation mechanism

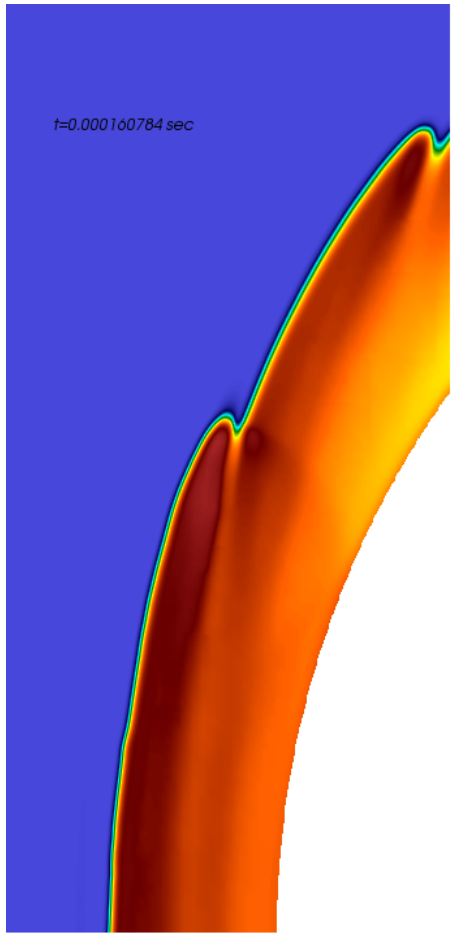
Schlieren of density



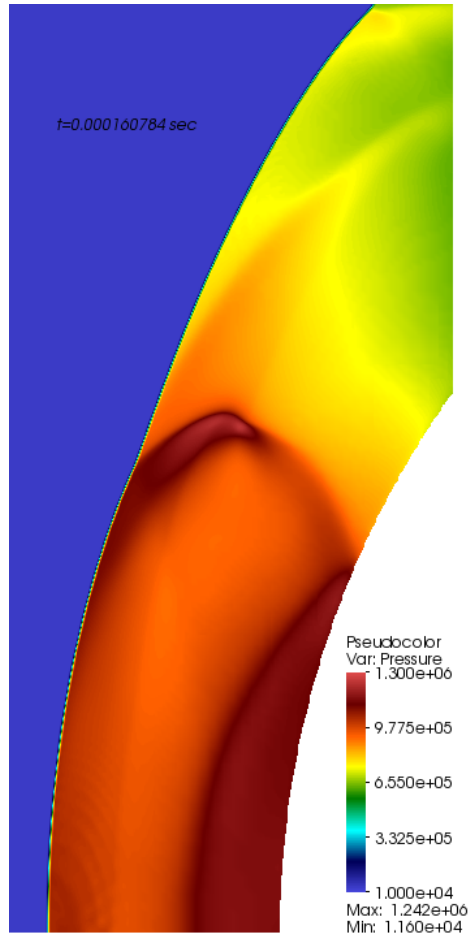
Temperature



Mass fraction OH

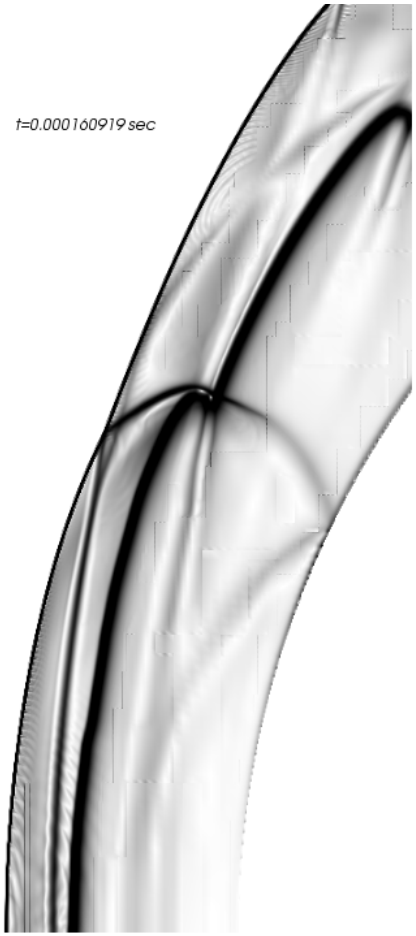


Pressure

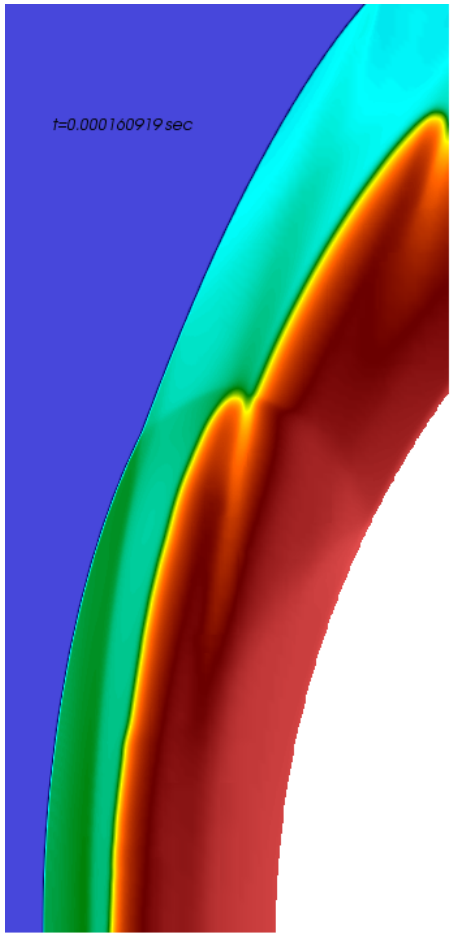


Oscillation mechanism

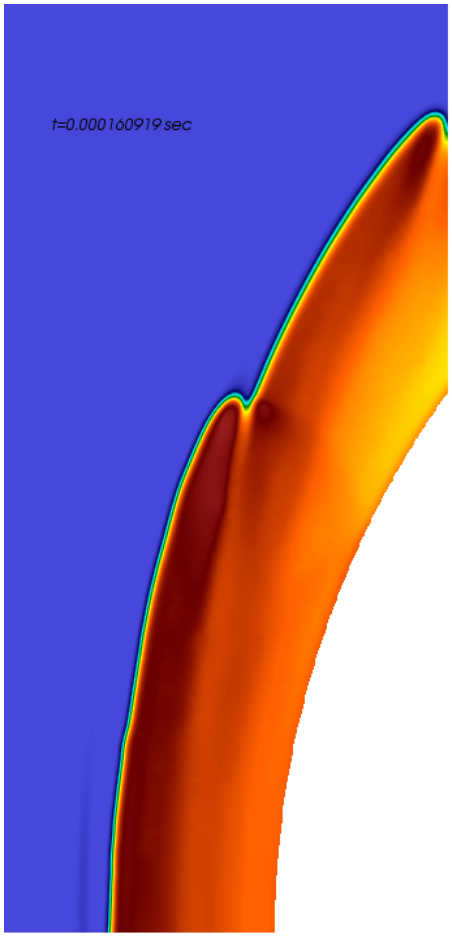
Schlieren of density



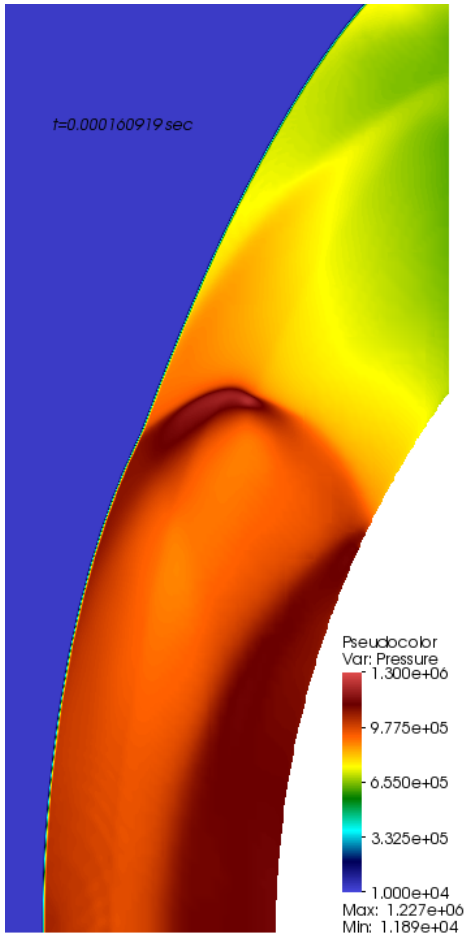
Temperature



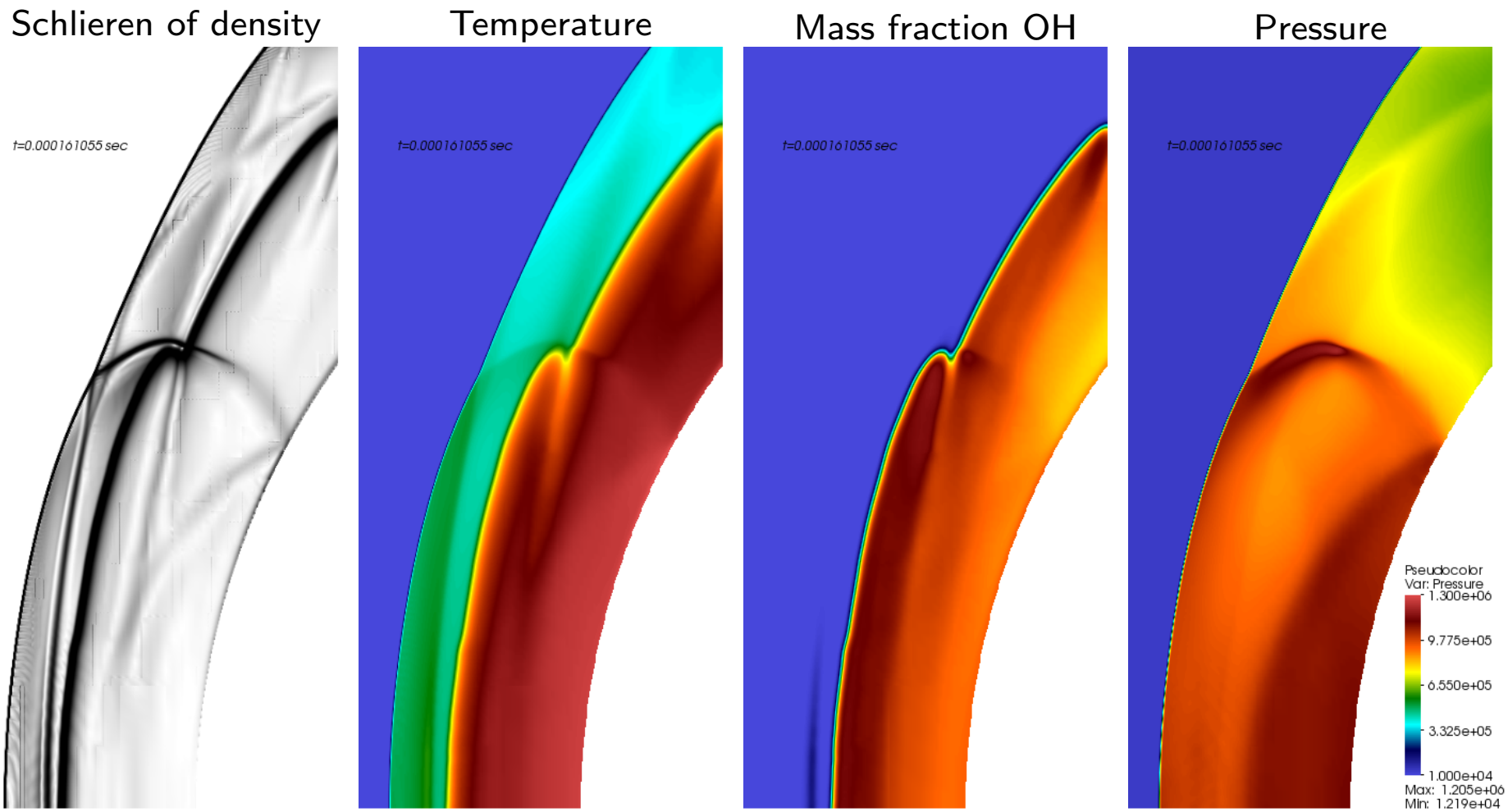
Mass fraction OH



Pressure



Oscillation mechanism

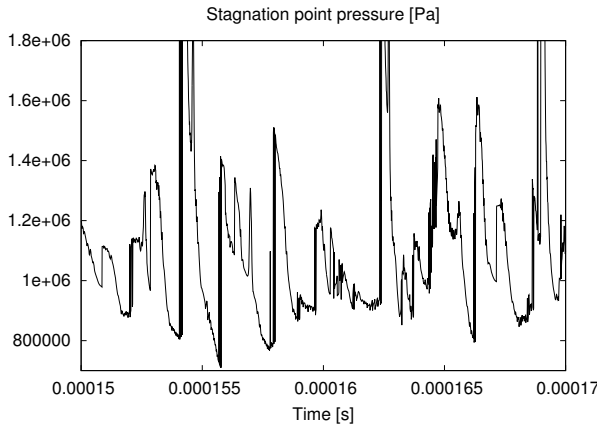


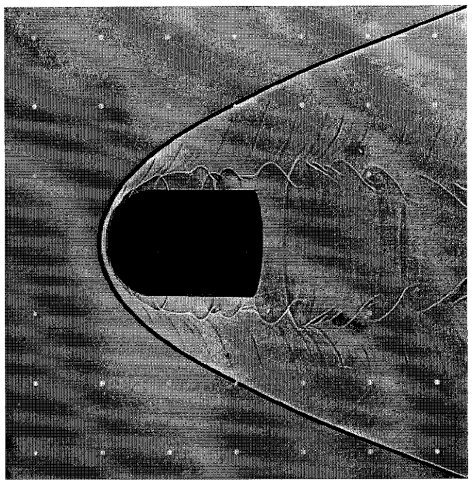
- Oscillation created by accelerated reaction due to slip line from previous triple point

Inviscid case – $M = 4.48$

- 4048 iterations with CFL=0.9 to $t = 170\,\mu\mathrm{s}$
- Oscillation frequency in last $20\,\mu\mathrm{s}$: $\sim 395\,\mathrm{kHz}$
- Experimental value: $\sim 425\,\mathrm{kHz}$

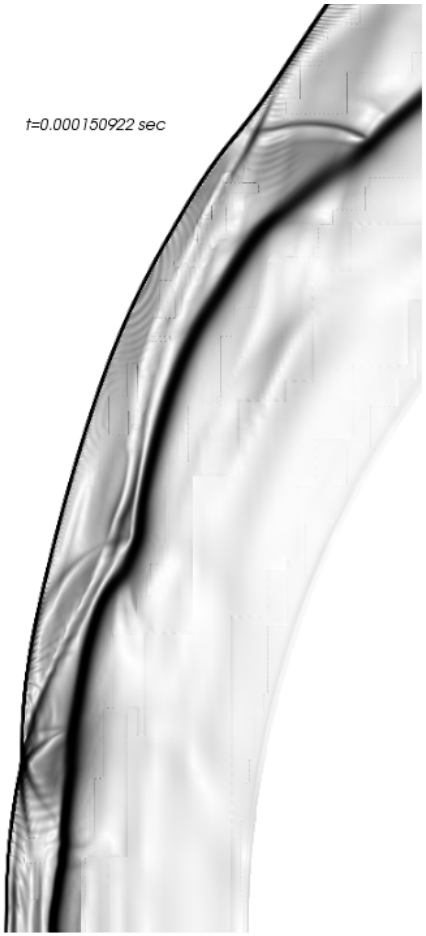
Schlieren plot of density



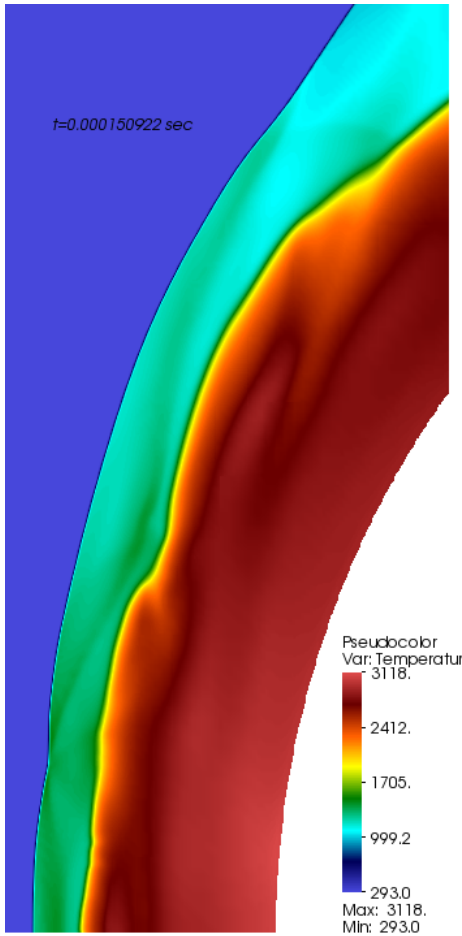


Perturbed oscillation mechanism

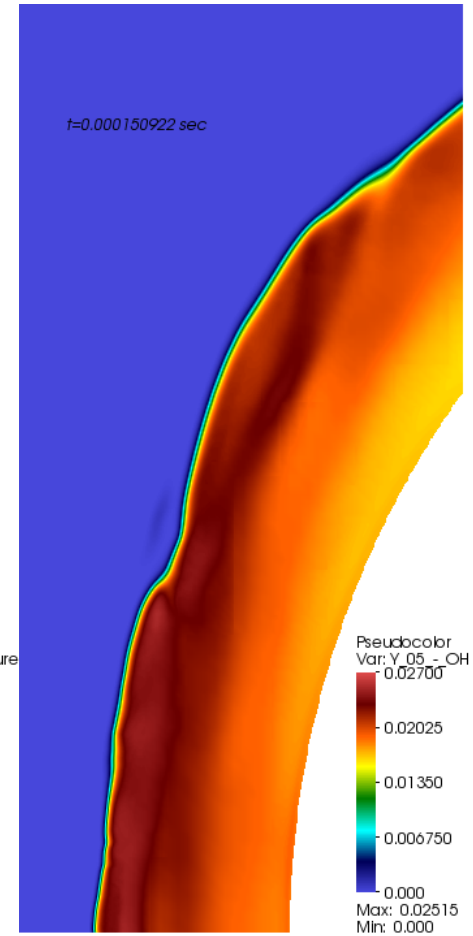
Schlieren of density



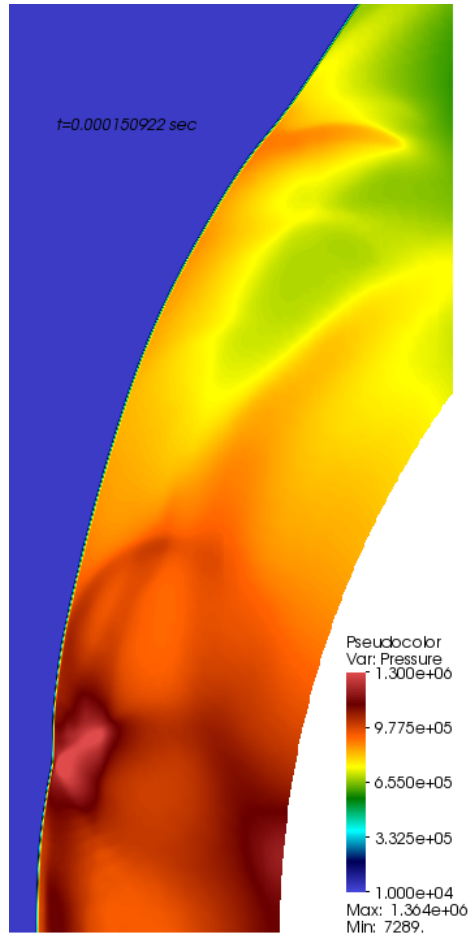
Temperature



Mass fraction OH

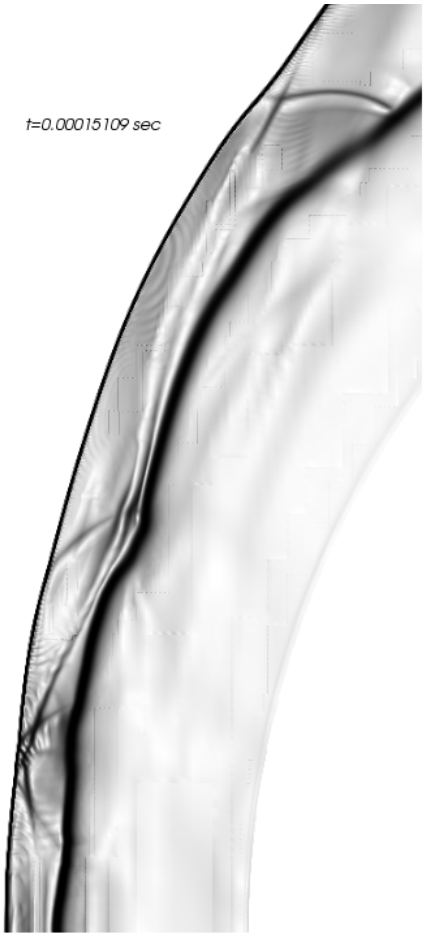


Pressure

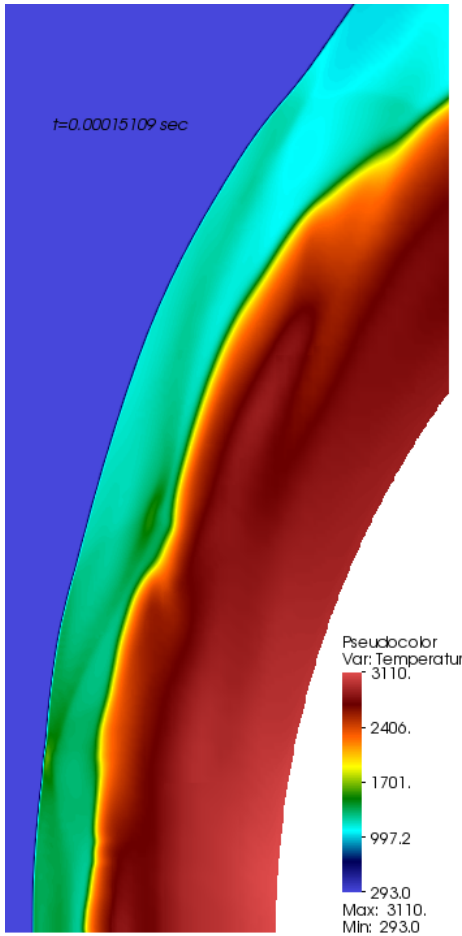


Perturbed oscillation mechanism

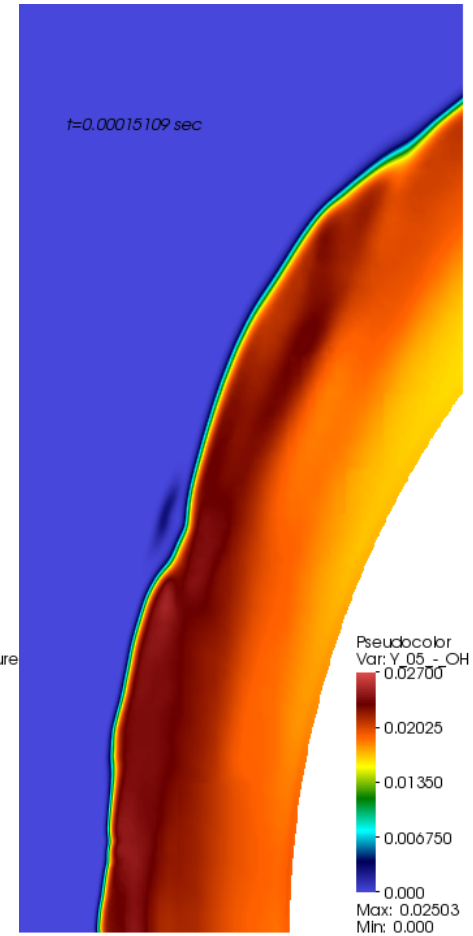
Schlieren of density



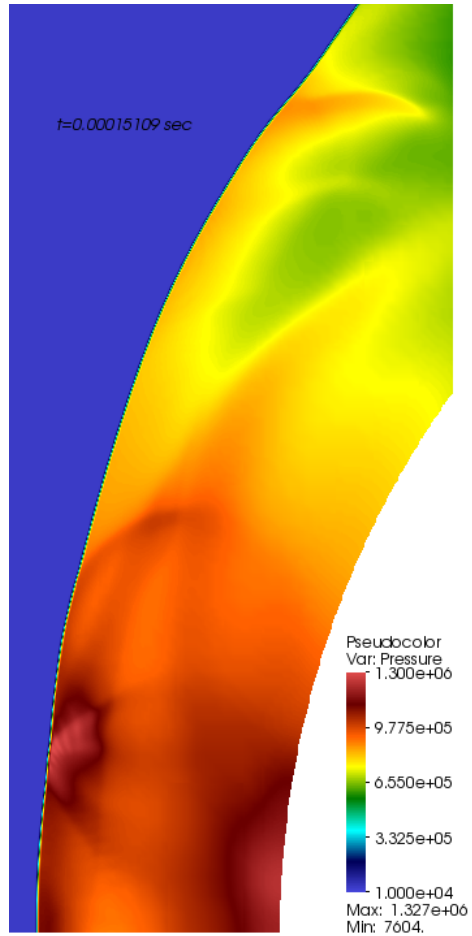
Temperature



Mass fraction OH

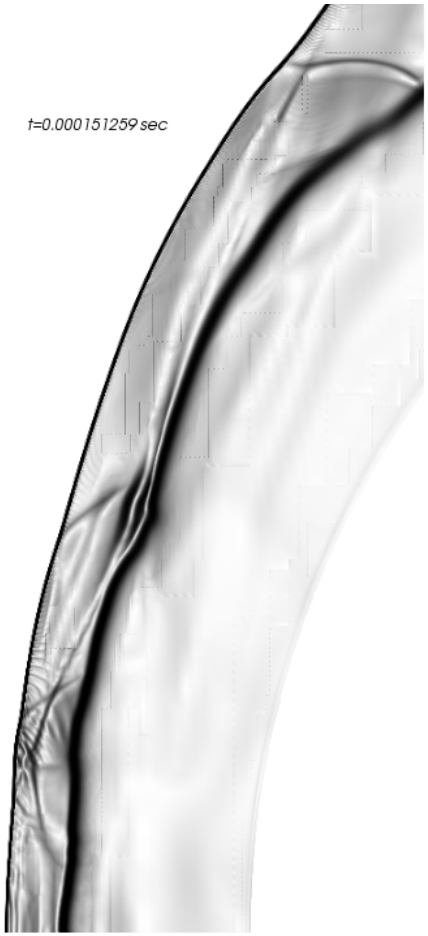


Pressure

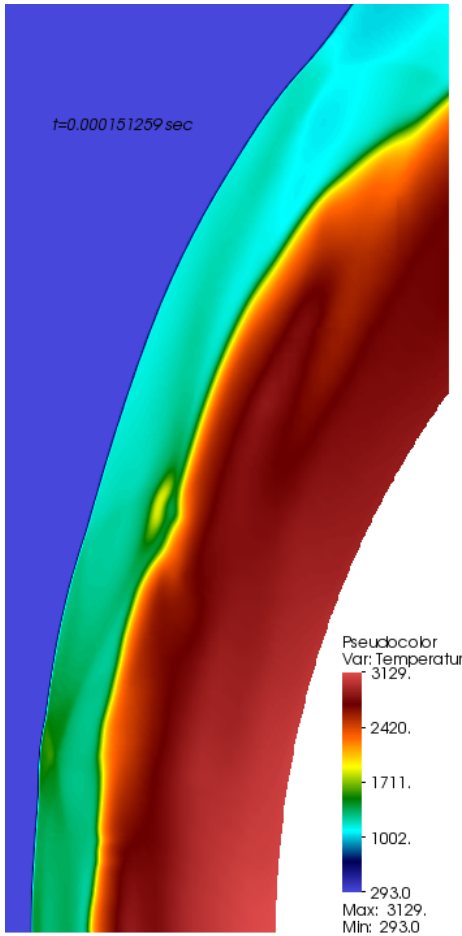


Perturbed oscillation mechanism

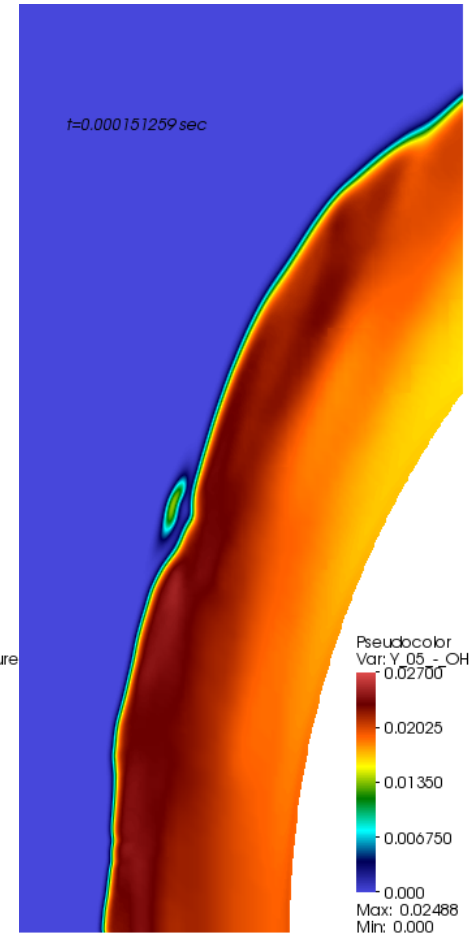
Schlieren of density



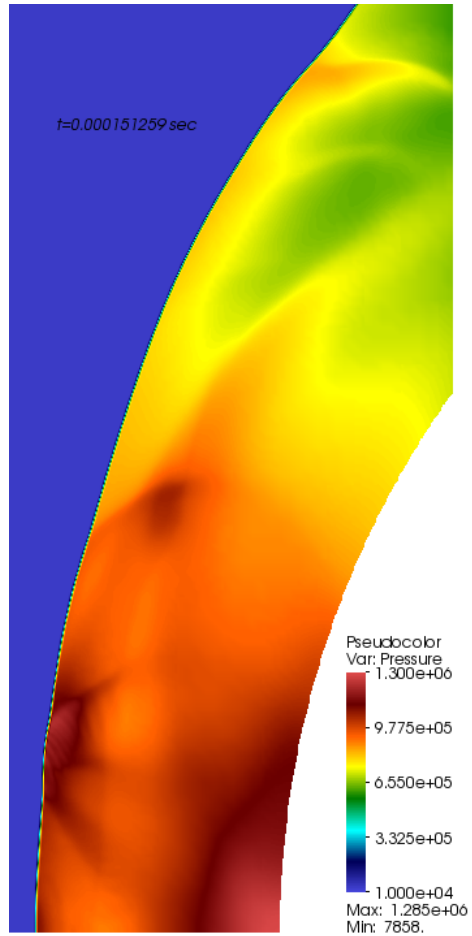
Temperature



Mass fraction OH

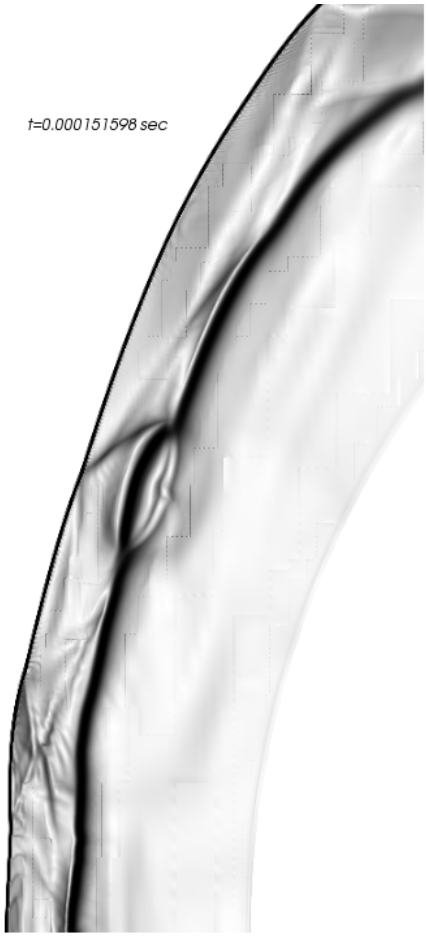


Pressure

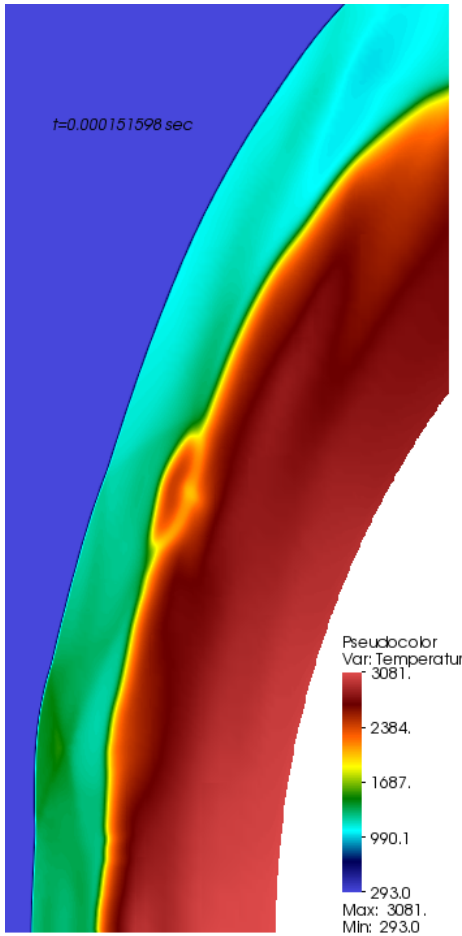


Perturbed oscillation mechanism

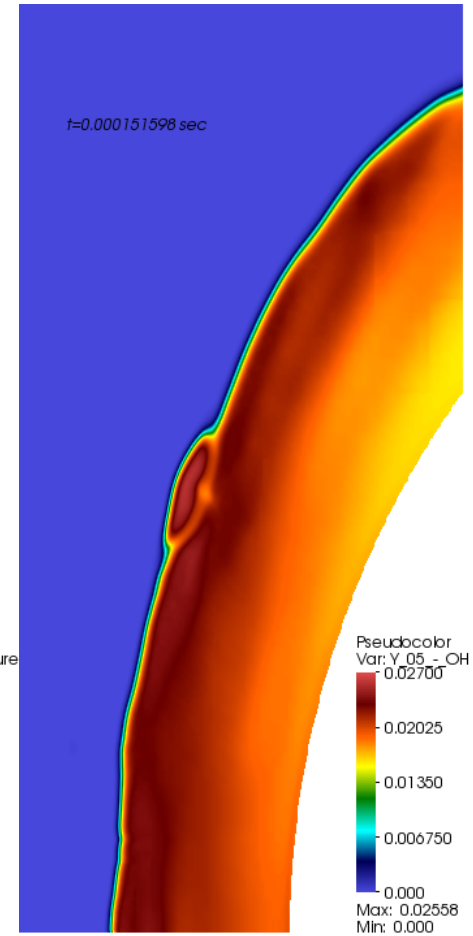
Schlieren of density



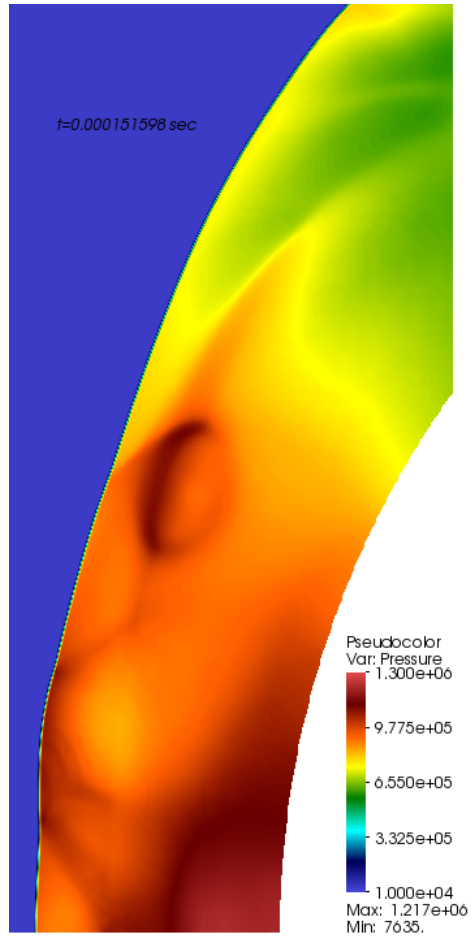
Temperature



Mass fraction OH

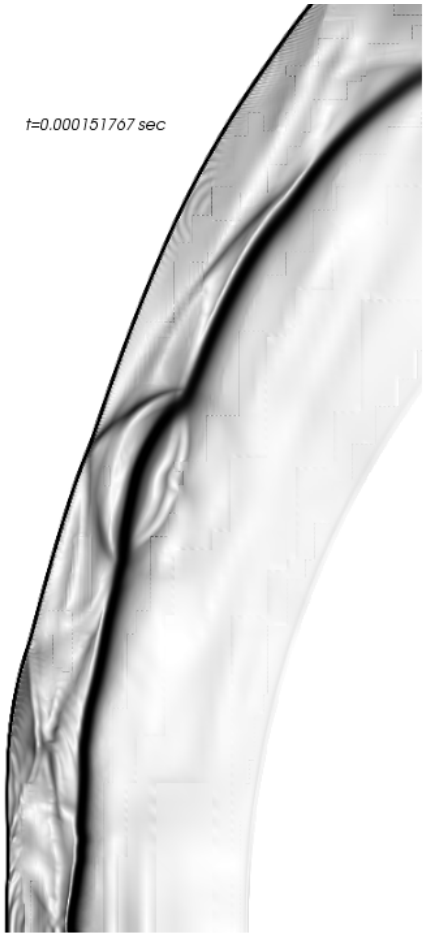


Pressure

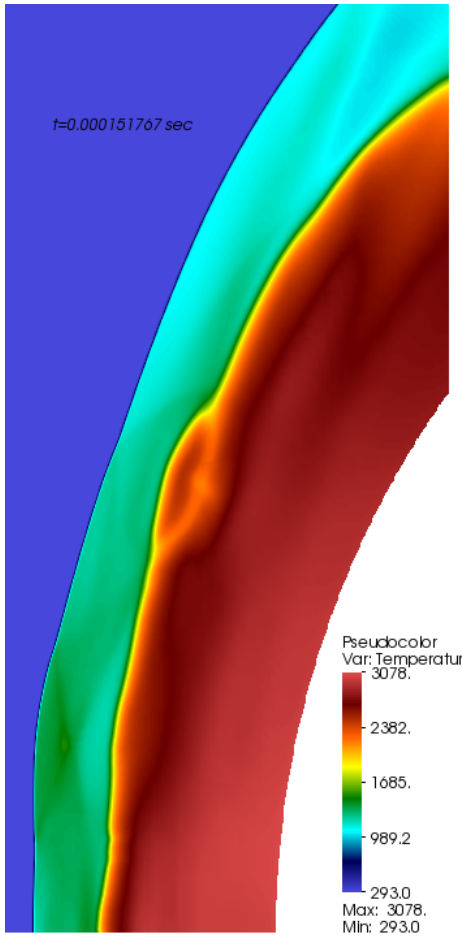


Perturbed oscillation mechanism

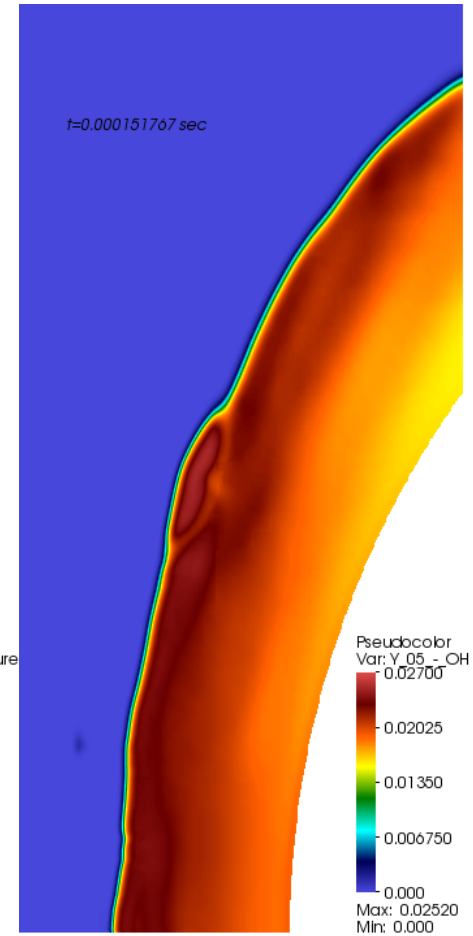
Schlieren of density



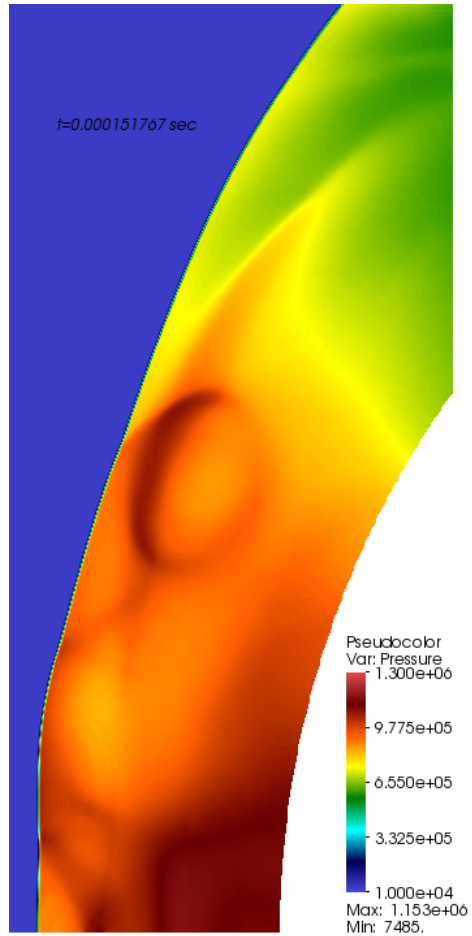
Temperature



Mass fraction OH

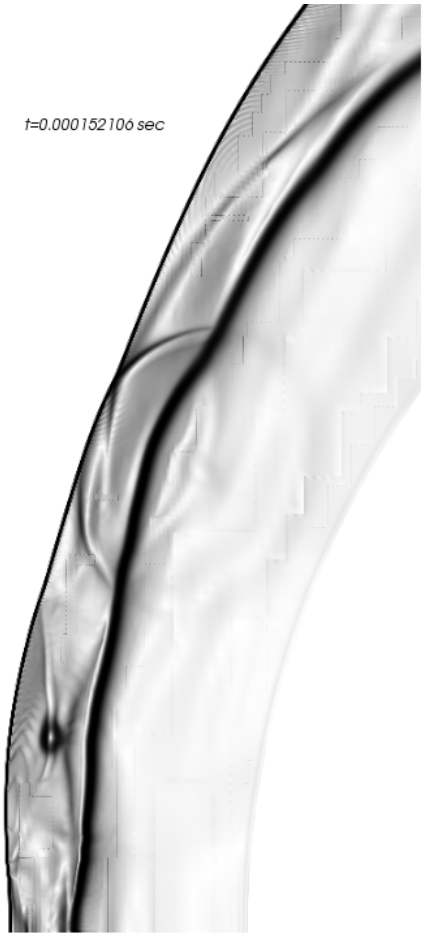


Pressure

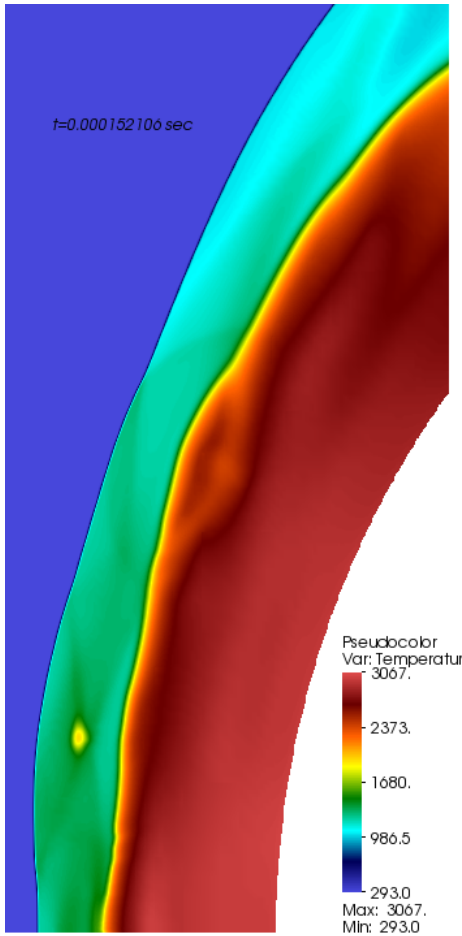


Perturbed oscillation mechanism

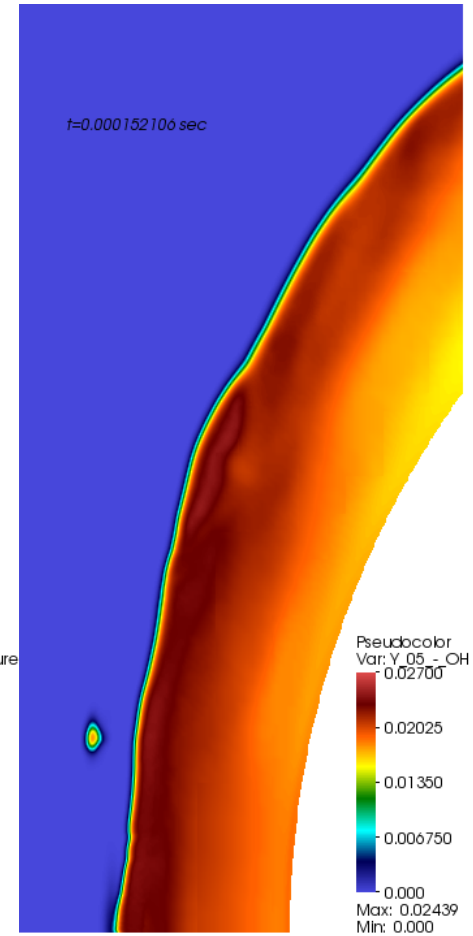
Schlieren of density



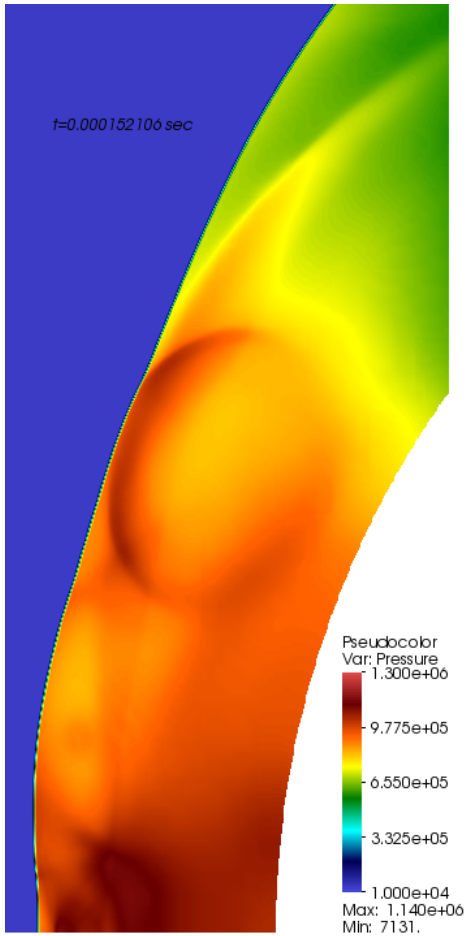
Temperature



Mass fraction OH

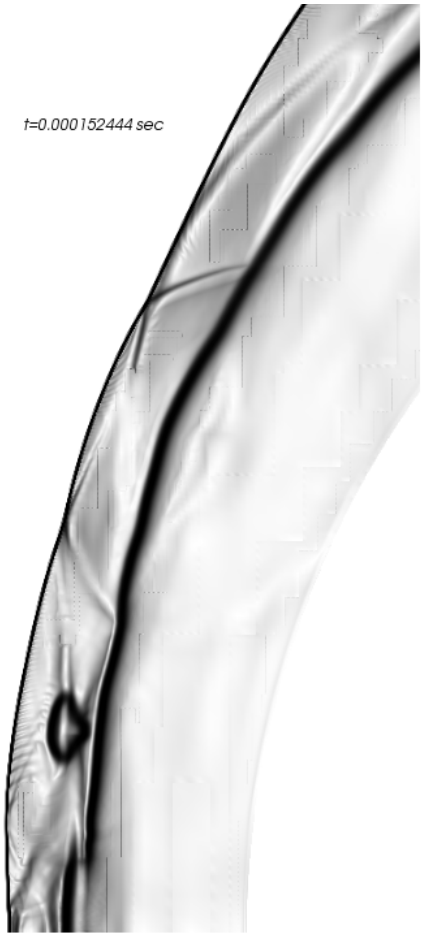


Pressure

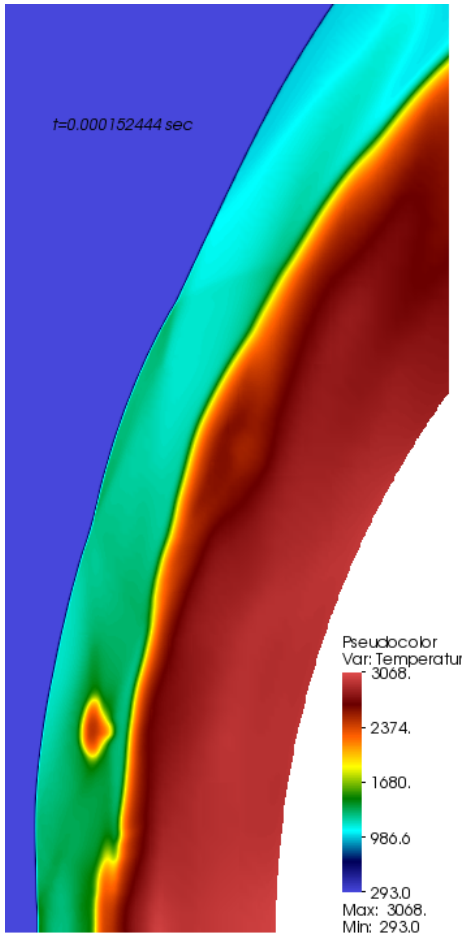


Perturbed oscillation mechanism

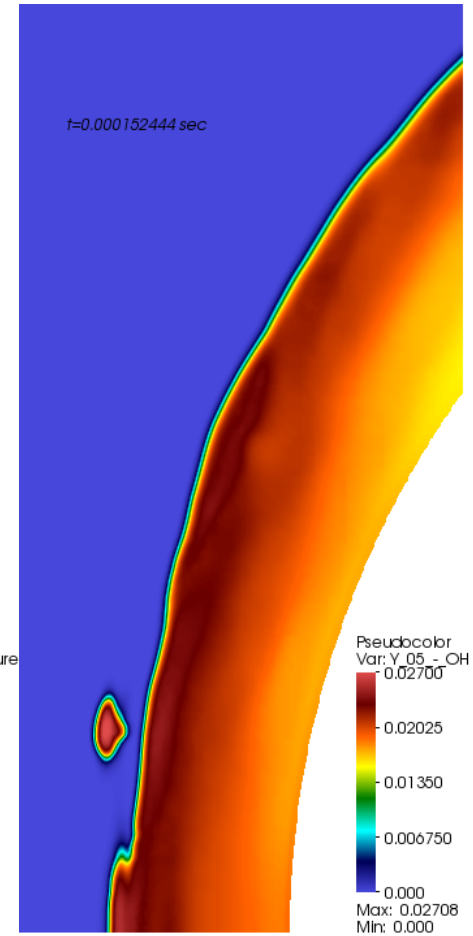
Schlieren of density



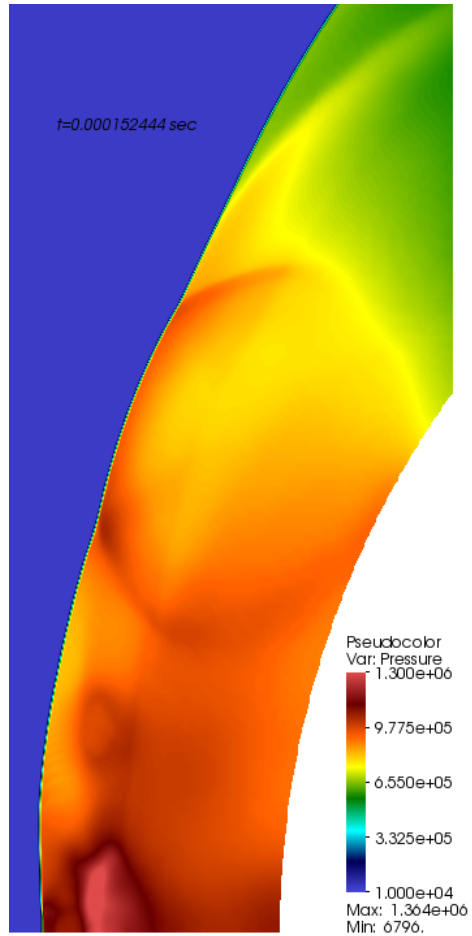
Temperature



Mass fraction OH

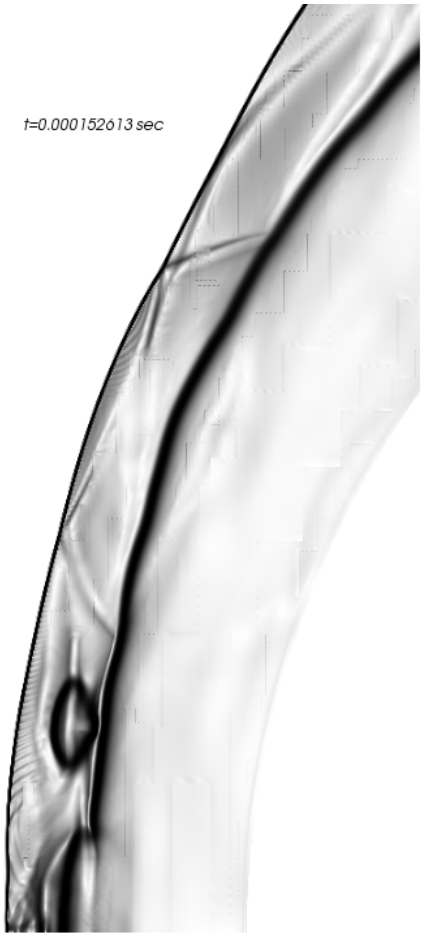


Pressure

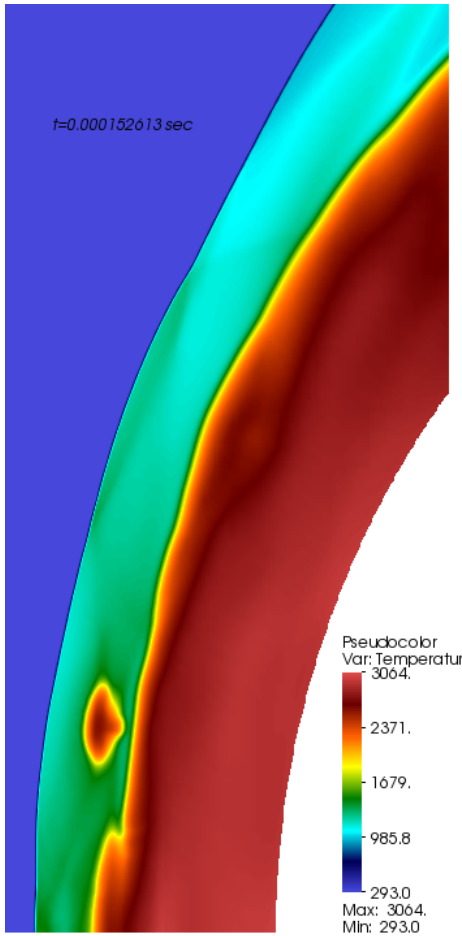


Perturbed oscillation mechanism

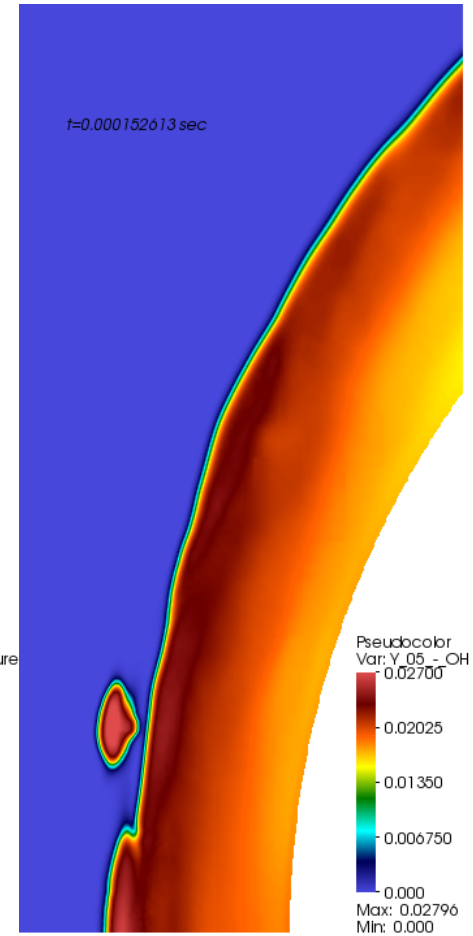
Schlieren of density



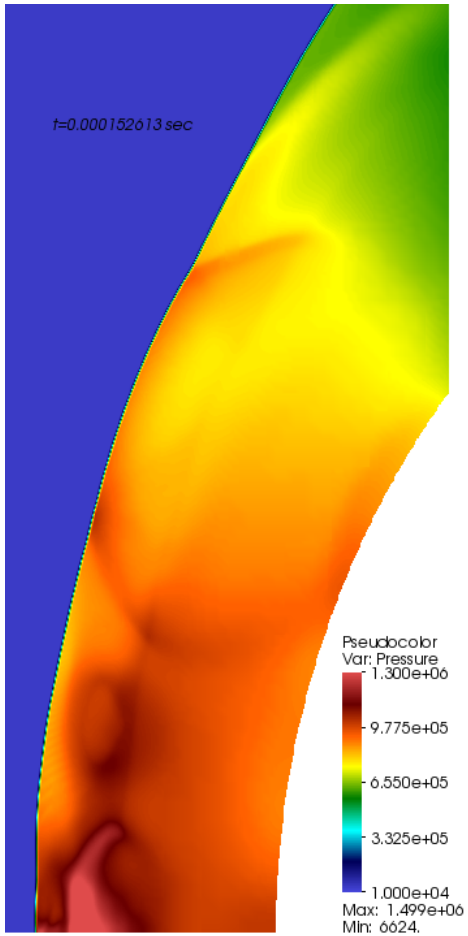
Temperature



Mass fraction OH

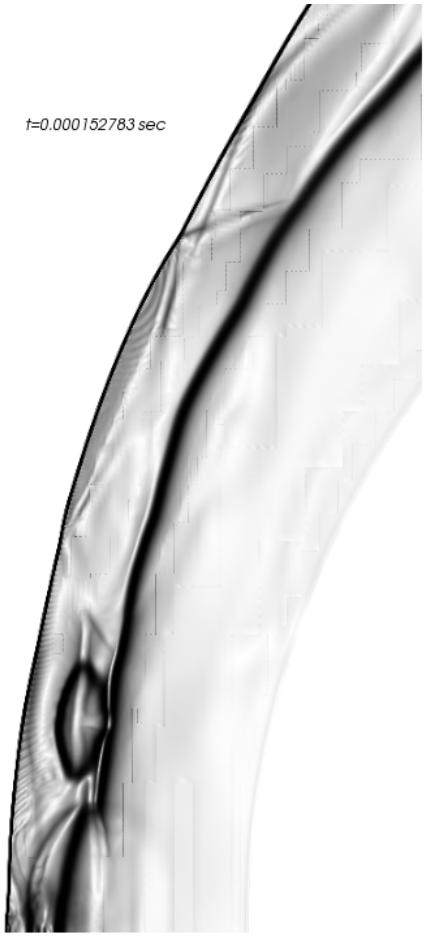


Pressure

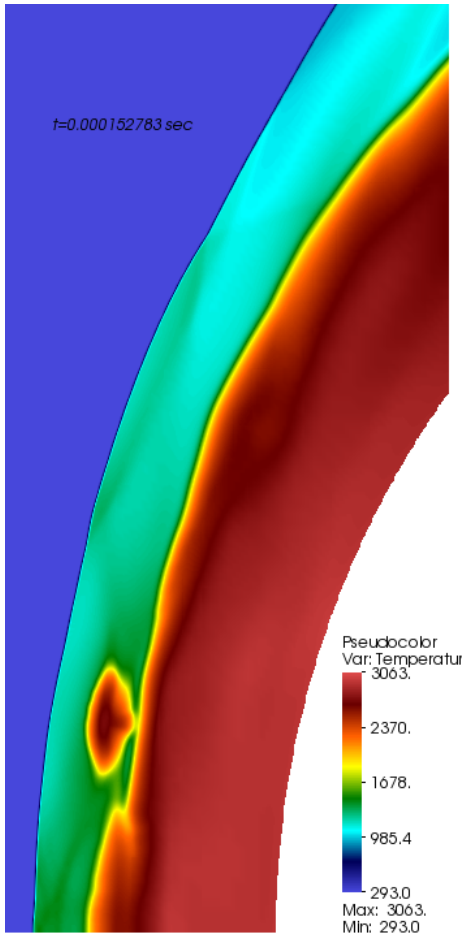


Perturbed oscillation mechanism

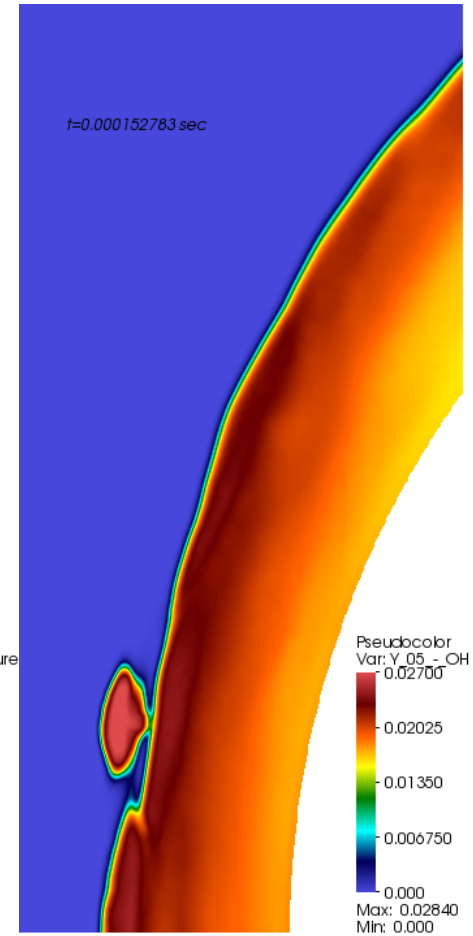
Schlieren of density



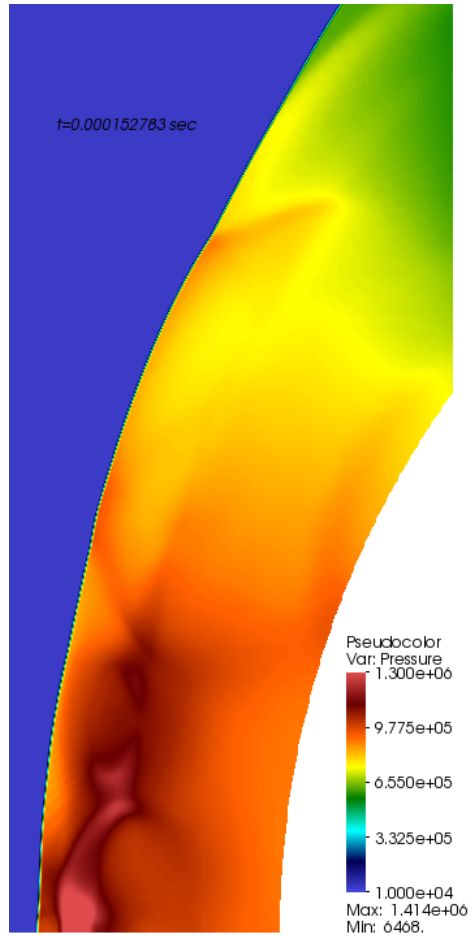
Temperature



Mass fraction OH

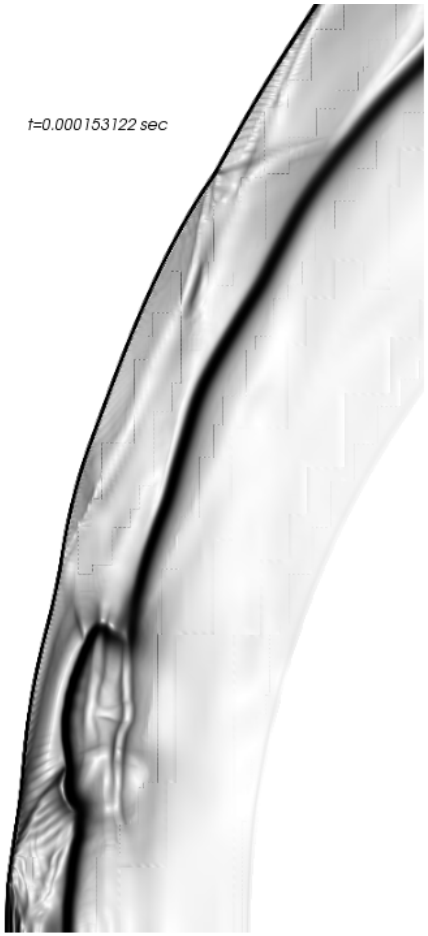


Pressure

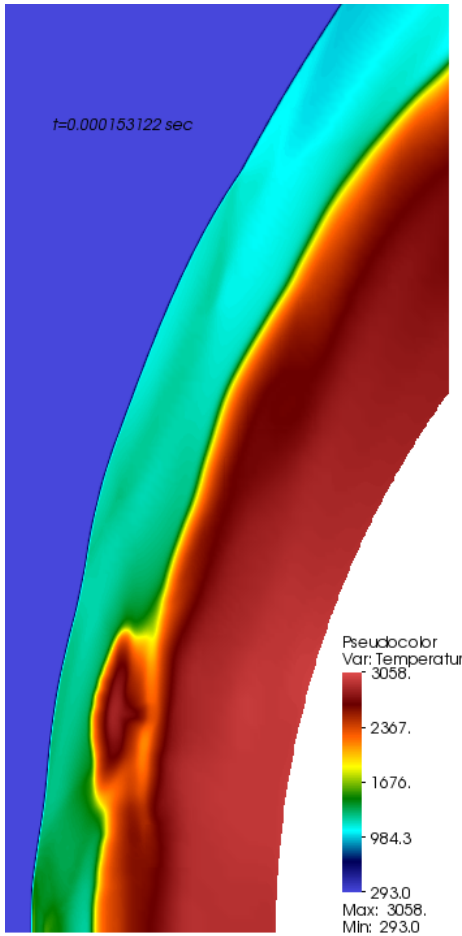


Perturbed oscillation mechanism

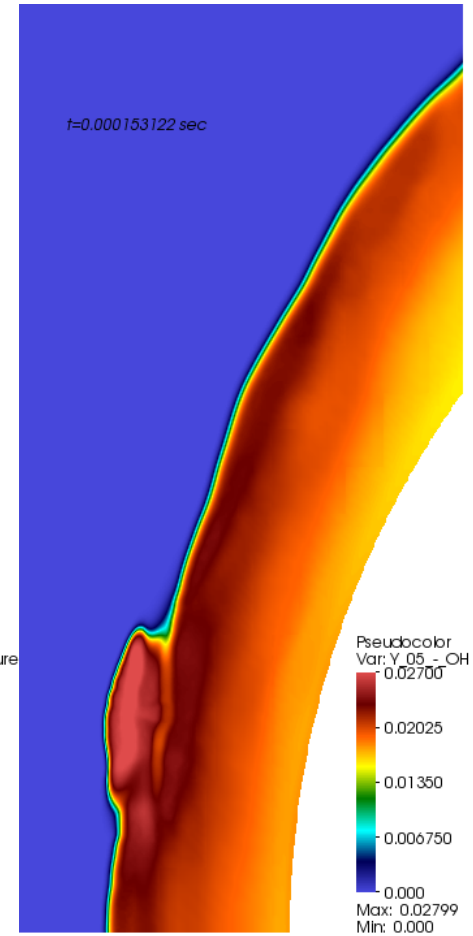
Schlieren of density



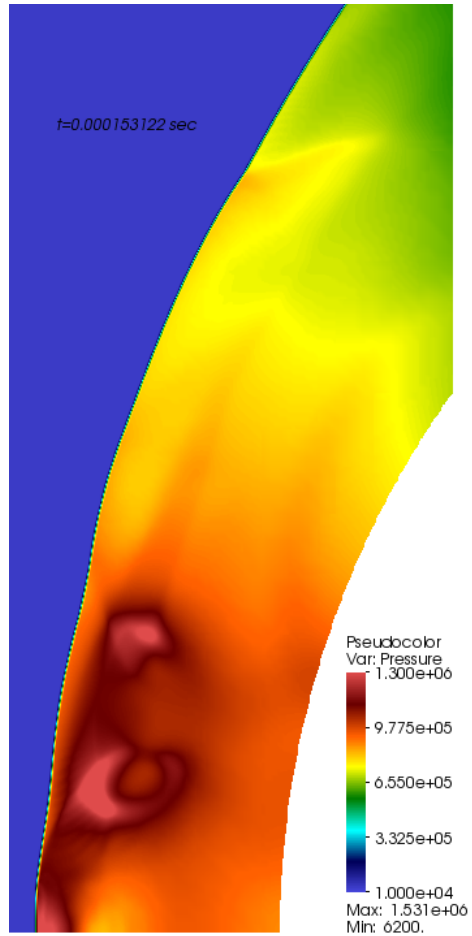
Temperature



Mass fraction OH

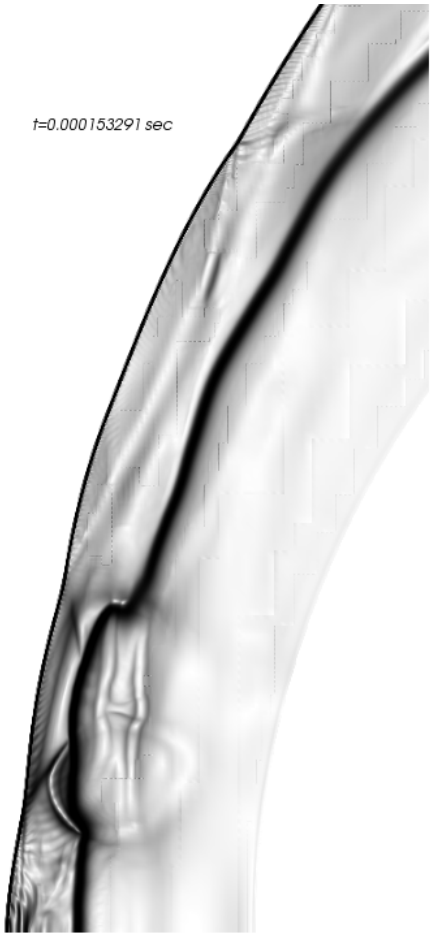


Pressure

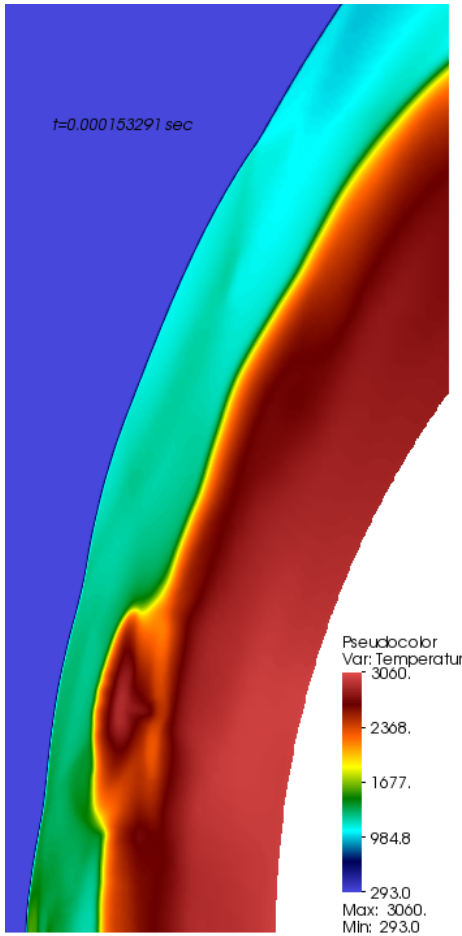


Perturbed oscillation mechanism

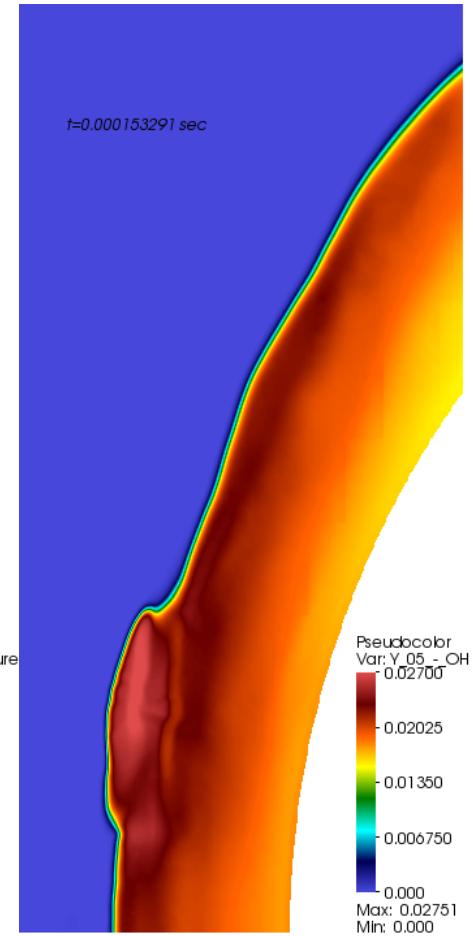
Schlieren of density



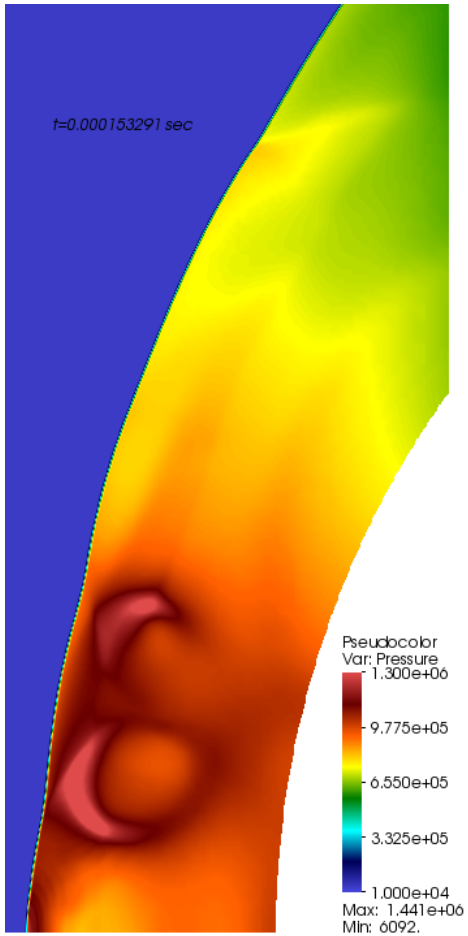
Temperature



Mass fraction OH

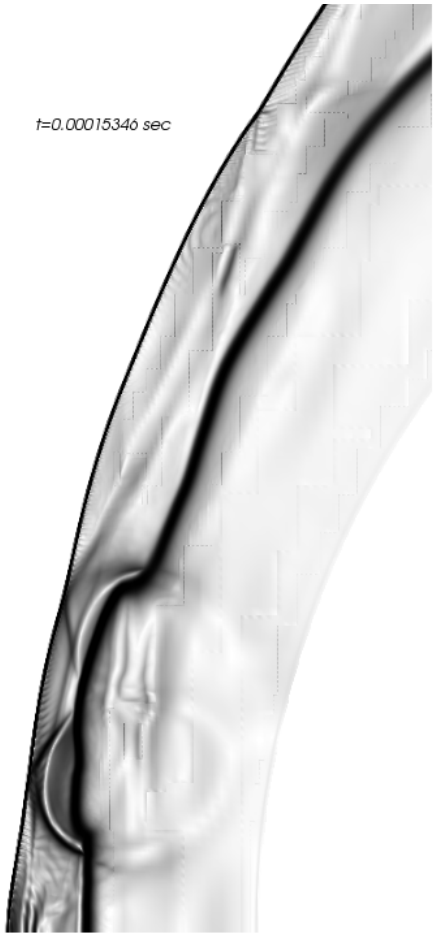


Pressure

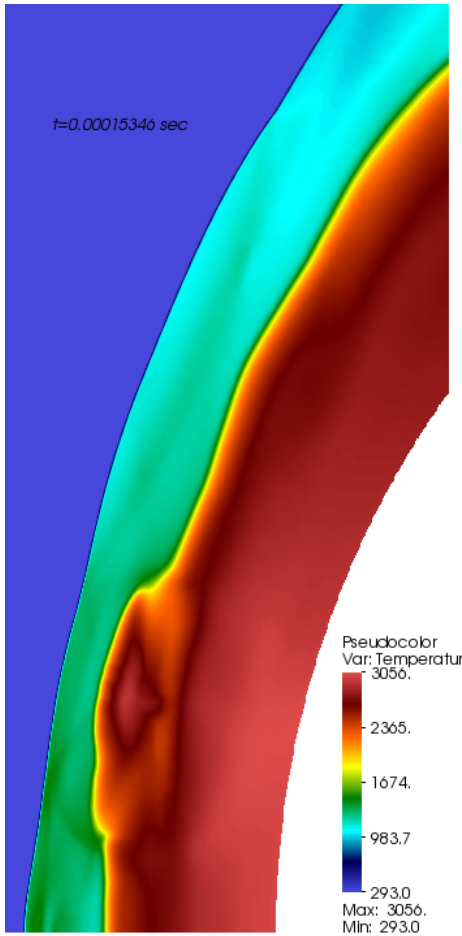


Perturbed oscillation mechanism

Schlieren of density



Temperature



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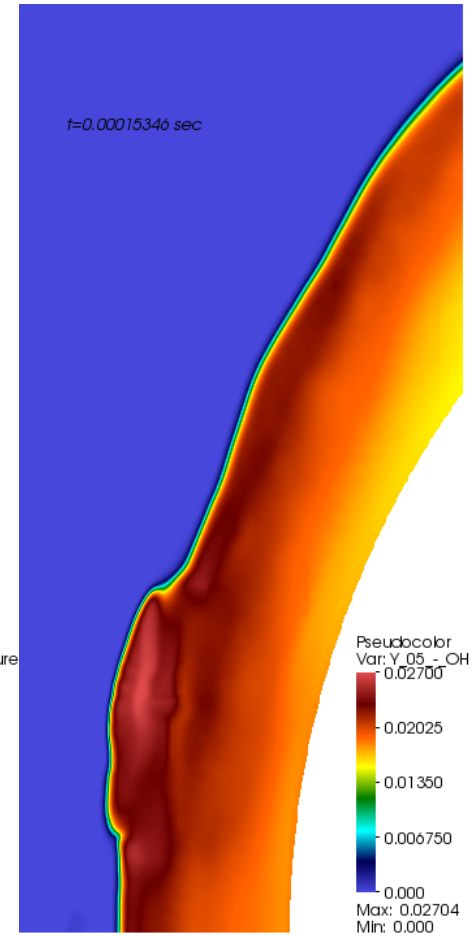
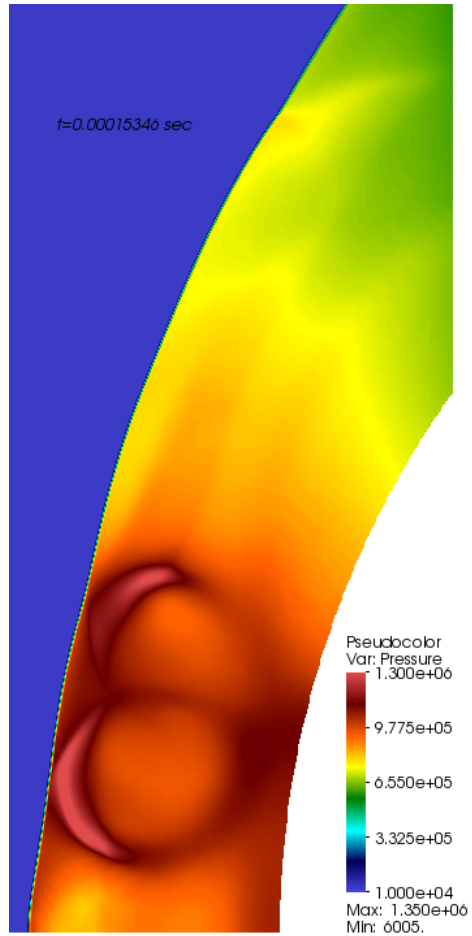
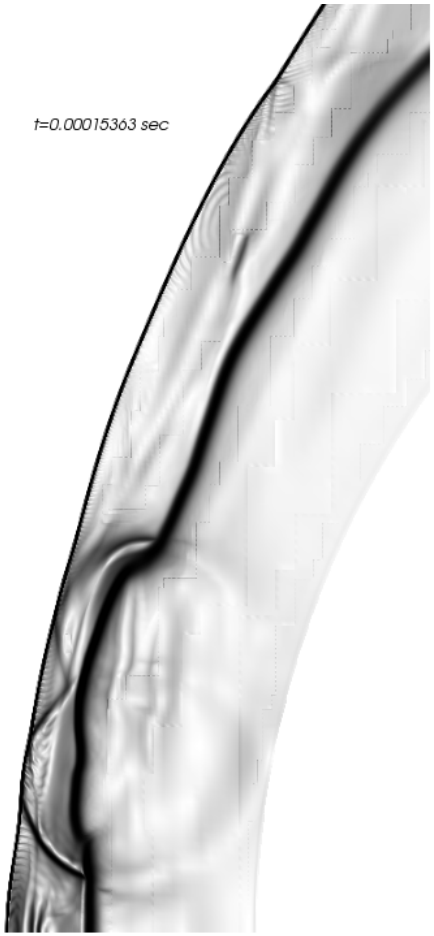


Pressure

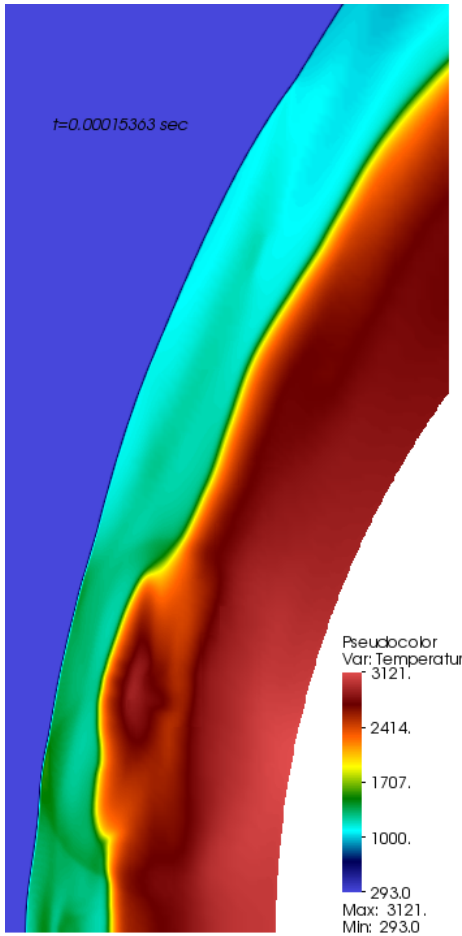


Perturbed oscillation mechanism

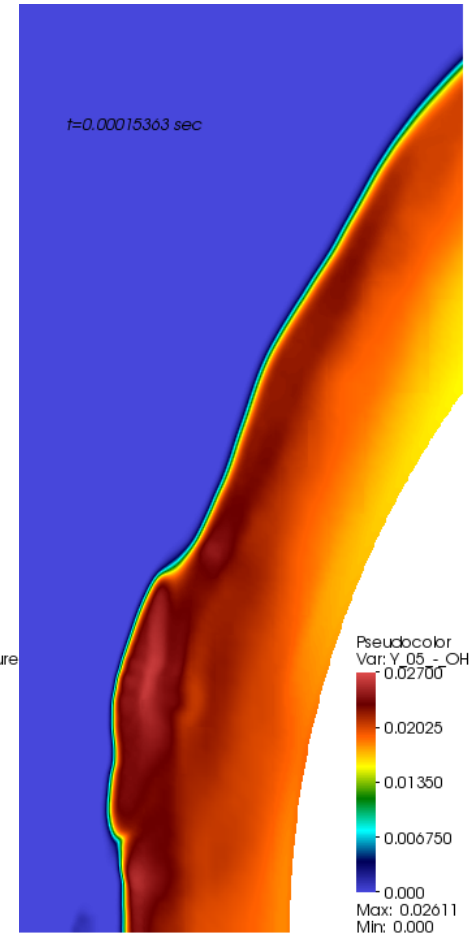
Schlieren of density



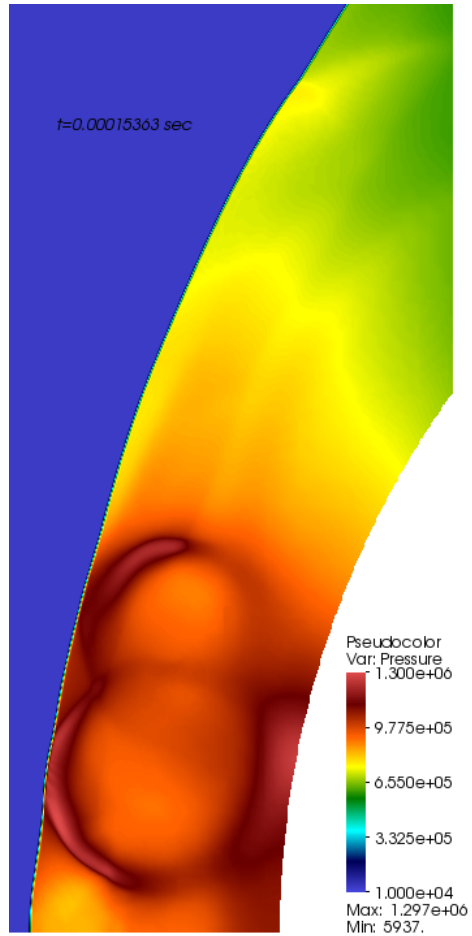
Temperature



Mass fraction OH

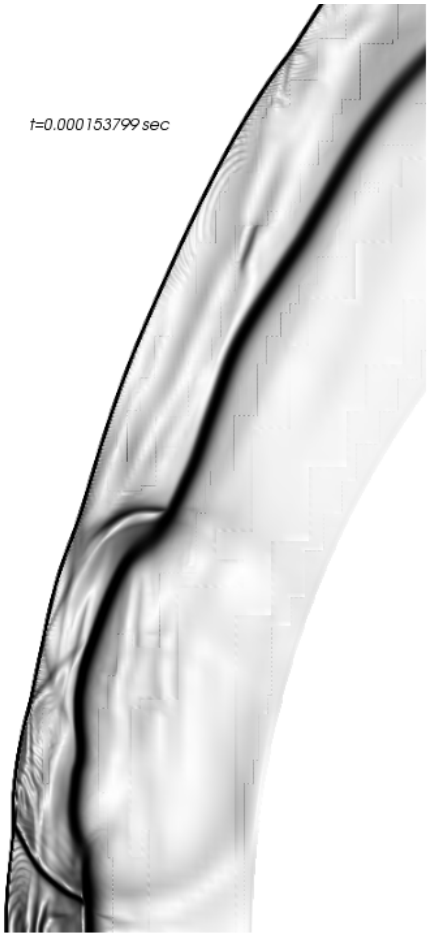


Pressure

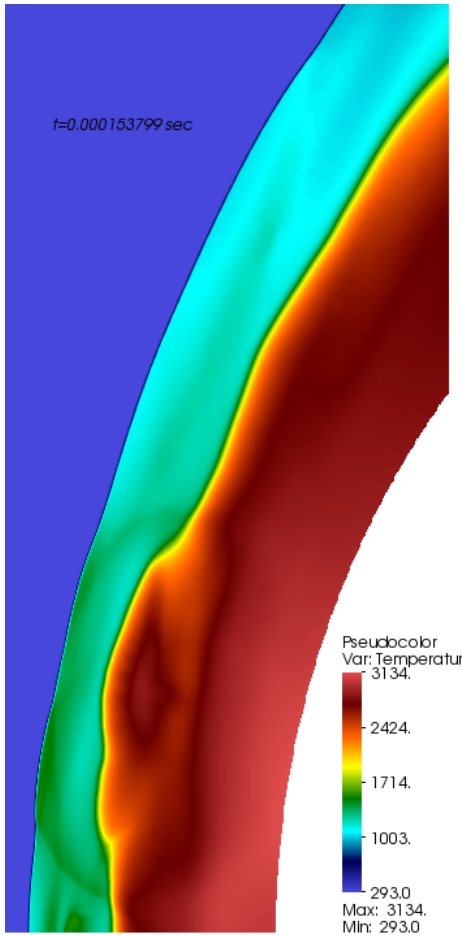


Perturbed oscillation mechanism

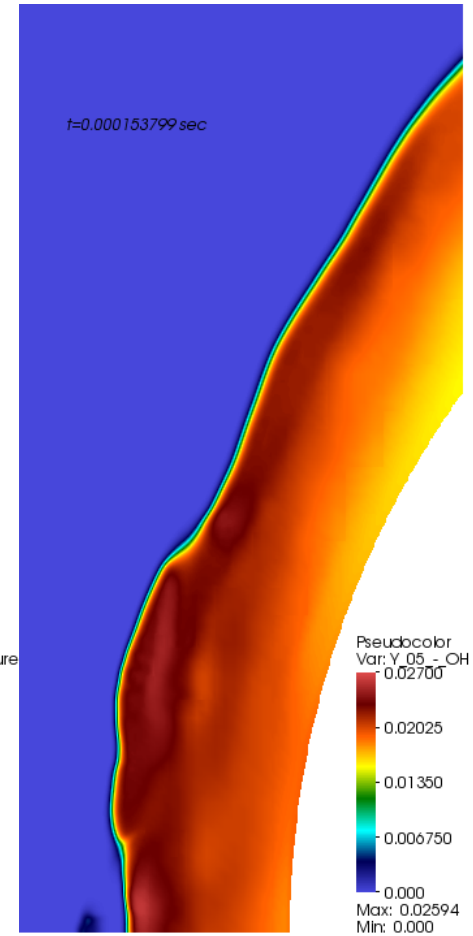
Schlieren of density



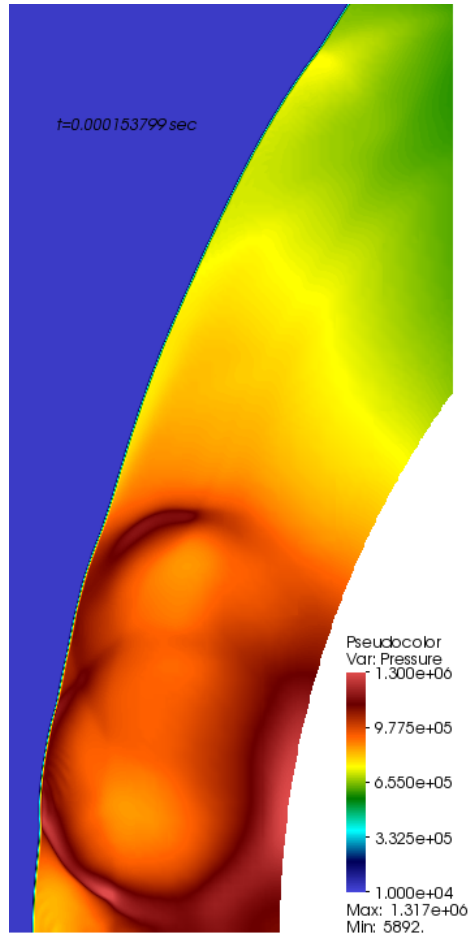
Temperature



Mass fraction OH

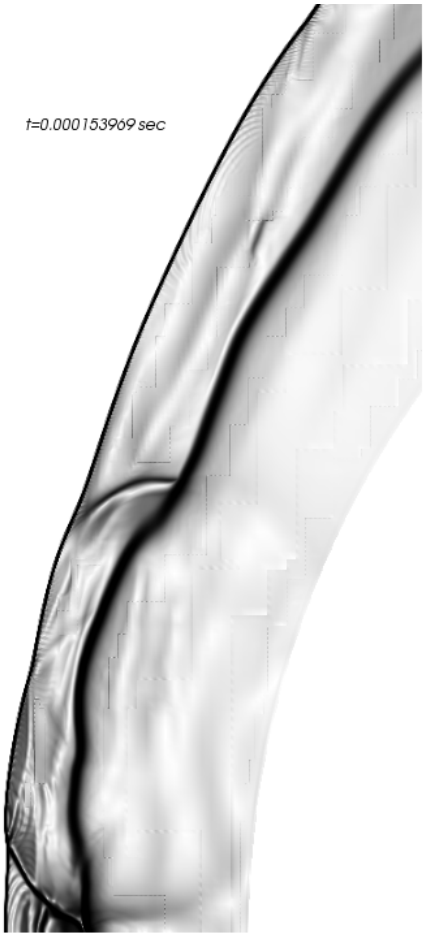


Pressure

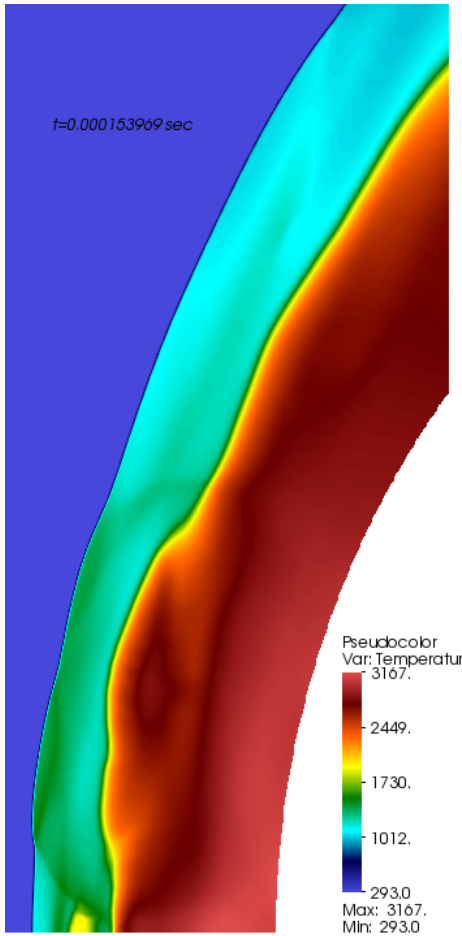


Perturbed oscillation mechanism

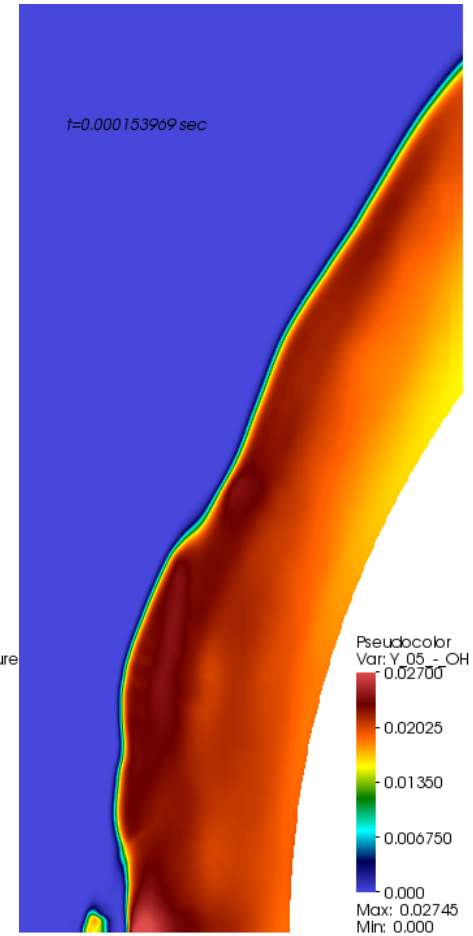
Schlieren of density



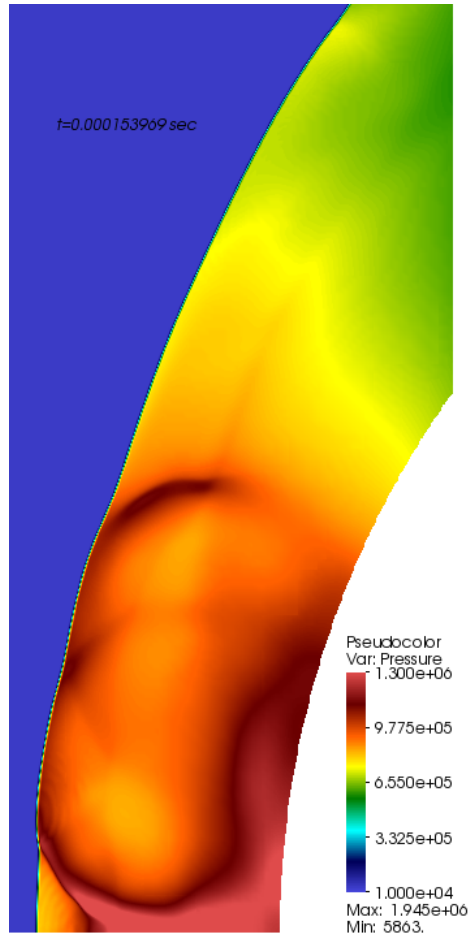
Temperature



Mass fraction OH

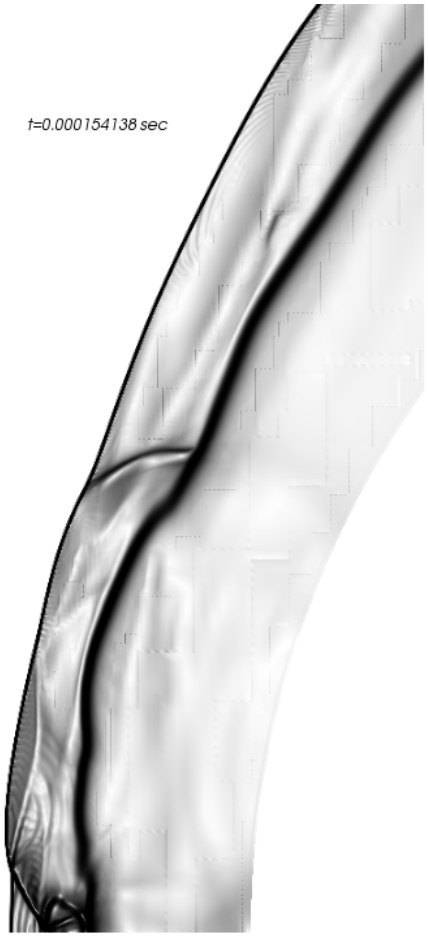


Pressure

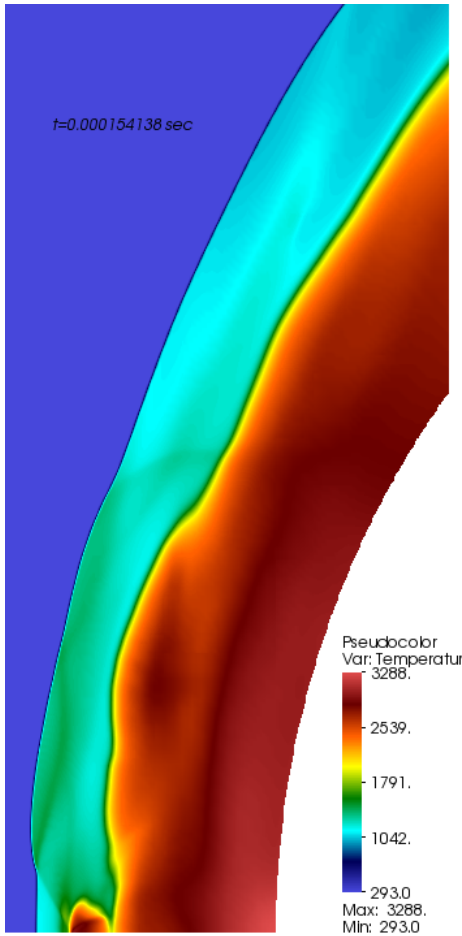


Perturbed oscillation mechanism

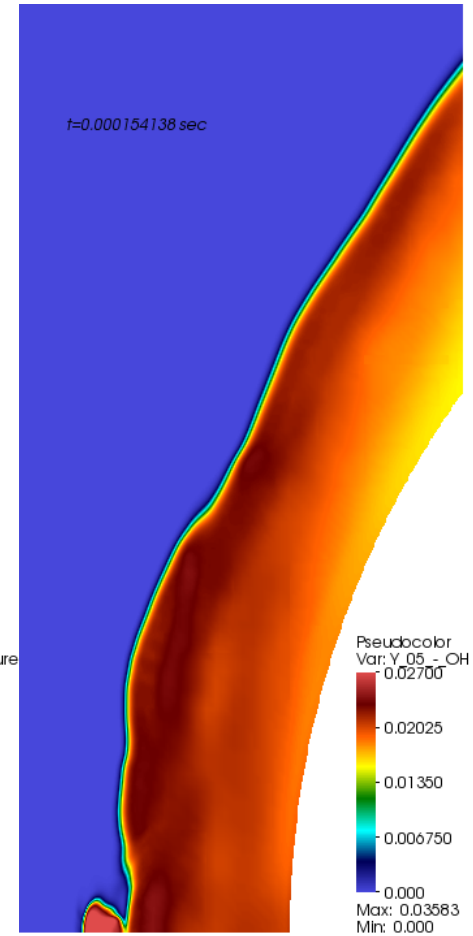
Schlieren of density



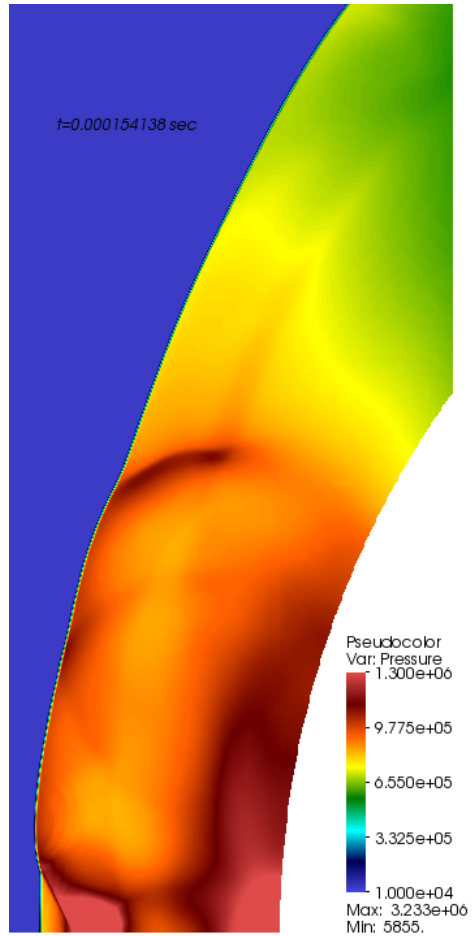
Temperature



Mass fraction OH

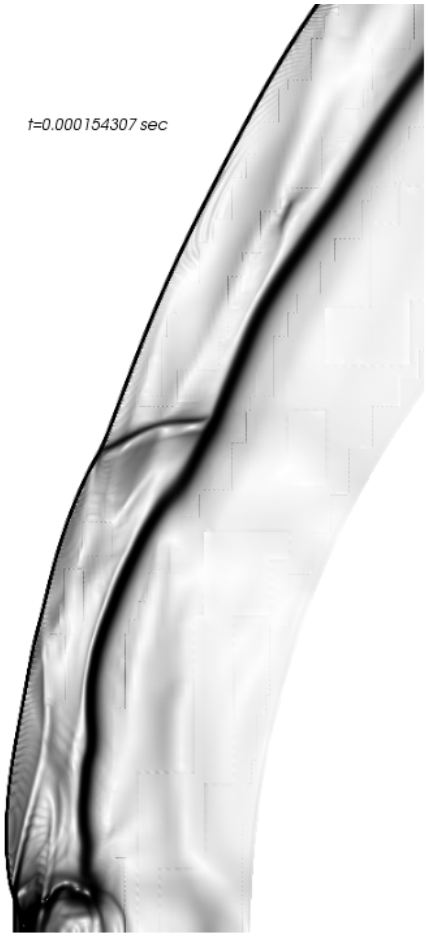


Pressure

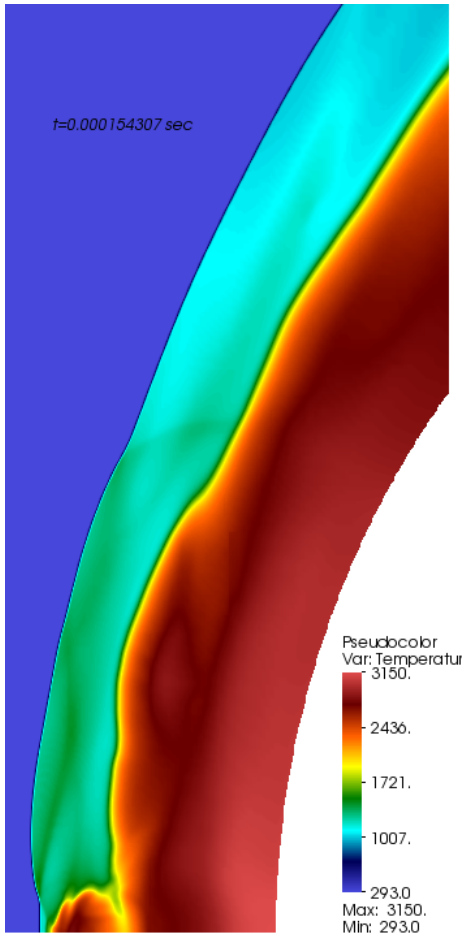


Perturbed oscillation mechanism

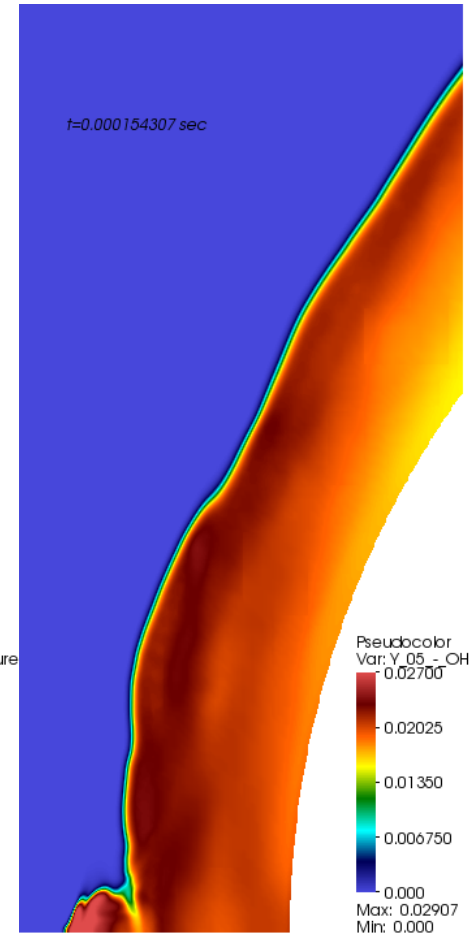
Schlieren of density



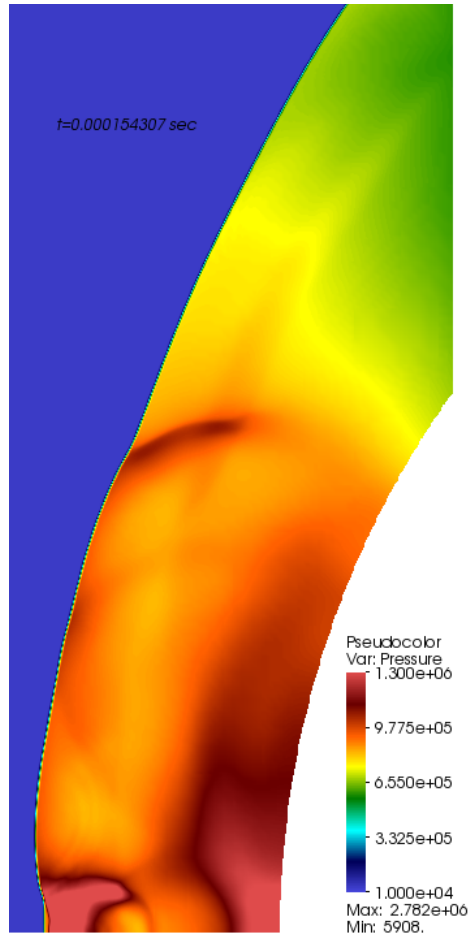
Temperature



Mass fraction OH

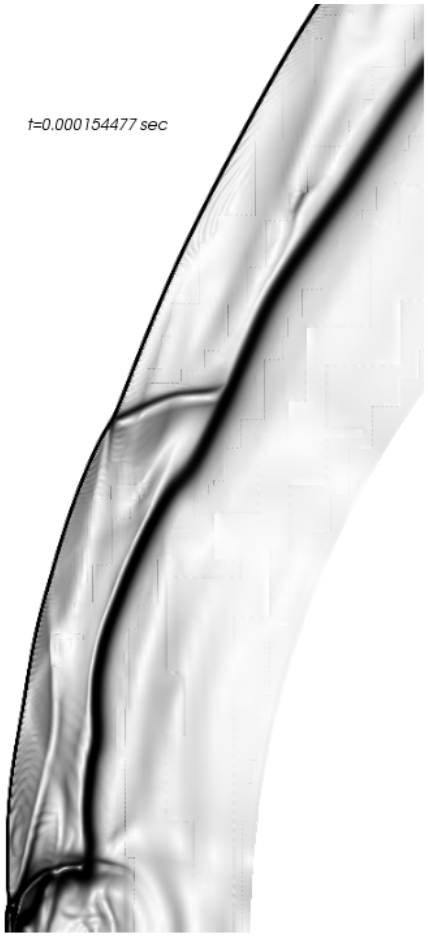


Pressure

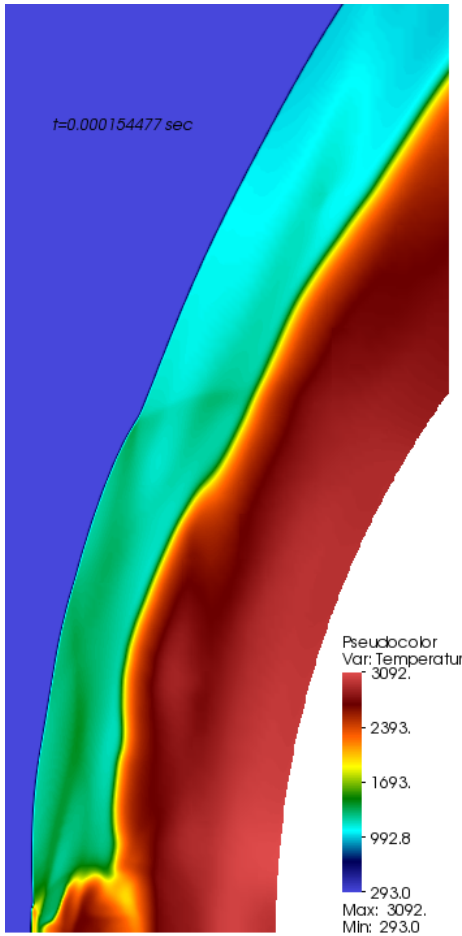


Perturbed oscillation mechanism

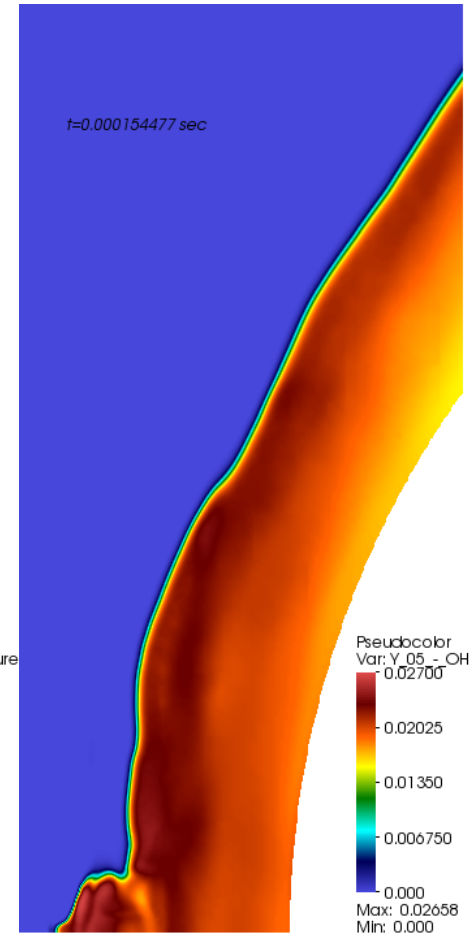
Schlieren of density



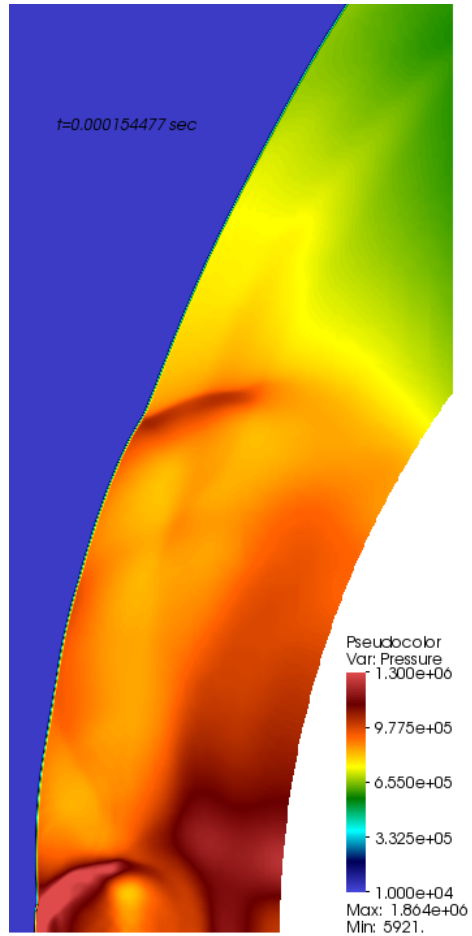
Temperature



Mass fraction OH

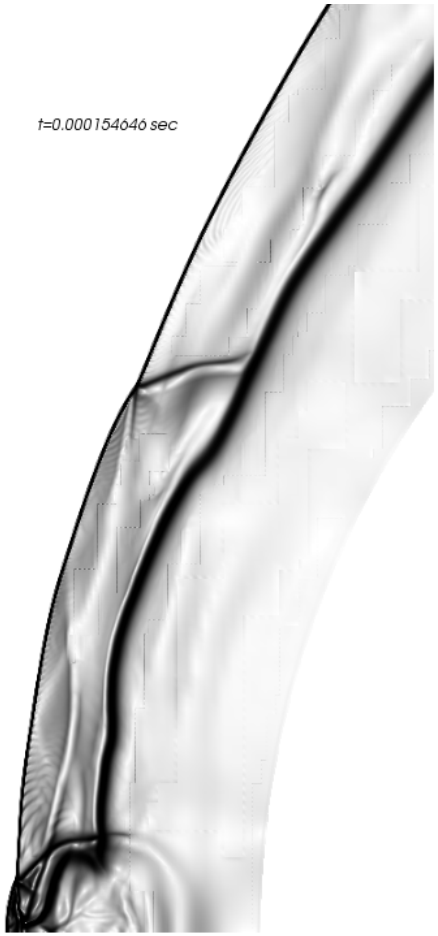


Pressure



Perturbed oscillation mechanism

Schlieren of density



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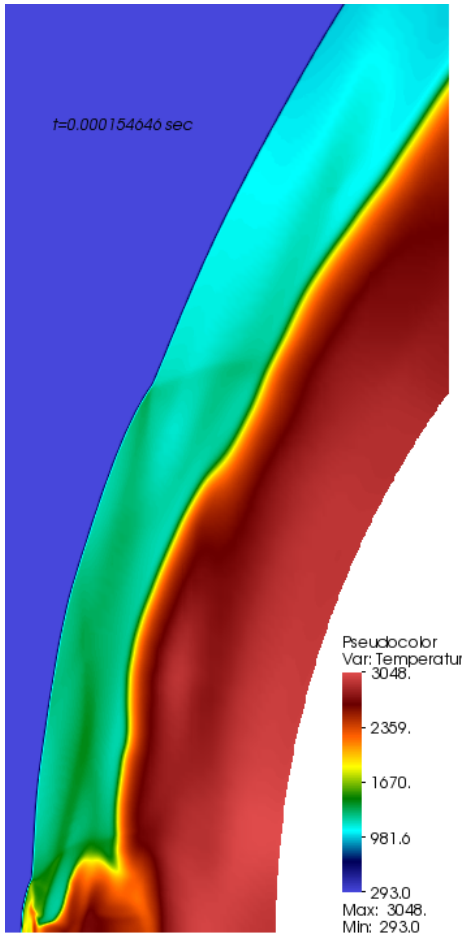
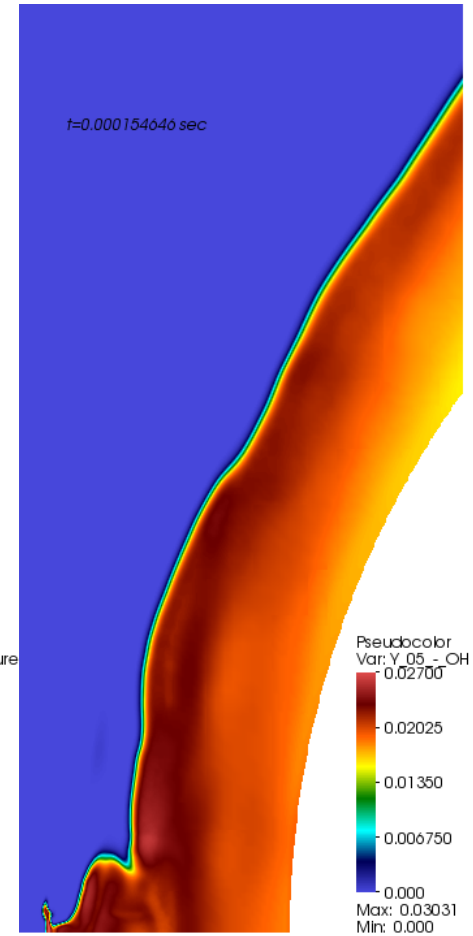
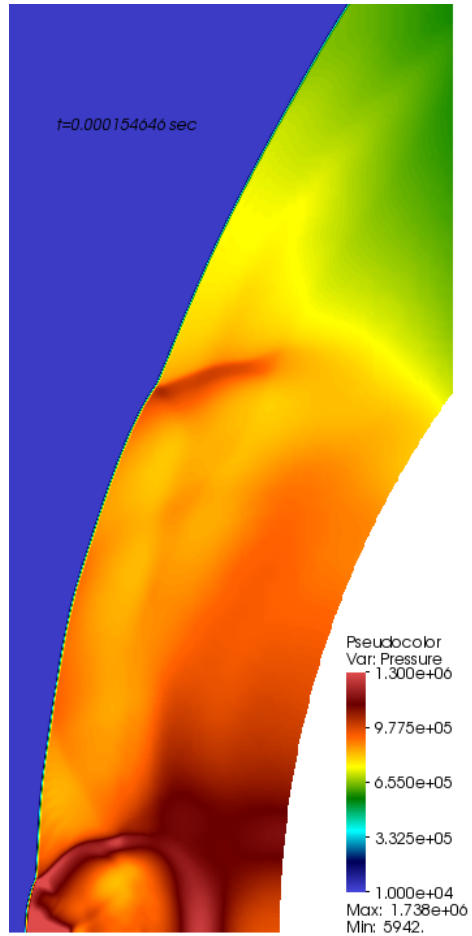


Mass fraction OH

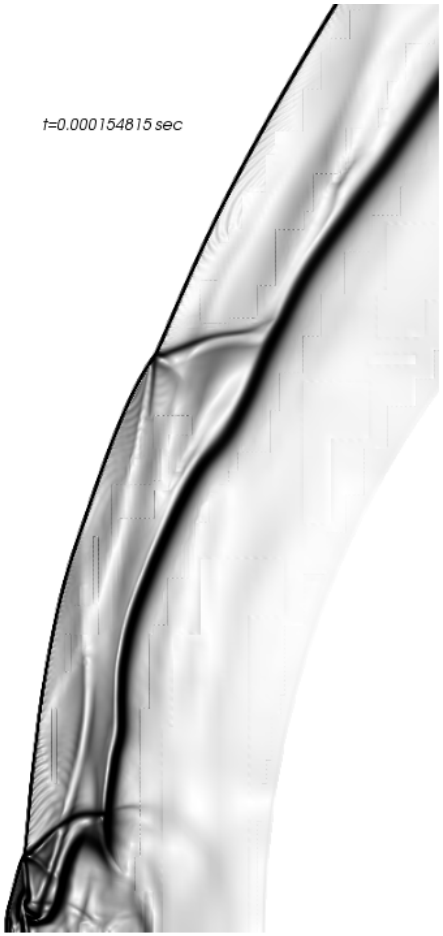


Pressure

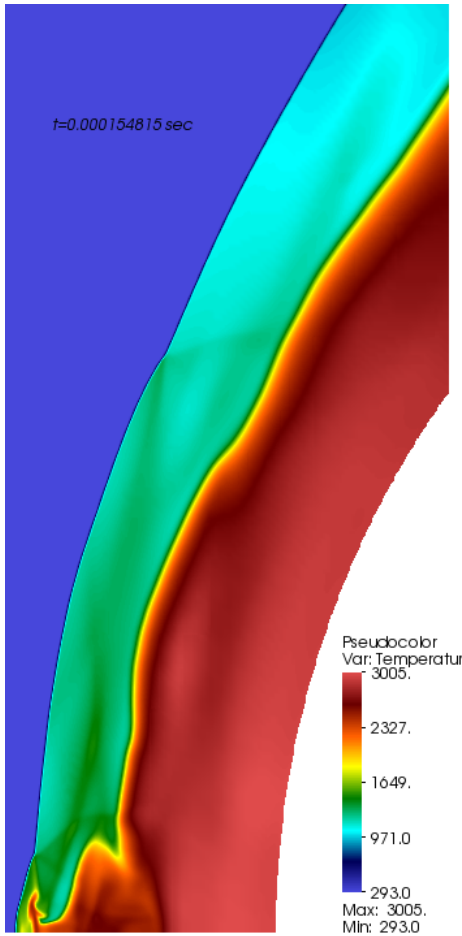


Perturbed oscillation mechanism

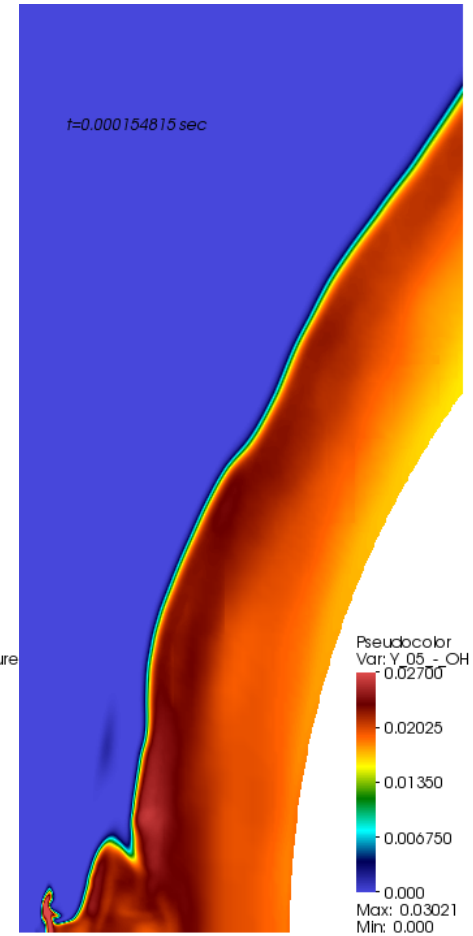
Schlieren of density



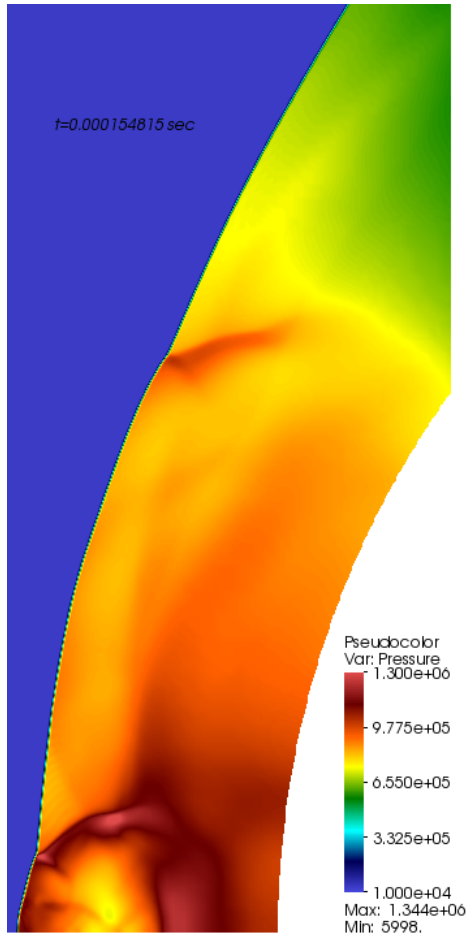
Temperature



Mass fraction OH

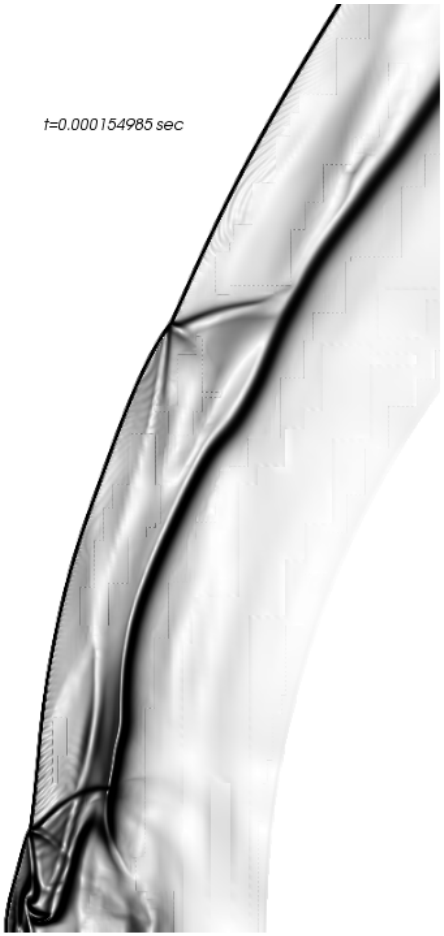


Pressure

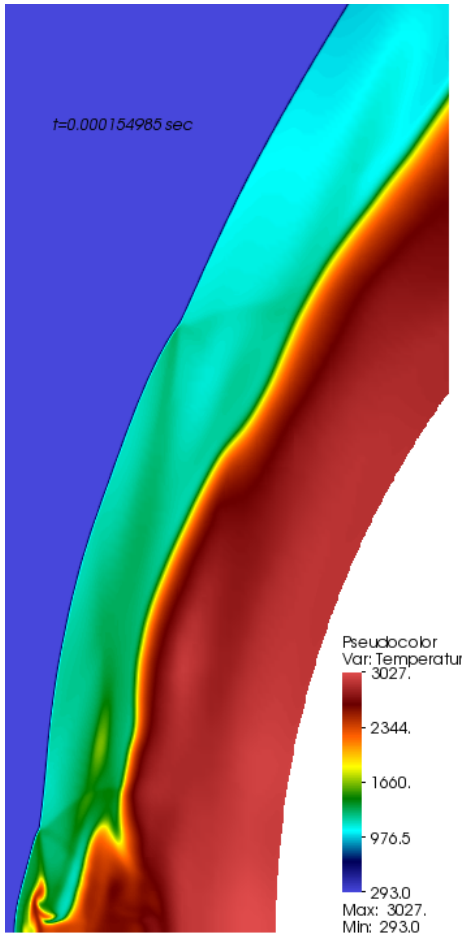


Perturbed oscillation mechanism

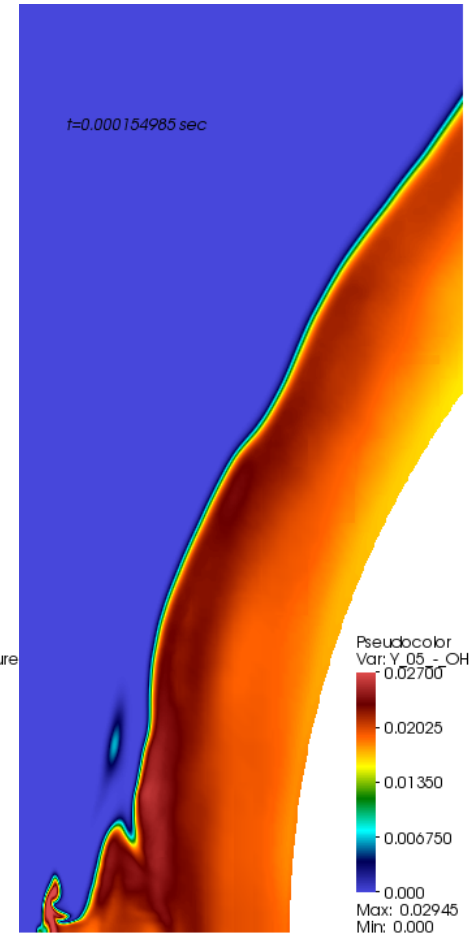
Schlieren of density



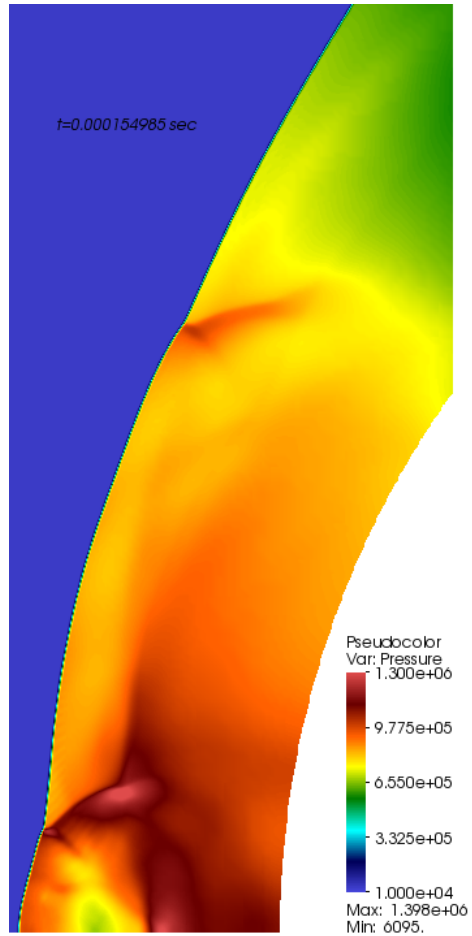
Temperature



Mass fraction OH



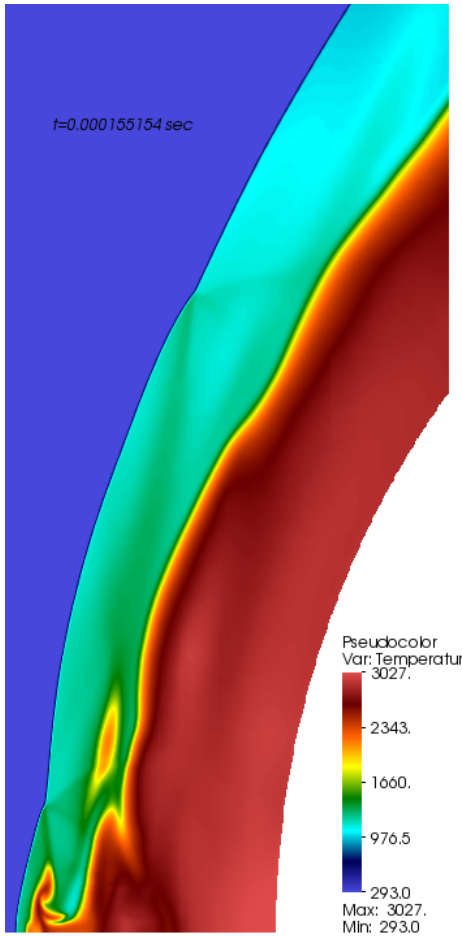
Pressure



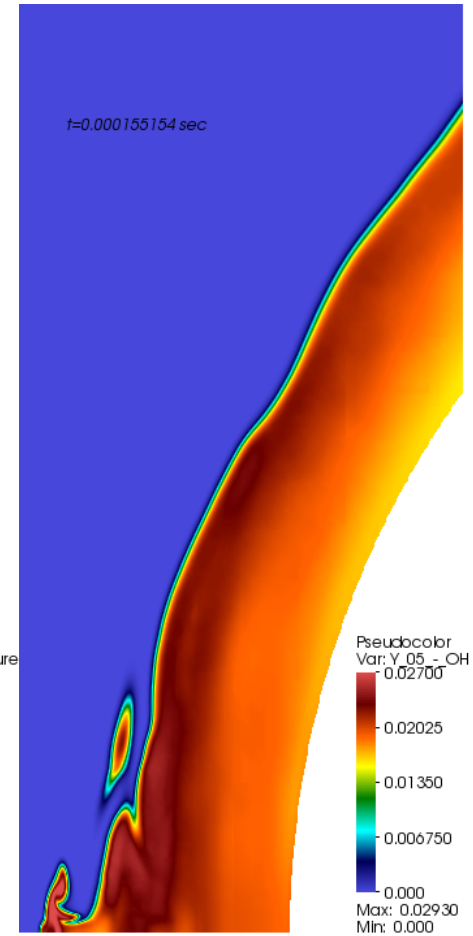
Perturbed oscillation mechanism

Schlieren of density

Temperature



Mass fraction OH



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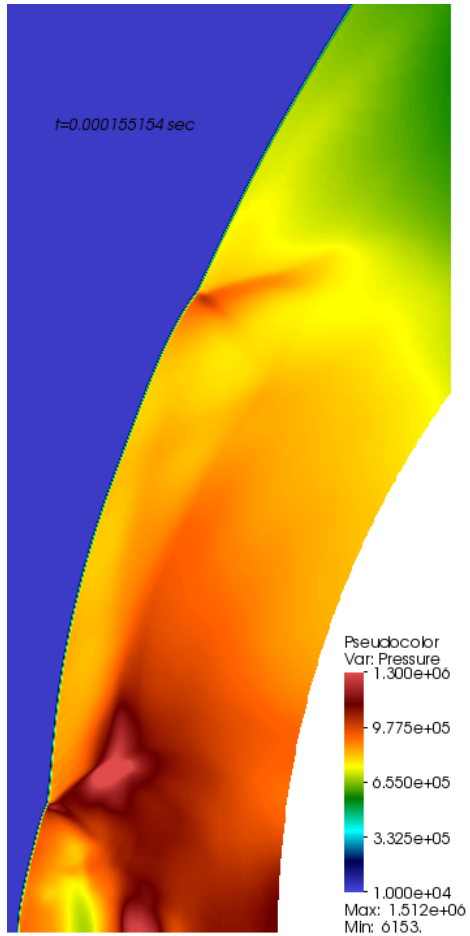
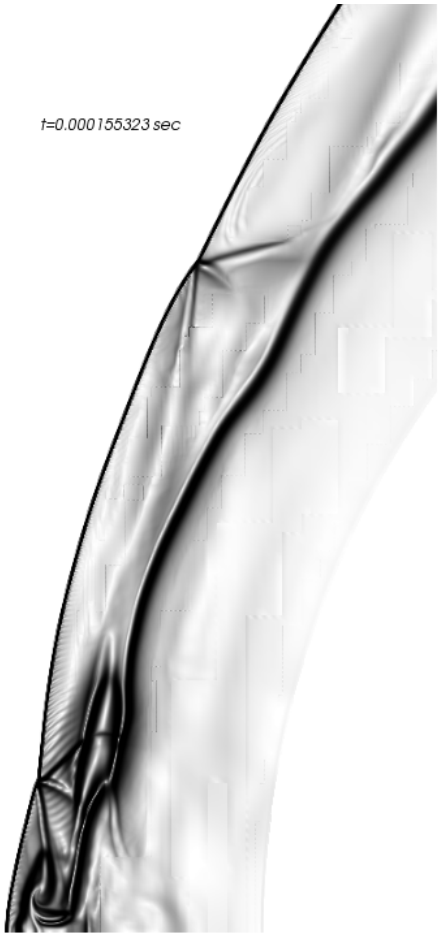
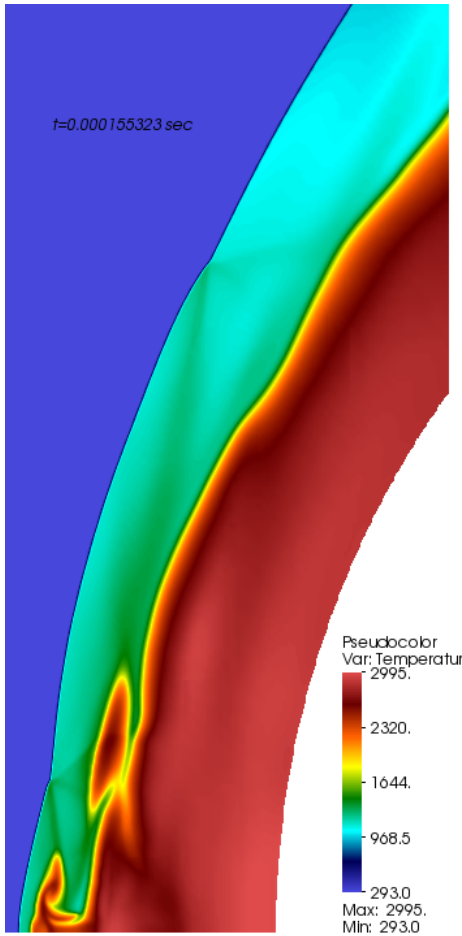


Perturbed oscillation mechanism

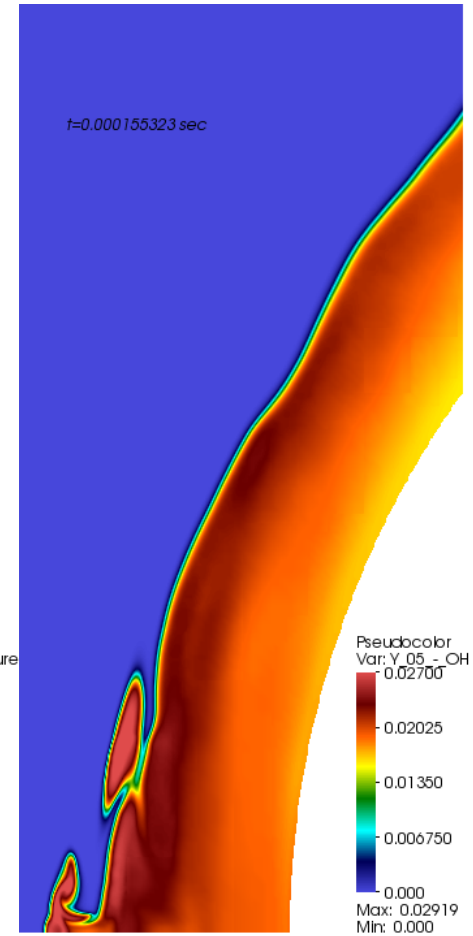
Schlieren of density



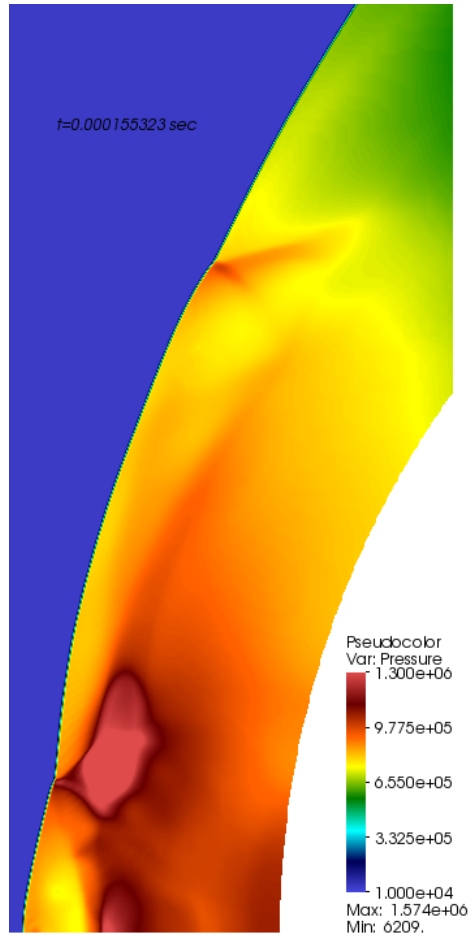
Temperature



Mass fraction OH



Pressure



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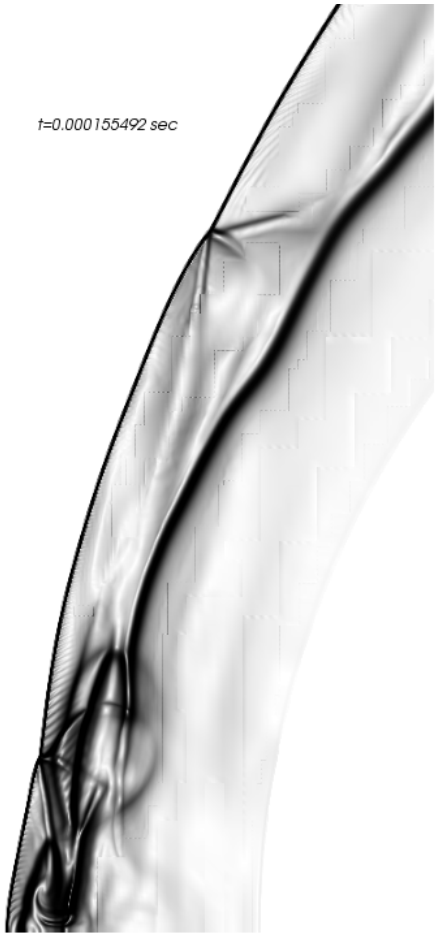
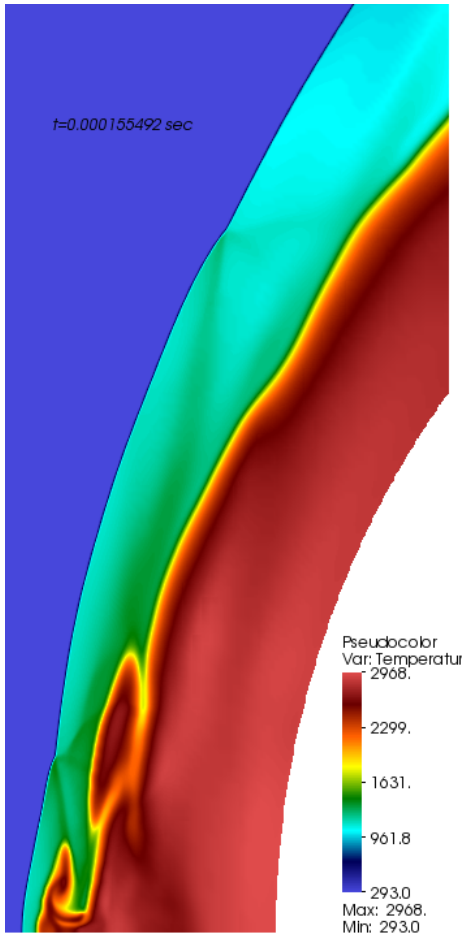


Temperature



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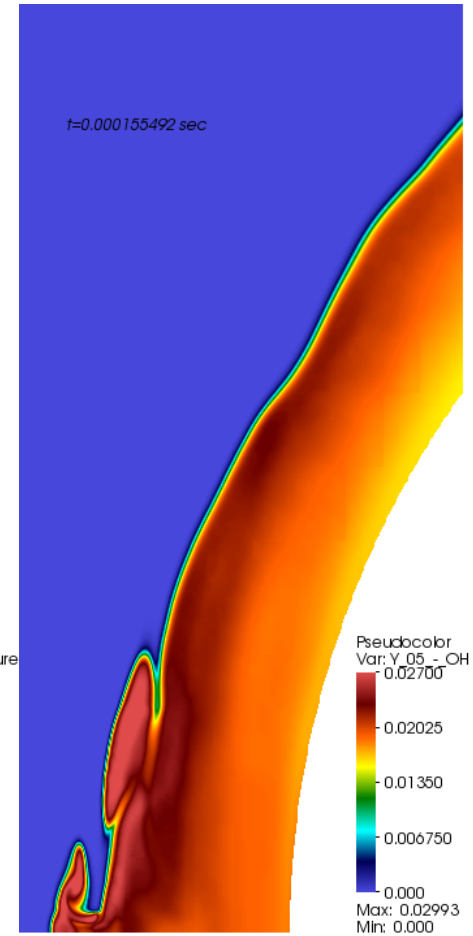
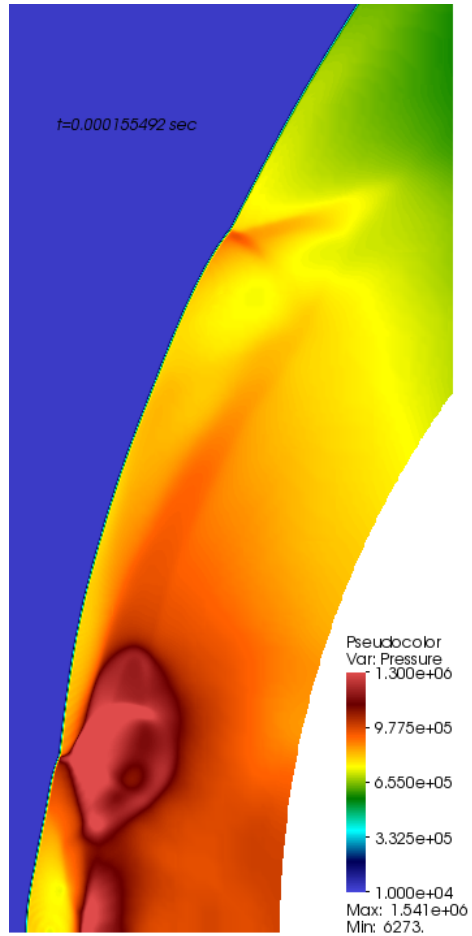


Pressure



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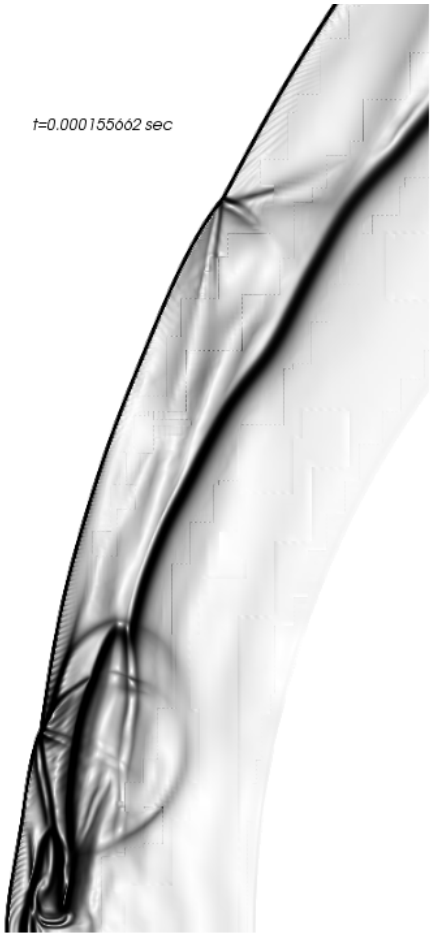
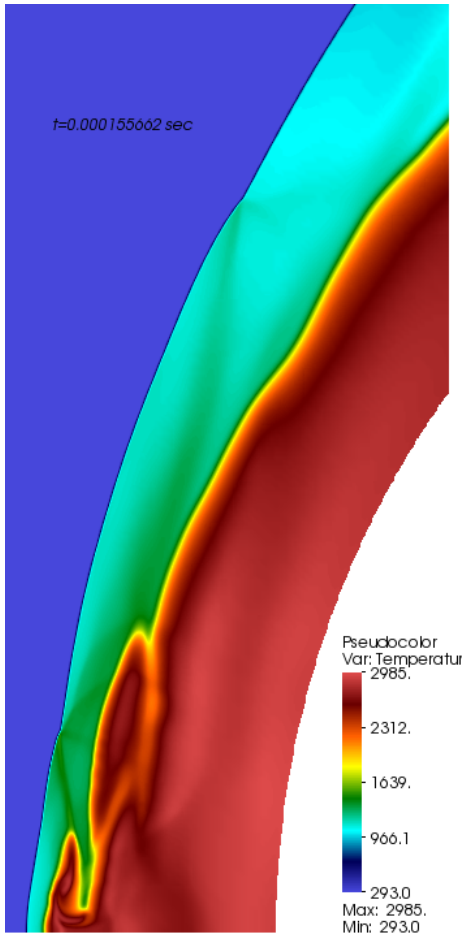
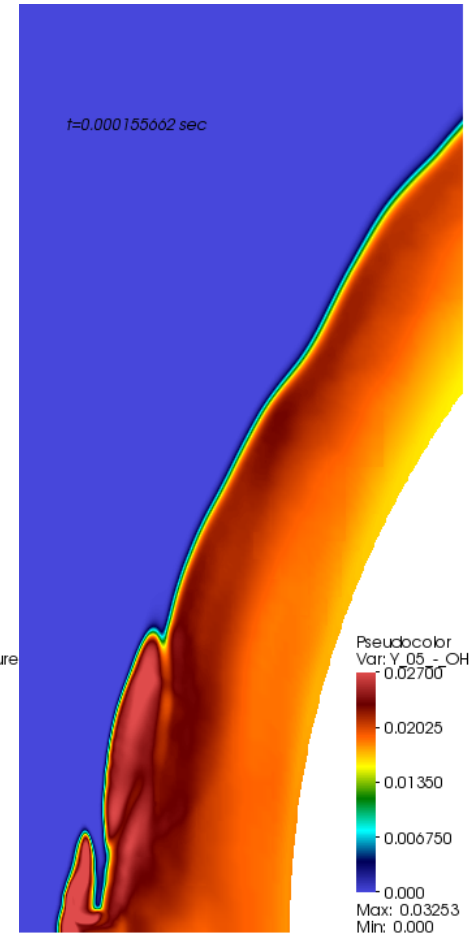


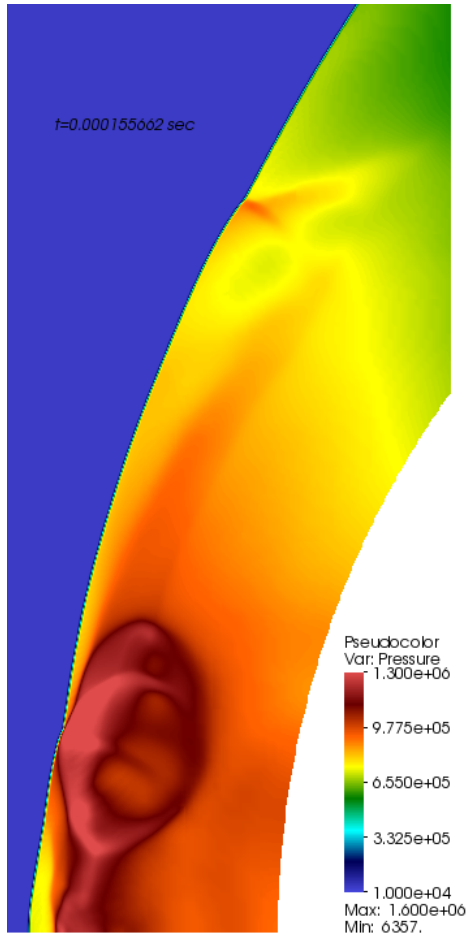
Temperature



Mass fraction OH



Pressure



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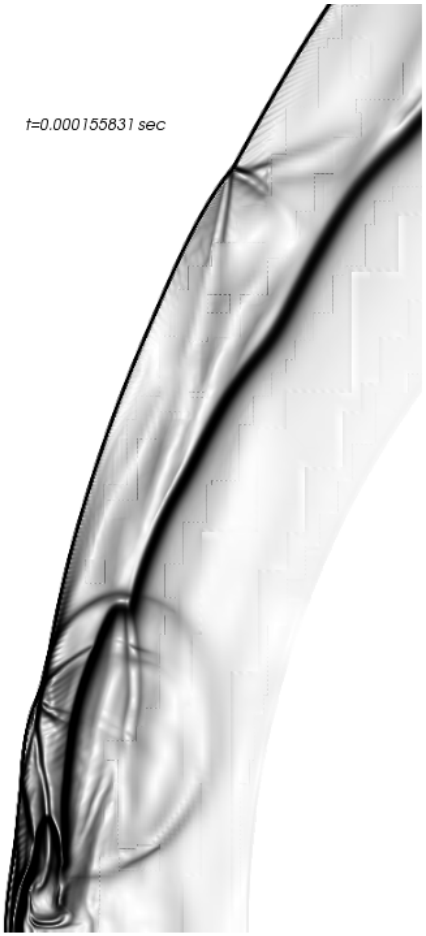
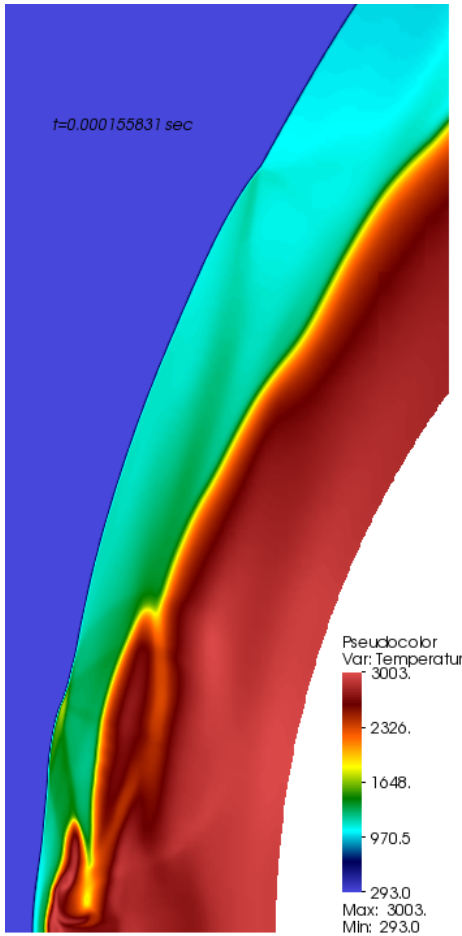


Temperature



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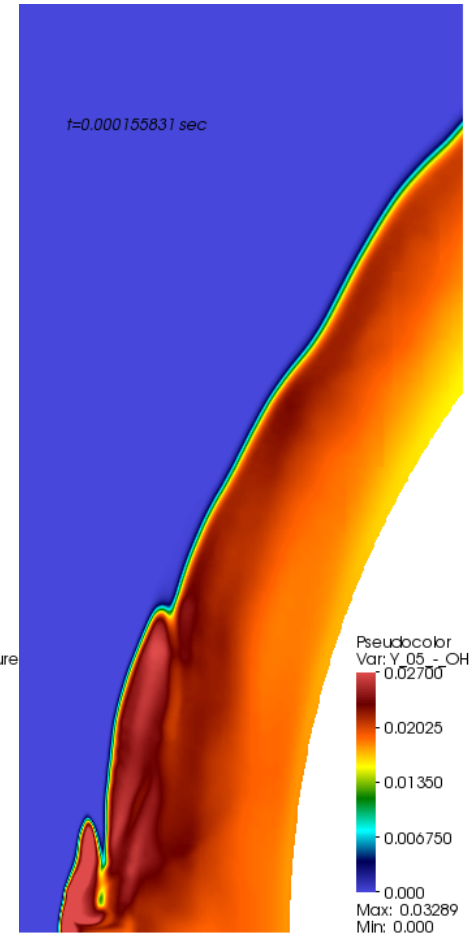

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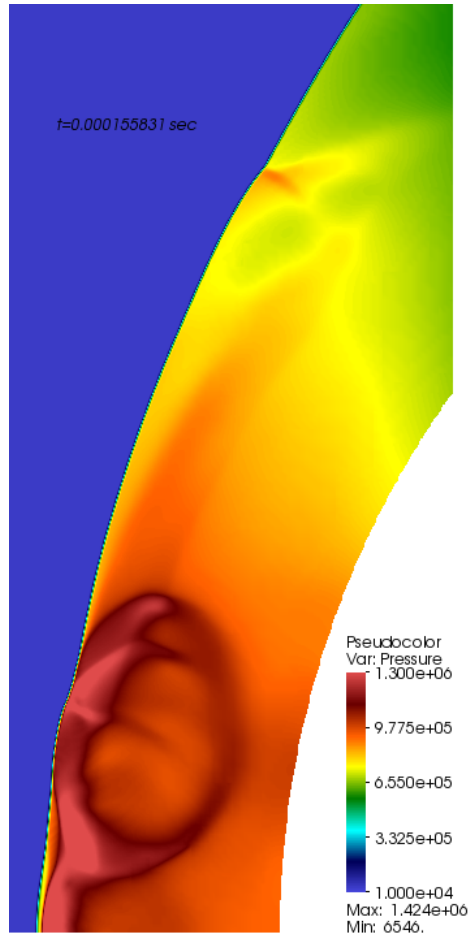

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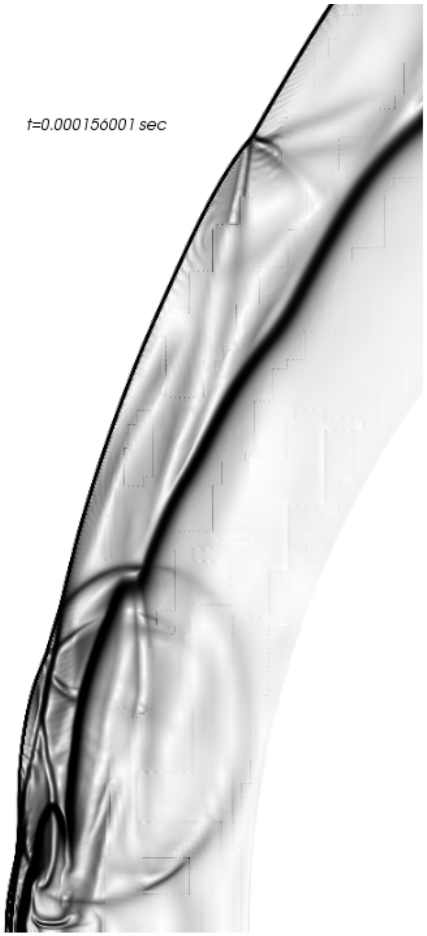
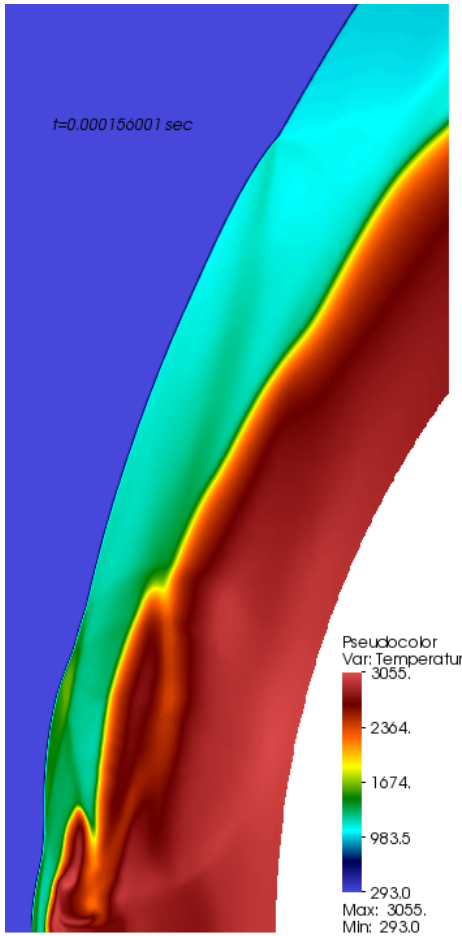


Temperature



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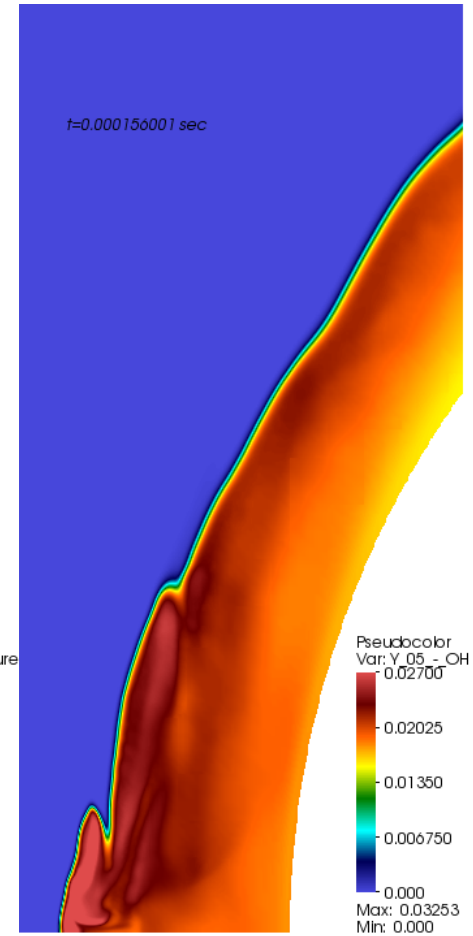
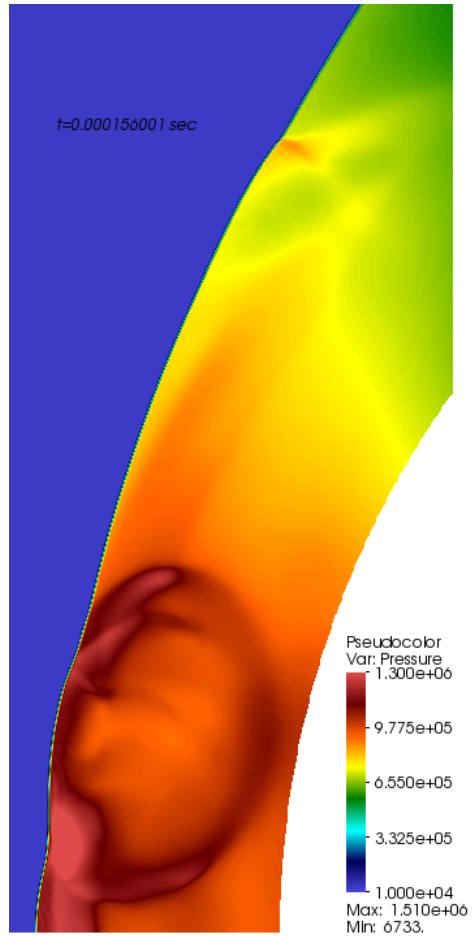


Pressure



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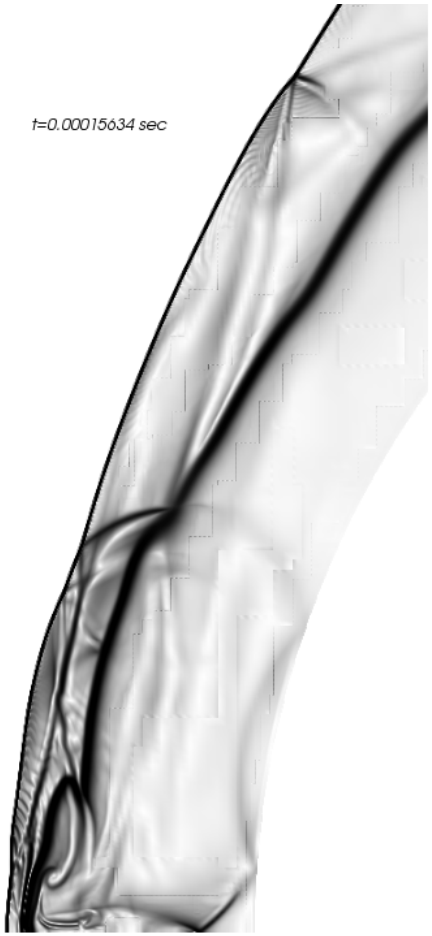
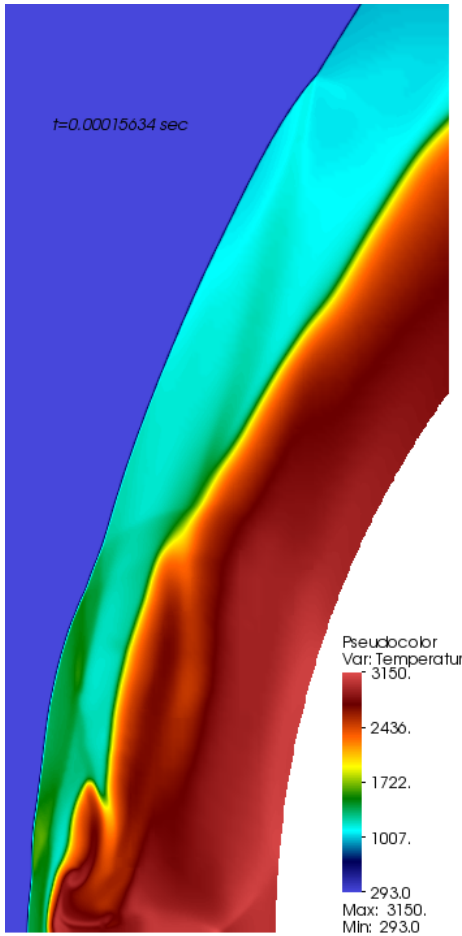


Temperature



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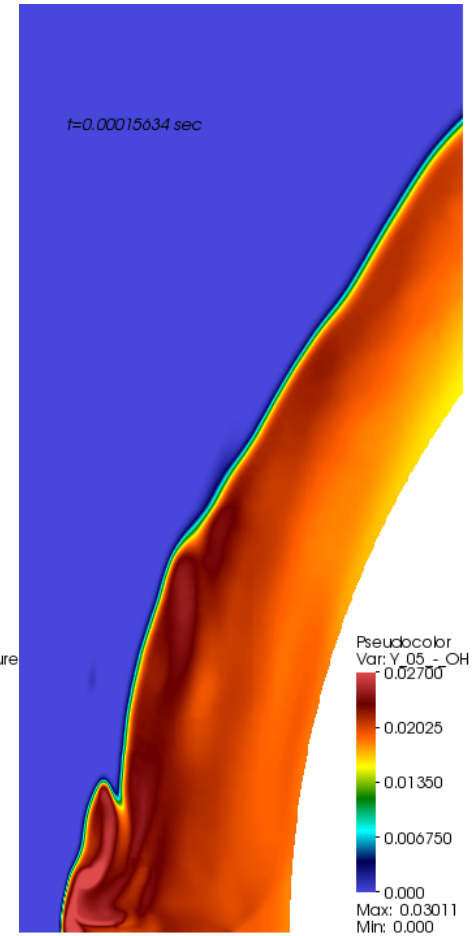
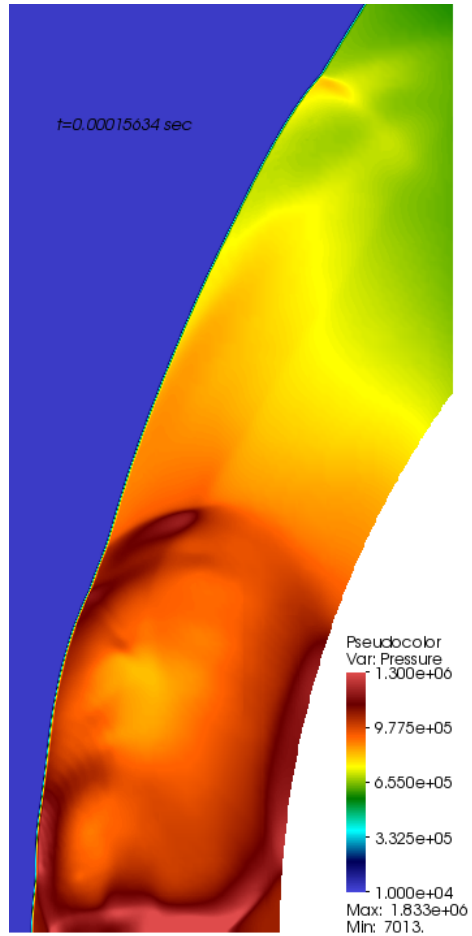


Pressure



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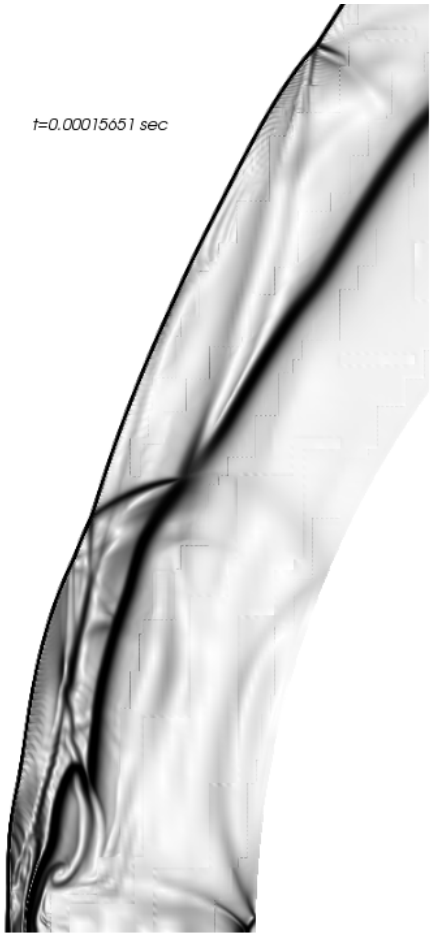
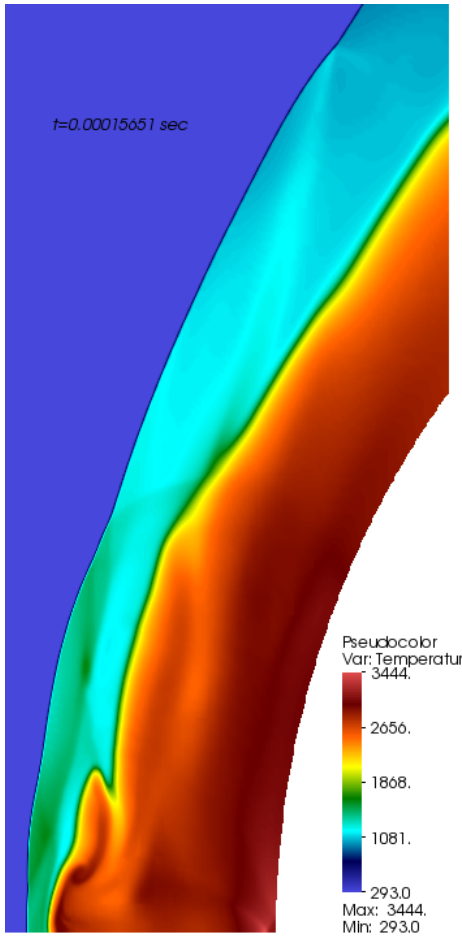


Temperature



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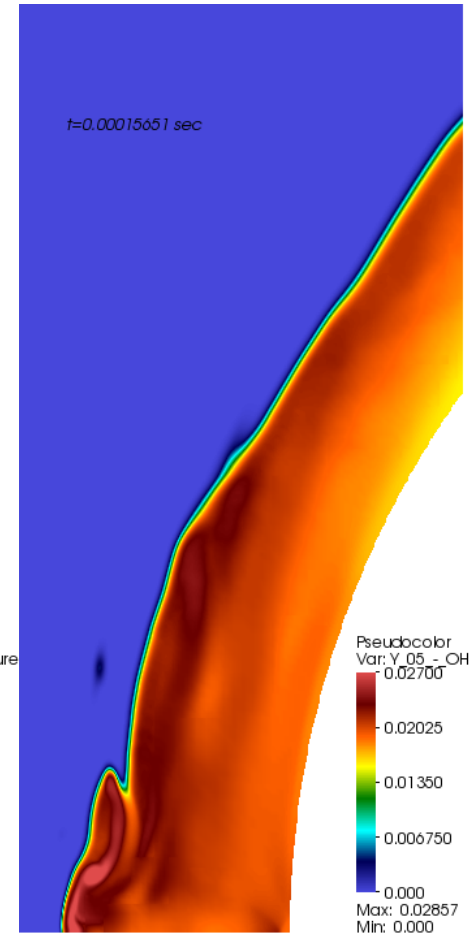
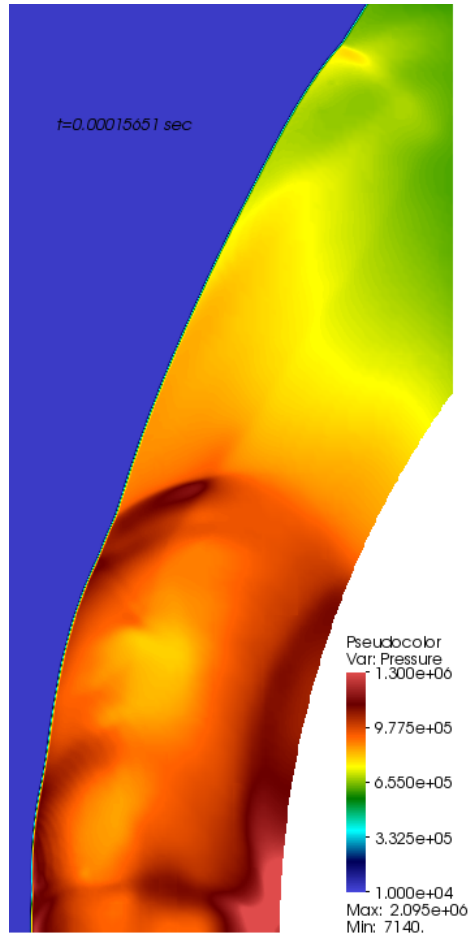


Pressure



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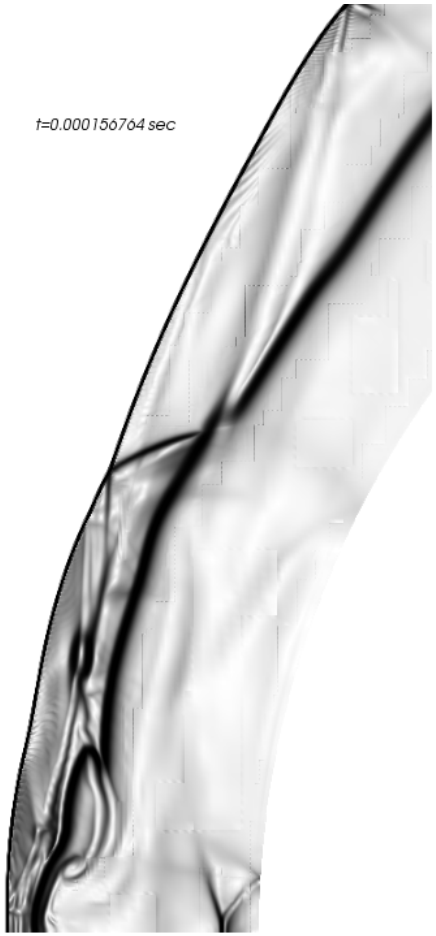
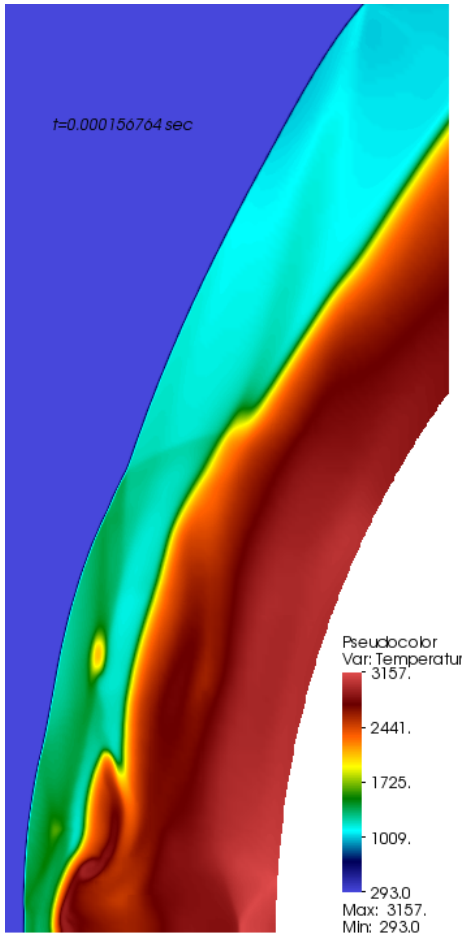


Temperature



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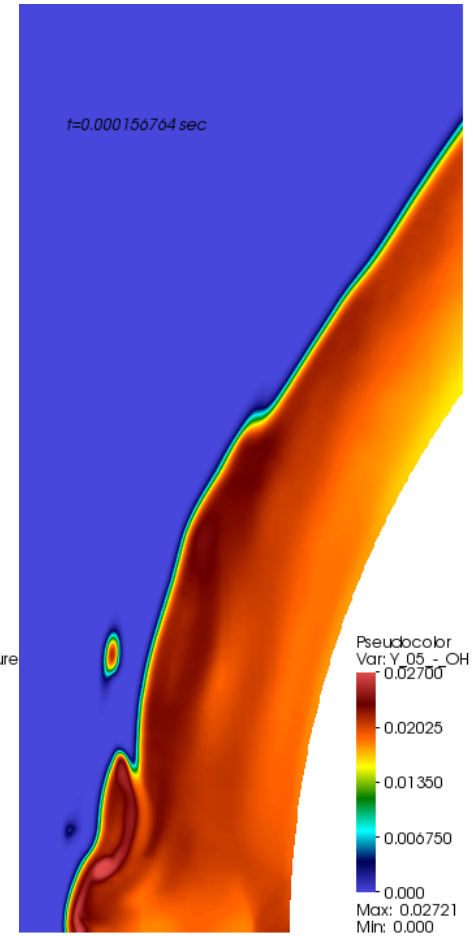
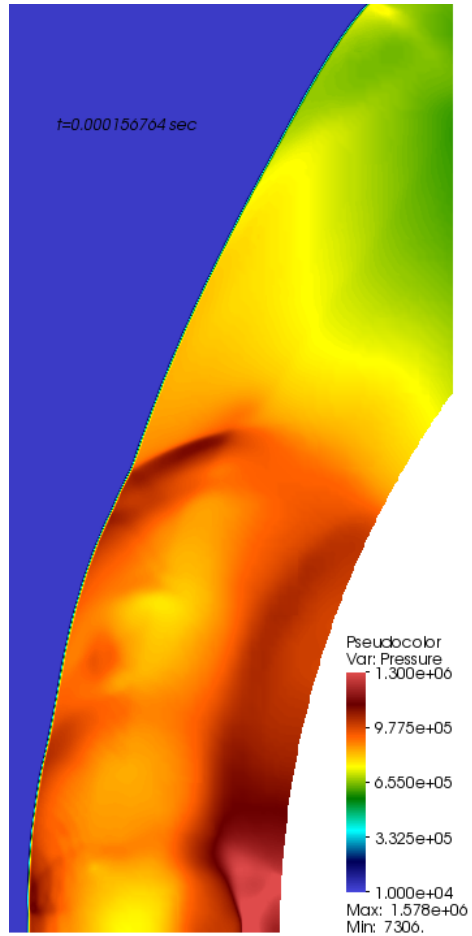


Pressure



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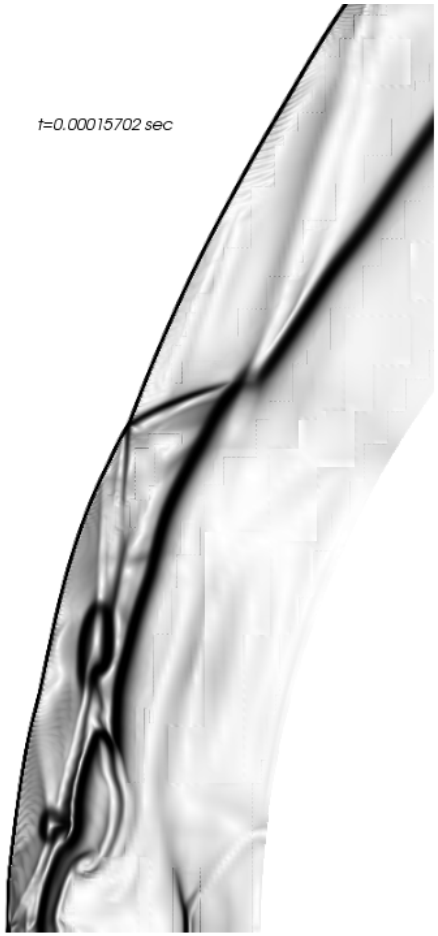

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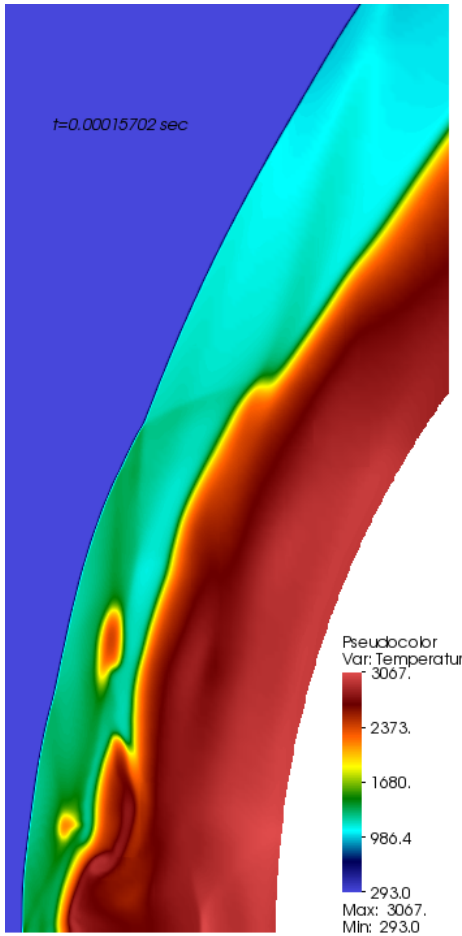

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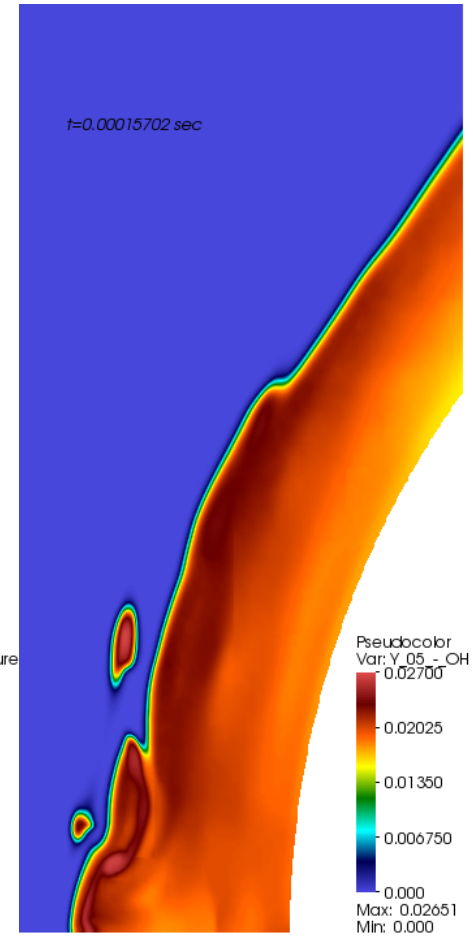

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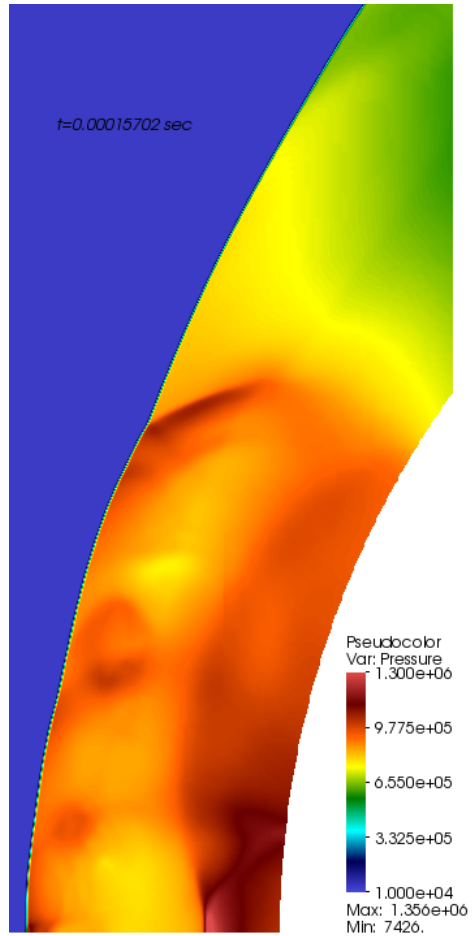

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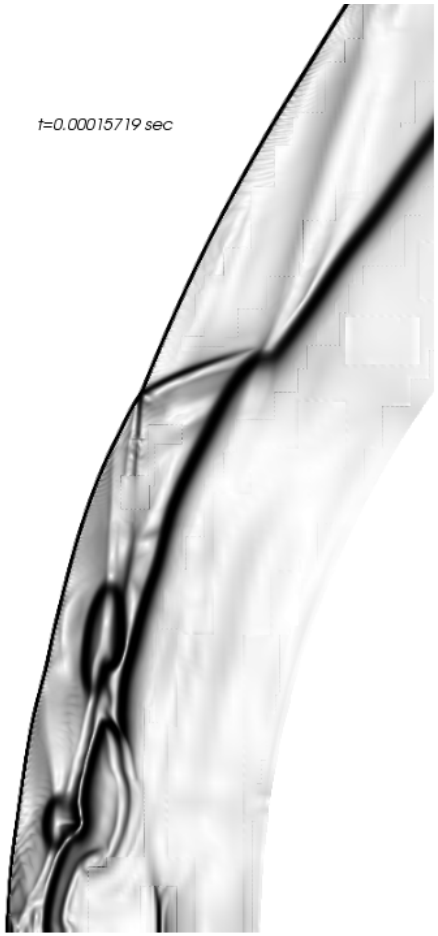

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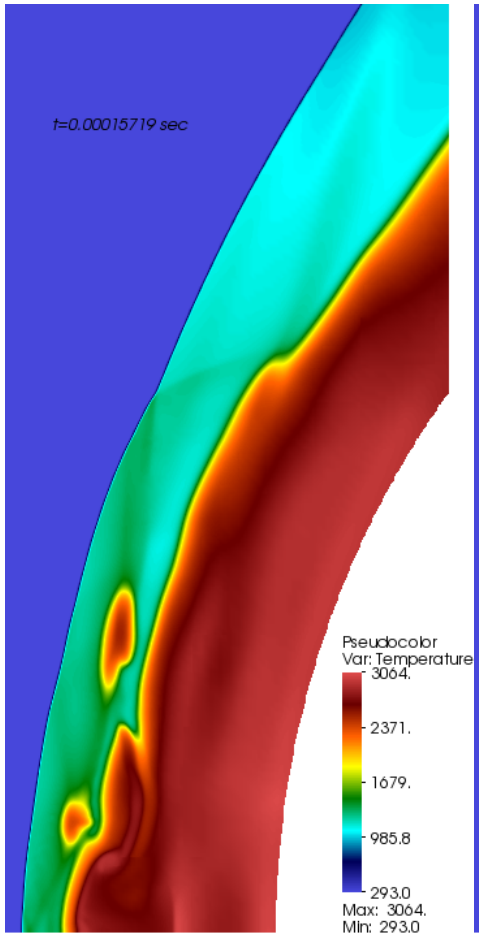

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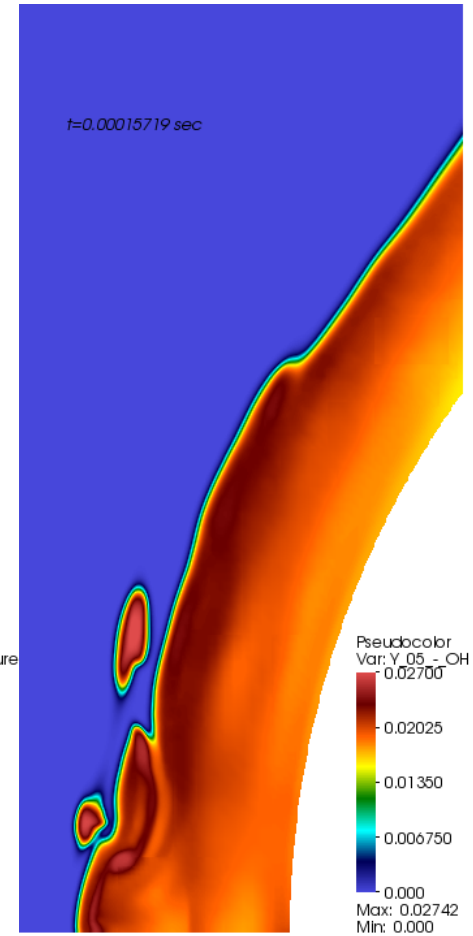

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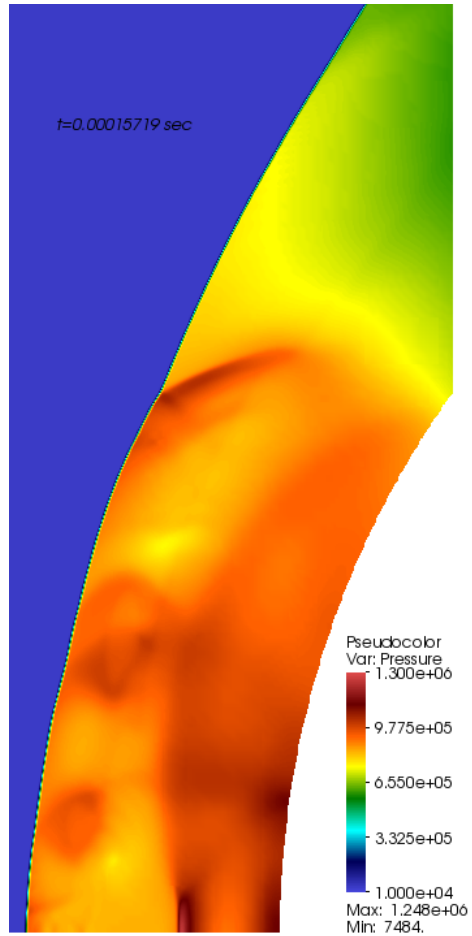

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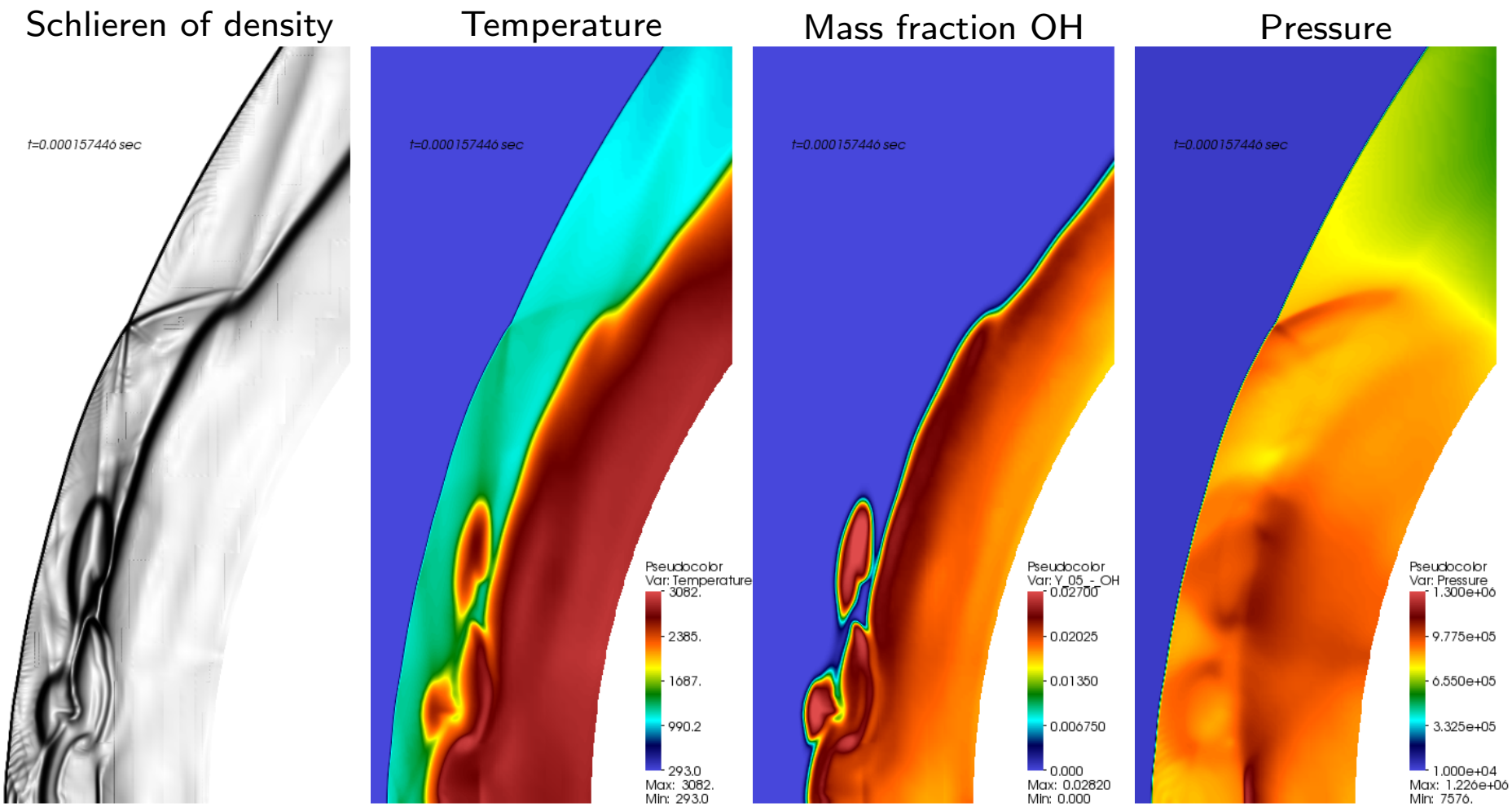

- Small perturbations can quickly create numerous triple points

Hybrid method

Convective numerical flux is defined as

$$\mathbf{F}^n_{inv} = \begin{cases} \mathbf{F}^n_{inv-WENO}, & \text{in } \mathcal{C} \\ \mathbf{F}^n_{inv-CD}, & \text{in } \overline{\mathcal{C}}, \end{cases}$$

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1. Lax-Liu entropy condition $|u_R \pm a_R| < |u_* \pm a_*| < |u_L \pm a_L|$ tested with a threshold to eliminate weak acoustic waves. Used intermediate states at cell interfaces:

$$u_* = \frac{\sqrt{\rho_L}u_L + \sqrt{\rho_R}u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \quad a_* = \sqrt{(\gamma_* - 1)(h_* - \frac{1}{2}u_*^2)}, \ldots$$

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2. Limiter-inspired discontinuity test based on mapped normalized pressure gradient θ_j

$$\phi(\theta_j) = \frac{2\theta_j}{(1+\theta_j)^2} \quad \text{with} \quad \theta_j = \frac{|p_{j+1} - p_j|}{|p_{j+1} + p_j|}, \quad \phi(\theta_j) > \alpha_{Map}$$

SAMR flux correction for Runge-Kutta method

Recall Runge-Kutta temporal update

$$\tilde{\mathbf{Q}}_j^{\upsilon} = \alpha_{\upsilon}\,\mathbf{Q}_j^{m} + \beta_{\upsilon}\,\tilde{\mathbf{Q}}_j^{\upsilon-1} + \gamma_{\upsilon}\,\frac{\Delta t}{\Delta x_n}\,\Delta\mathbf{F}^{n}(\tilde{\mathbf{Q}}^{\upsilon-1})$$

[Pantano et al., 2007]

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rewrite scheme as

$$\mathbf{Q}^{m+1} = \mathbf{Q}^{m} - \sum_{\upsilon=1}^{\Upsilon} \varphi_{\upsilon}\,\frac{\Delta t}{\Delta x_n}\,\Delta\mathbf{F}^{n}(\tilde{\mathbf{Q}}^{\upsilon-1}) \quad \text{with} \quad \varphi_{\upsilon} = \gamma_{\upsilon} \prod_{\nu=\upsilon+1}^{\Upsilon} \beta_{\nu}$$

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2. $\delta\mathbf{F}^{1,l+1}_{i-\frac{1}{2},j} := \delta\mathbf{F}^{1,l+1}_{i-\frac{1}{2},j} + \frac{1}{r_{l+1}^2}\sum_{\iota=0}^{r_{l+1}-1}\sum_{\upsilon=1}^{\Upsilon}\varphi_{\upsilon}\mathbf{F}^{1,l+1}_{v+\frac{1}{2},w+\iota}\left(\tilde{\mathbf{Q}}^{\upsilon-1}(t+\kappa\Delta t_{l+1})\right)$

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Flux correction to be used

1. $\delta\mathbf{F}^{1,l+1}_{i-\frac{1}{2},j} := -\varphi_1\mathbf{F}^{1,l}_{i-\frac{1}{2},j}(\tilde{\mathbf{Q}}^0)\,, \qquad \delta\mathbf{F}^{1,l+1}_{i-\frac{1}{2},j} := \delta\mathbf{F}^{1,l+1}_{i-\frac{1}{2},j} - \sum_{\upsilon=2}^{\Upsilon}\varphi_{\upsilon}\mathbf{F}^{1,l}_{i-\frac{1}{2},j}(\tilde{\mathbf{Q}}^{\upsilon-1})$

2. $\delta\mathbf{F}^{1,l+1}_{i-\frac{1}{2},j} := \delta\mathbf{F}^{1,l+1}_{i-\frac{1}{2},j} + \frac{1}{r_{l+1}^2}\sum_{\iota=0}^{r_{l+1}-1}\sum_{\upsilon=1}^{\Upsilon}\varphi_{\upsilon}\mathbf{F}^{1,l+1}_{v+\frac{1}{2},w+\iota}\left(\tilde{\mathbf{Q}}^{\upsilon-1}(t+\kappa\Delta t_{l+1})\right)$

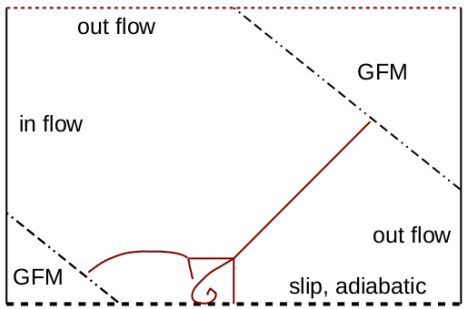
Storage-efficient SSPRK(3,3):

υ	α_{υ}	β_{υ}	γ_{υ}	φ_{υ}
1	1	0	1	$\frac{1}{6}$
2	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{6}$
3	$\frac{1}{2}$	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$

[Pantano et al., 2007]

DNS of shear layer in detonation triple point

- Calorically perfect two-species model with $\gamma = 1.29499$ and $h_0 = 54,000\,\mathrm{J/mol}$ and one-step Arrhenius reaction with parameters $E_a = 30,000\,\mathrm{J/mol}$, $A = 6 \cdot 10^5\,\mathrm{s}^{-1}$, $W = 0.029\,\mathrm{kg/mol}$ $\longrightarrow$ 1d ZND theory predicts $d_{\mathrm{CJ}} = 1587.8\,\mathrm{m/s}$
- For dynamic viscosity, heat conductivity, and mass diffusion simple Sutherland models are used
- Distance $L(t) = d_{\mathrm{CJ}} \sin(\theta) t$ is used to define a Reynolds number as $\mathrm{Re} = \frac{\rho_0 a_0 L(t)}{\mu_0}$
- Viscous shear layer thickness, thermal heat conduction layer thickness, and mass diffusion layer thickness grow as $\delta_{\mathrm{visc}} \approx \sqrt{\frac{\mu}{\rho} t}$, $\delta_{\mathrm{cond}} \approx \sqrt{\frac{k_{\mathrm{ref}}}{\rho c_v} t}$, $\delta_{\mathrm{mass,i}} \approx \sqrt{\frac{D_i}{\rho} t}$
- Only shock thickness not resolved $\longrightarrow$ "pseudo-DNS"
- Computations with WENO/CD/RK3 use SAMR base mesh 320 $\times$ 160 and up to 8 levels refined by factor 2, domain: $40\,\mathrm{mm} \times 20\,\mathrm{mm}$
- Computations with MUSCL scheme use base mesh 590 $\times$ 352 and up to 7 levels refined by factor 2, domain: $40\,\mathrm{mm} \times 22\,\mathrm{mm}$



Setup

DNS of shear layer in detonation triple point

- Calorically perfect two-species model with $\gamma = 1.29499$ and $h_0 = 54,000\,\mathrm{J/mol}$ and one-step Arrhenius reaction with parameters $E_a = 30,000\,\mathrm{J/mol}$, $A = 6 \cdot 10^5\,\mathrm{s}^{-1}$, $W = 0.029\,\mathrm{kg/mol}$ $\longrightarrow$ 1d ZND theory predicts $d_{\mathrm{CJ}} = 1587.8\,\mathrm{m/s}$
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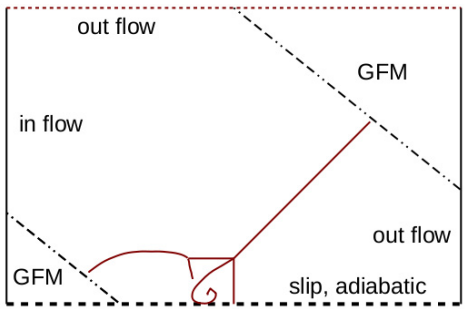
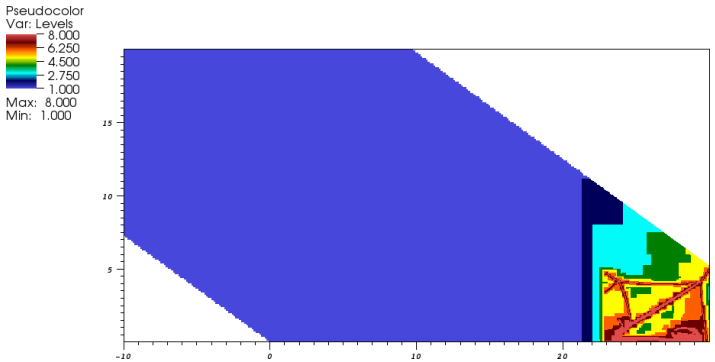


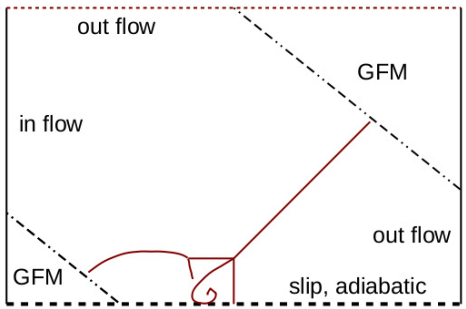
Setup



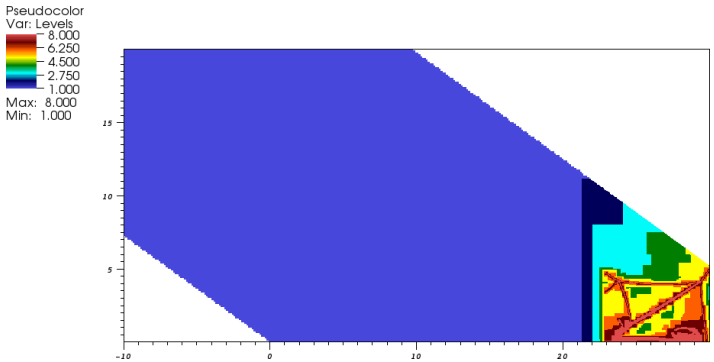
Refinement

DNS of shear layer in detonation triple point

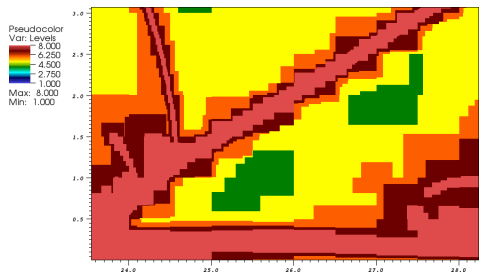
- Calorically perfect two-species model with $\gamma = 1.29499$ and $h_0 = 54,000\,\mathrm{J/mol}$ and one-step Arrhenius reaction with parameters $E_a = 30,000\,\mathrm{J/mol}$, $A = 6 \cdot 10^5\,\mathrm{s}^{-1}$, $W = 0.029\,\mathrm{kg/mol}$ $\longrightarrow$ 1d ZND theory predicts $d_{\mathrm{CJ}} = 1587.8\,\mathrm{m/s}$
- For dynamic viscosity, heat conductivity, and mass diffusion simple Sutherland models are used
- Distance $L(t) = d_{\mathrm{CJ}} \sin(\theta) t$ is used to define a Reynolds number as $\mathrm{Re} = \frac{\rho_0 a_0 L(t)}{\mu_0}$
- Viscous shear layer thickness, thermal heat conduction layer thickness, and mass diffusion layer thickness grow as $\delta_{\mathrm{visc}} \approx \sqrt{\frac{\mu}{\rho} t}$, $\delta_{\mathrm{cond}} \approx \sqrt{\frac{k_{\mathrm{ref}}}{\rho c_v} t}$, $\delta_{\mathrm{mass,i}} \approx \sqrt{\frac{D_i}{\rho} t}$
- Only shock thickness not resolved $\longrightarrow$ "pseudo-DNS"
- Computations with WENO/CD/RK3 use SAMR base mesh 320 $\times$ 160 and up to 8 levels refined by factor 2, domain: $40\,\mathrm{mm} \times 20\,\mathrm{mm}$
- Computations with MUSCL scheme use base mesh 590 $\times$ 352 and up to 7 levels refined by factor 2, domain: $40\,\mathrm{mm} \times 22\,\mathrm{mm}$



Setup



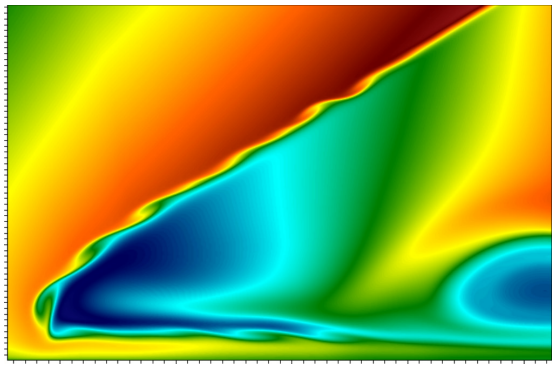
Refinement



Enlarged

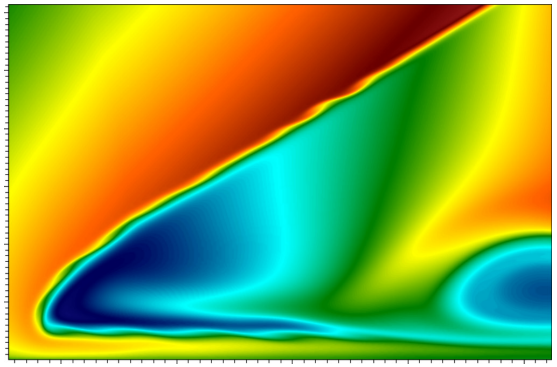
Computational results for shear layer

WENO/CD - 6 levels



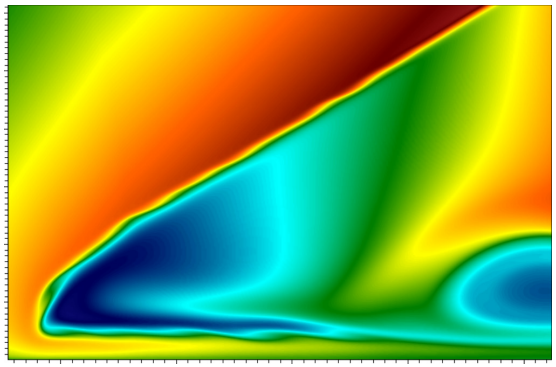
$\Delta x_{\min} = 3.91 \cdot 10^{-6}\,\mathrm{m}$

WENO/CD - 7 levels



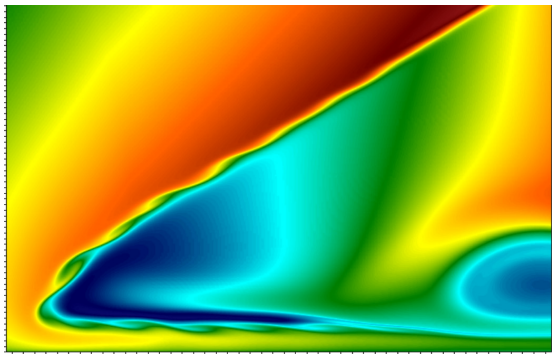
$\Delta x_{\min} = 1.95 \cdot 10^{-6}\,\mathrm{m}$

WENO/CD - 8 levels



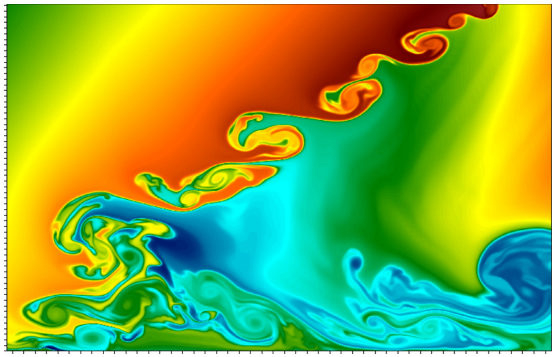
$\Delta x_{\min} = 9.77 \cdot 10^{-7}\,\mathrm{m}$

MUSCL - 7 levels



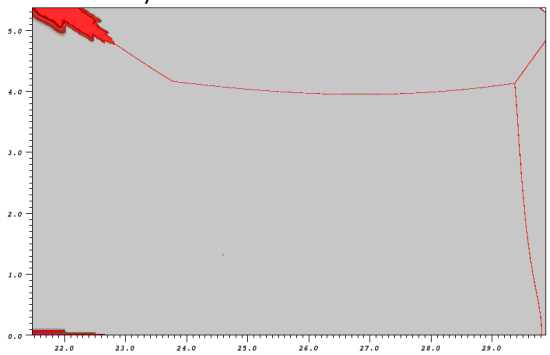
$\Delta x_{\min} = 1.05 \cdot 10^{-6}\,\mathrm{m}$

MUSCL - 7 levels - Euler



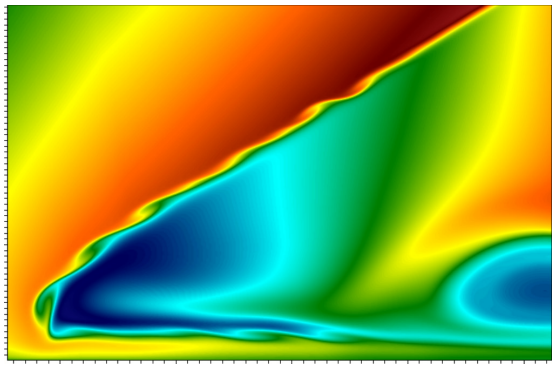
$\Delta x_{\min} = 1.05 \cdot 10^{-6}\,\mathrm{m}$

Usage of WENO for WENO/CD - 8 levels



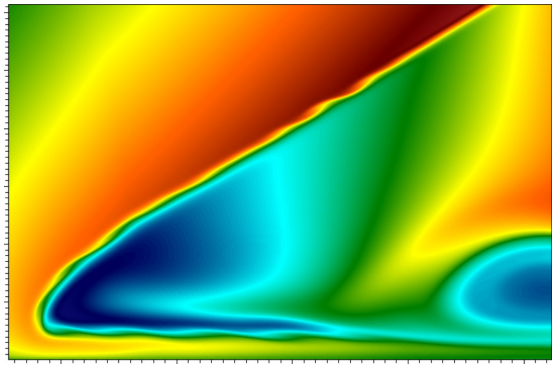
Computational results for shear layer

WENO/CD - 6 levels



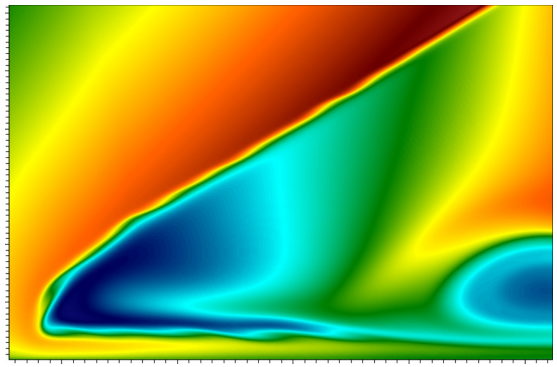
$\Delta x_{\min} = 3.91 \cdot 10^{-6}\,\mathrm{m}$

WENO/CD - 7 levels



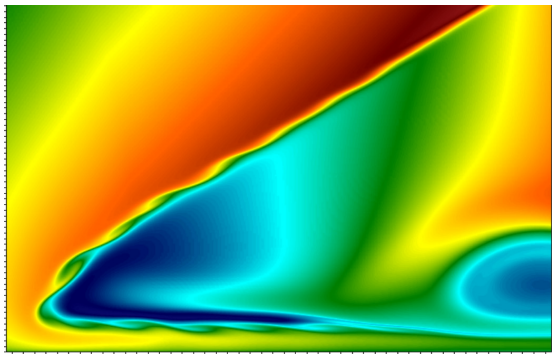
$\Delta x_{\min} = 1.95 \cdot 10^{-6}\,\mathrm{m}$

WENO/CD - 8 levels



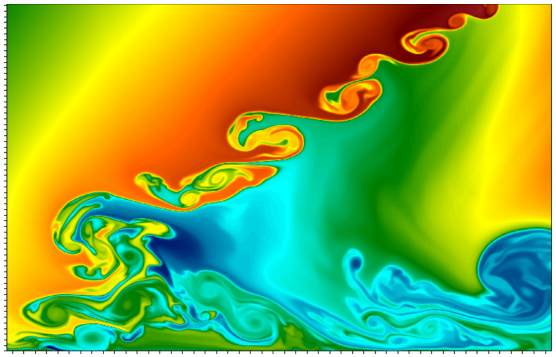
$\Delta x_{\min} = 9.77 \cdot 10^{-7}\,\mathrm{m}$

MUSCL - 7 levels



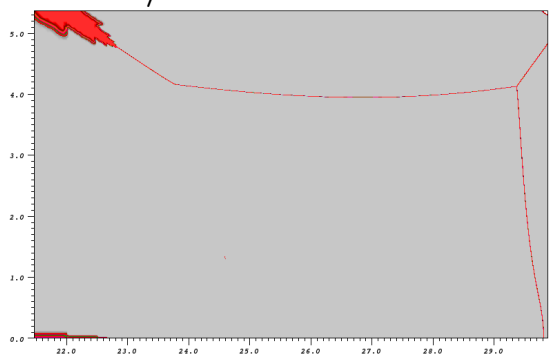
$\Delta x_{\min} = 1.05 \cdot 10^{-6}\,\mathrm{m}$

MUSCL - 7 levels - Euler



$\Delta x_{\min} = 1.05 \cdot 10^{-6}\,\mathrm{m}$

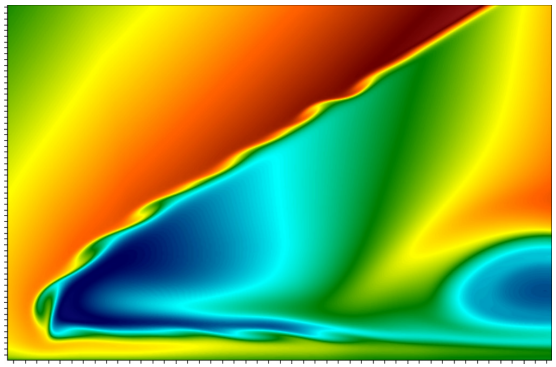
Usage of WENO for WENO/CD - 8 levels



- WENO/CD/RK3 gives results comparable to 4x finer resolved optimal 2nd-order scheme, but CPU times with SAMR 2-3x larger

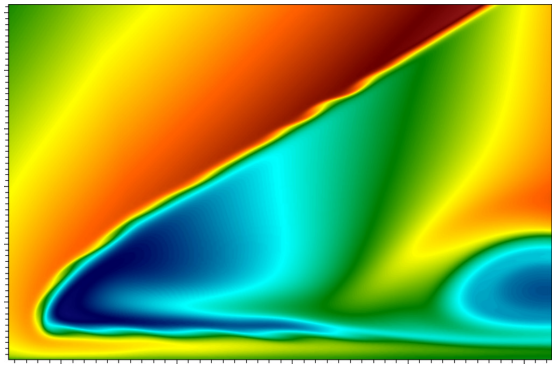
Computational results for shear layer

WENO/CD - 6 levels



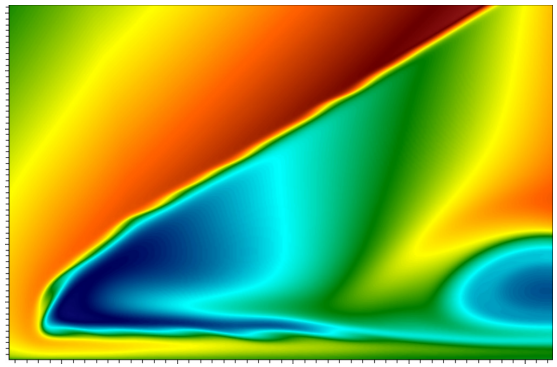
$\Delta x_{\min} = 3.91 \cdot 10^{-6}\,\mathrm{m}$

WENO/CD - 7 levels



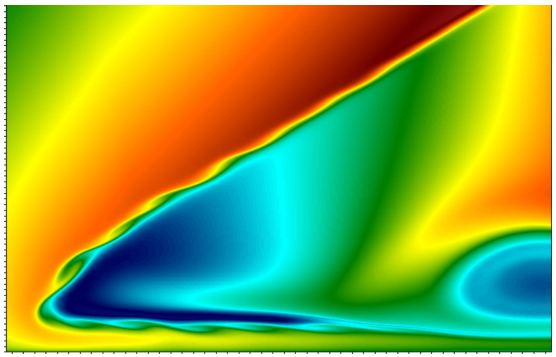
$\Delta x_{\min} = 1.95 \cdot 10^{-6}\,\mathrm{m}$

WENO/CD - 8 levels



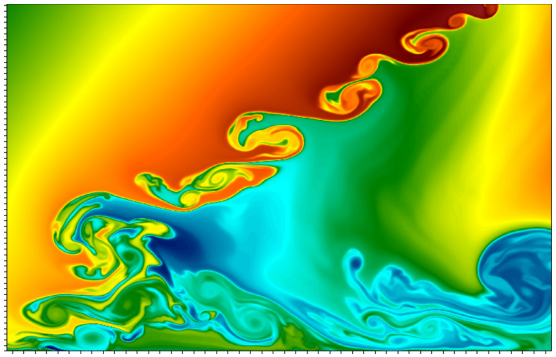
$\Delta x_{\min} = 9.77 \cdot 10^{-7}\,\mathrm{m}$

MUSCL - 7 levels



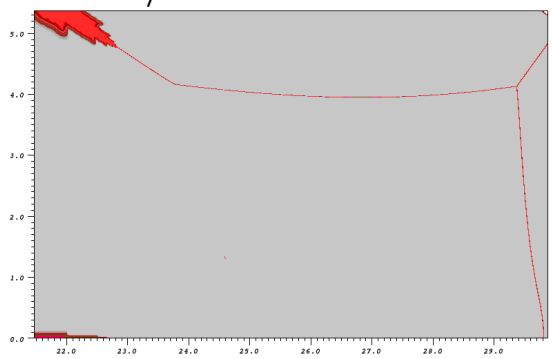
$\Delta x_{\min} = 1.05 \cdot 10^{-6}\,\mathrm{m}$

MUSCL - 7 levels - Euler



$\Delta x_{\min} = 1.05 \cdot 10^{-6}\,\mathrm{m}$

Usage of WENO for WENO/CD - 8 levels



- WENO/CD/RK3 gives results comparable to 4x finer resolved optimal 2nd-order scheme, but CPU times with SAMR 2-3x larger
- Gain in CPU time from higher-order scheme roughly one order

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