

Droplet formation

Stéphane Zaleski

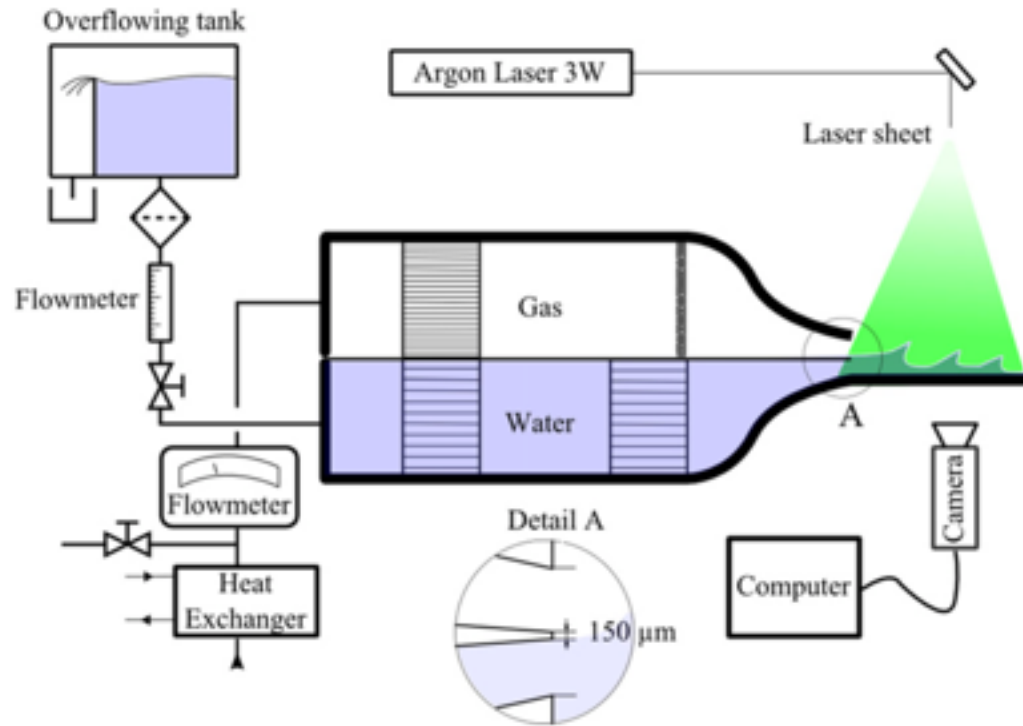
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CNRS & Université Pierre et Marie Curie – UPMC – Paris 6*

web site <http://www.ida.upmc.fr/~zaleski>

D'Alembert 



Grenoble experiment



Descamps et al, 2008
Matas et al., 2011
Jérôme et al, 2013
Fuster et al, 2013
Ling et al, 2015

and of course *Hopfinger,*
Lasheras, Cartellier,
Villermaux, Hoepffner,
Popinet, Boeck, Rossi ...

1) Is it possible to do a real Direct Numerical Simulation of atomisation, resolving all the scales ?

2) What can we learn from these very detailed simulations ?



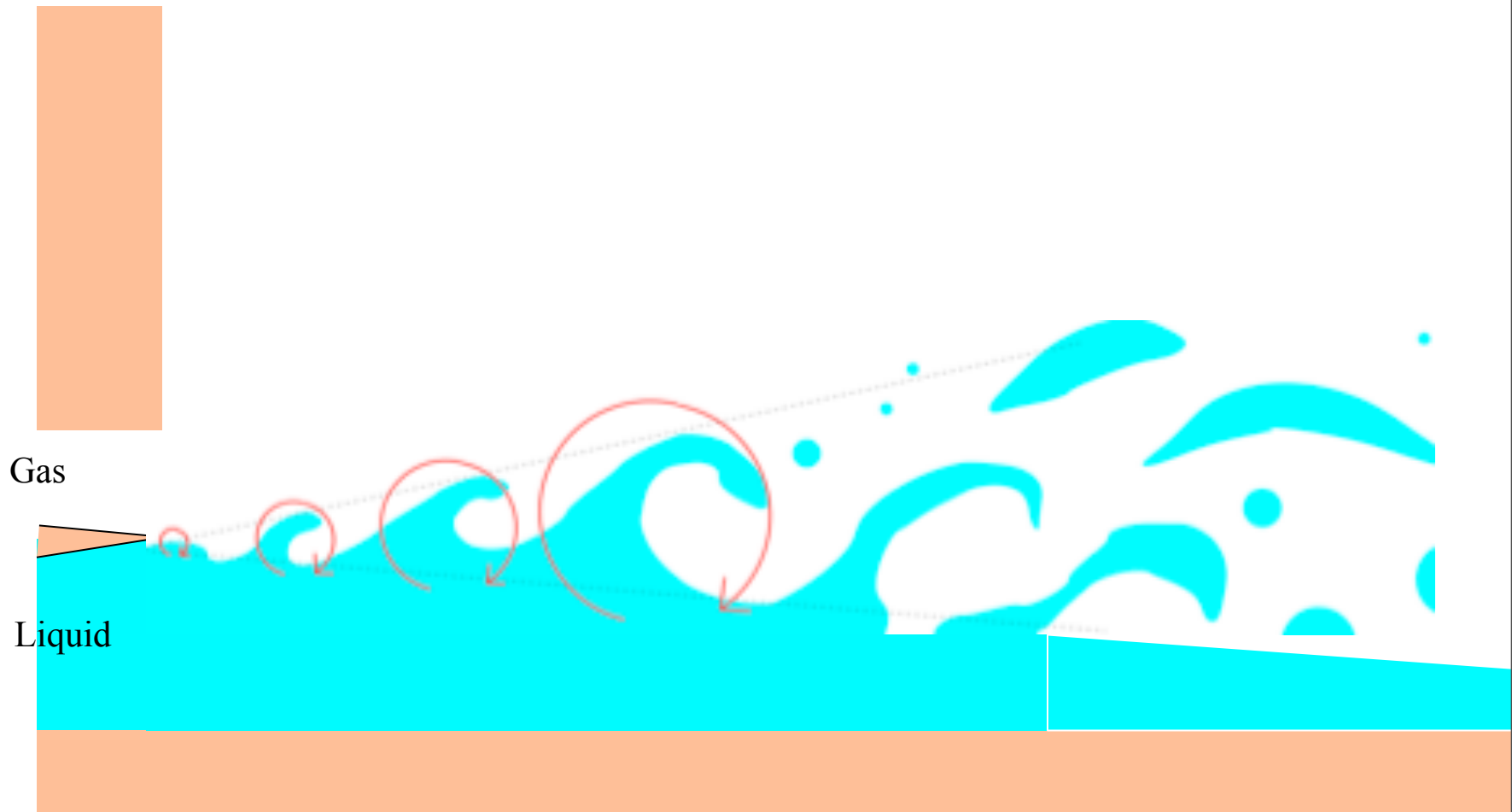
1) 2D flows

2) 3D flows



2D simulations of the planar « Grenoble » setup.

The Grenoble quasi 2D experiment set up



Navier-Stokes equations with interfaces

$$\partial_t(\rho \mathbf{u}) + \nabla \times (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \times (2\mu \mathbf{D}) + \sigma \kappa \delta_s \mathbf{n} + \rho \mathbf{g},$$

where the strain-rate tensor is:

$$D_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right),$$

and both fluids are considered incompressible

$$\nabla \cdot \mathbf{u} = 0.$$

Compressible fluids: possible but difficult and less relevant.

Surface tension

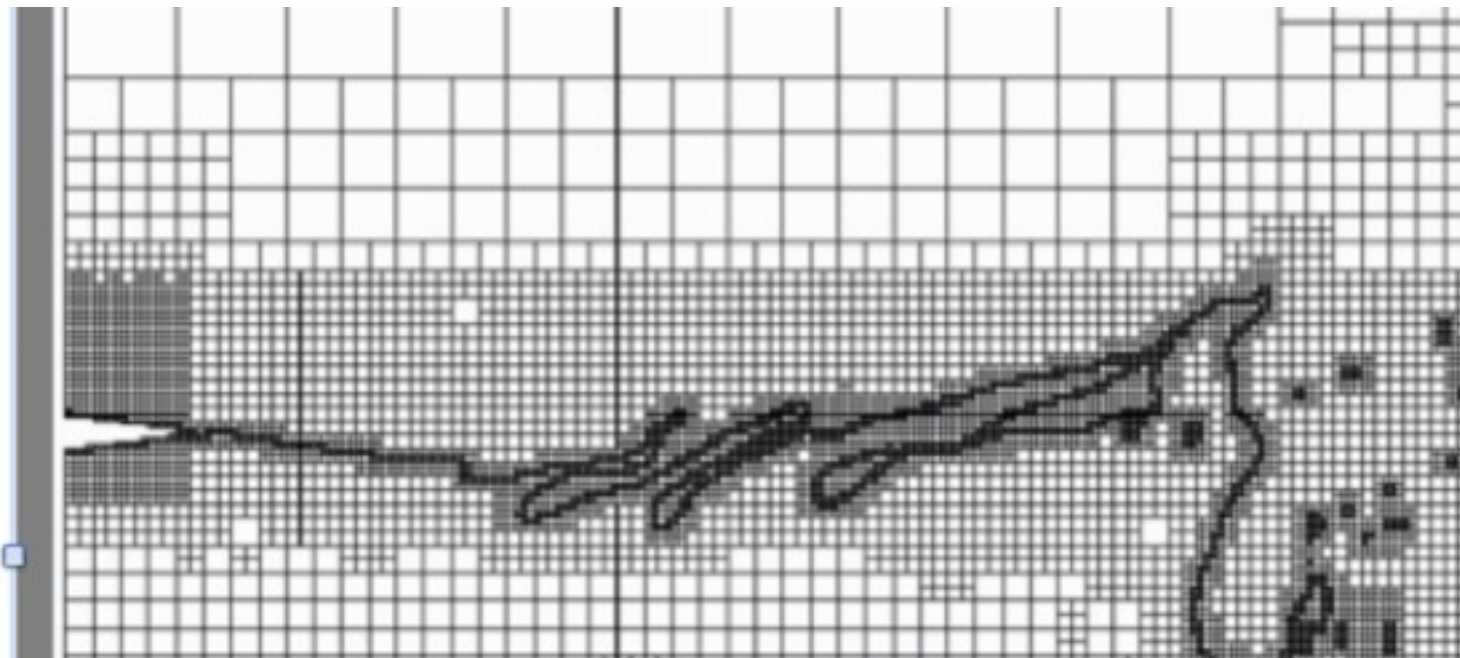
Treatment of surface tension by Continuous Surface Force
(« **CSF** » method, Brackbill, Kothe and Zemach JCP 1993)

$$\sigma \kappa \mathbf{n} \delta_S \approx \sigma \kappa^h \nabla^h C$$

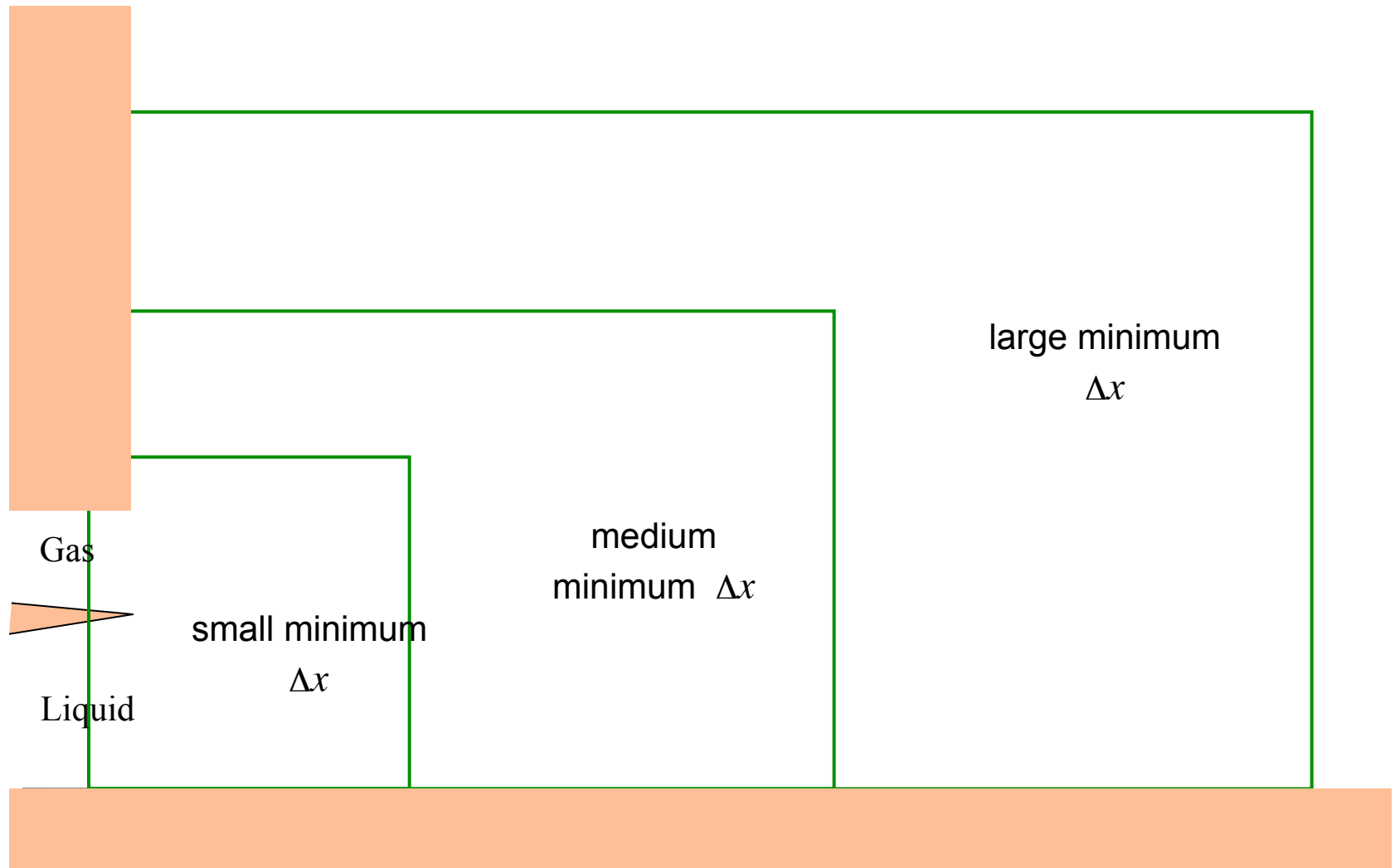
Many methods for κ .



Use Gerris flow solver (S. Popinet) with adaptive oct-tree and quad-tree grids

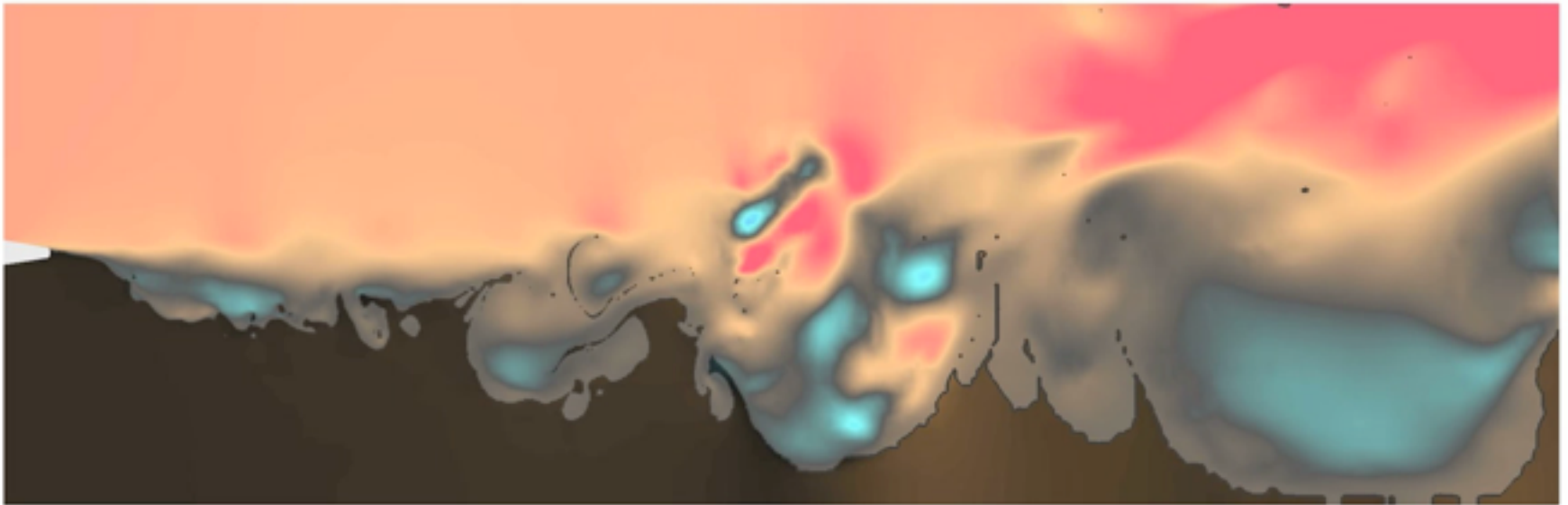


Navier-Stokes with variable minimum grid size according to a subdivision of the computational domain.



Simulation with a separator plate at density ratio ($1/r = 100$)

m	r	Re_g	Re_l	We_g	We_l	M
0.017	0,01	2640	290	19	8	2,4



Movie by Daniel Fuster and Jérôme Hoepffner using the Gerris Flow solver

Simulation with a separator plate at density ratio ($1/r = 100$)

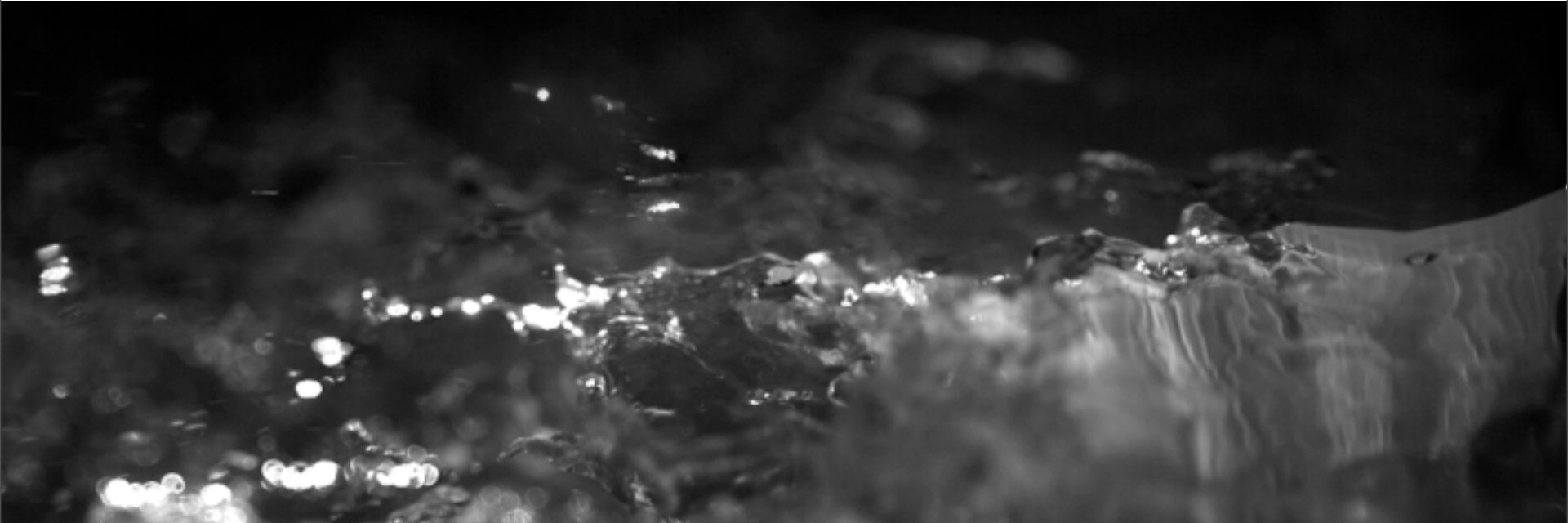
m	r	Re_g	Re_l	We_g	We_l	M
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Movie by Daniel Fuster and Jérôme Hoepffner using the Gerris Flow solver



Compare to experiments in Grenoble (Cartellier, Matas) . Flow from right to left.
Video with help of Jérôme Hoepffner and Jon Soundar.





Compare to experiments in Grenoble (Cartellier, Matas) . Flow from right to left.
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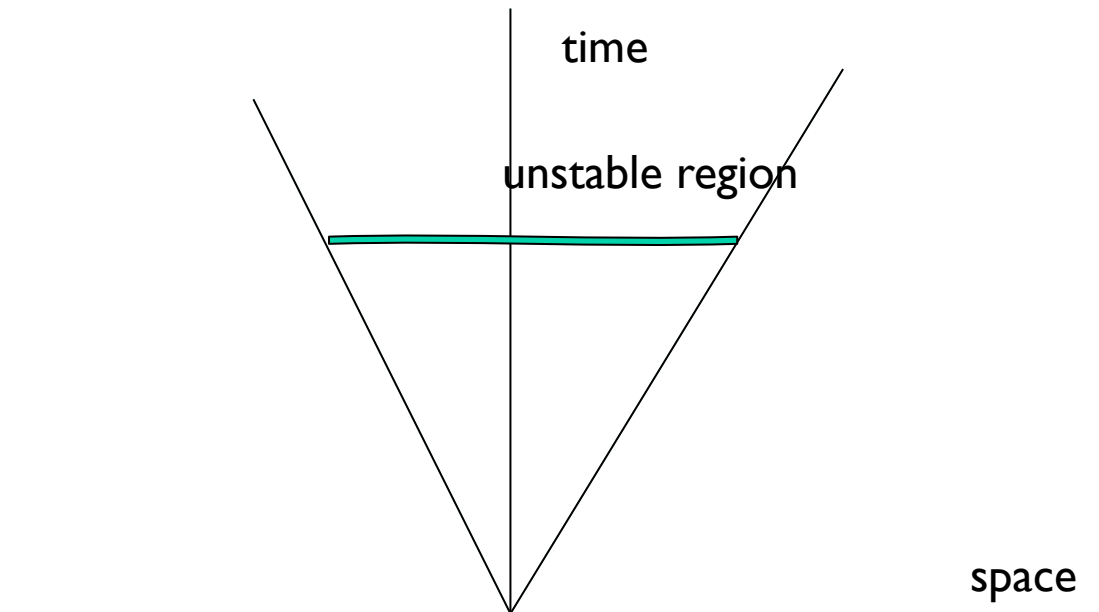
We need linear theory for spatially developing flows.

For that, we need to know what are **absolute and convective** instabilities !



Convective/absolute instabilities

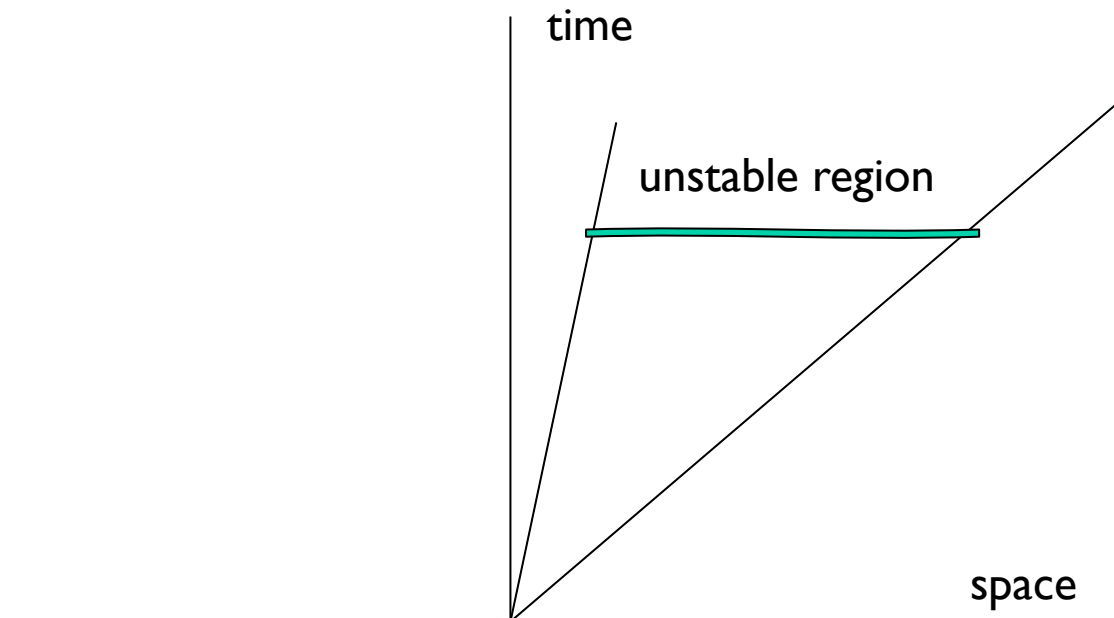
- 1) **Absolute**: a spatially localized perturbation at $x=0$ and $t=0$ grows in the entire space



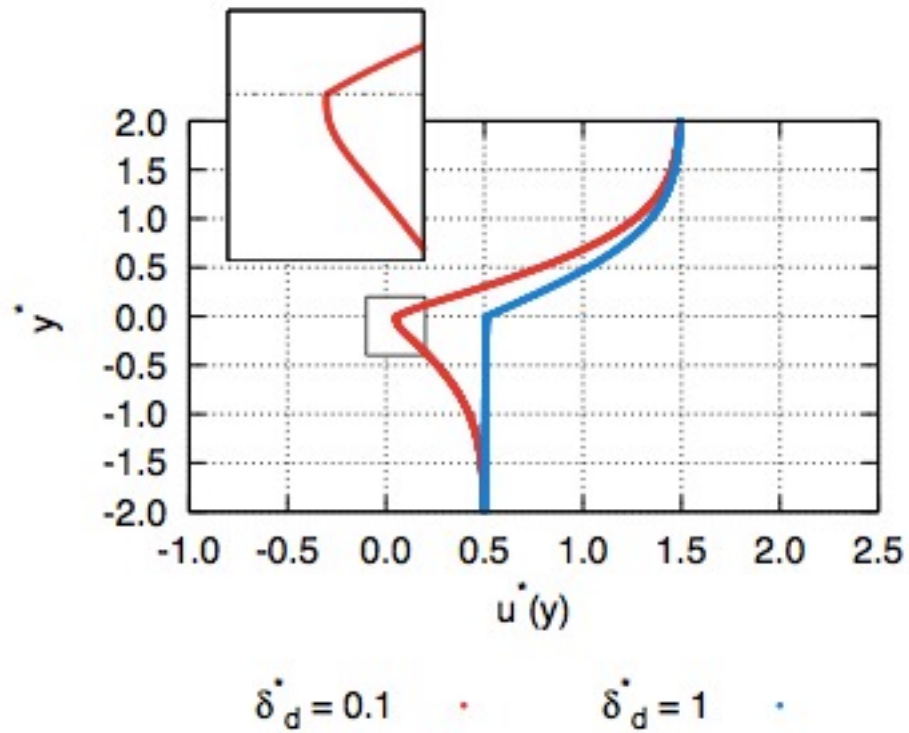
corresponds to a **well-defined oscillator frequency** in the entire domain, a so-called « **global mode** »

Convective/absolute instabilities

- 2) Convective instability: a spatially localized perturbation at $t=0$ is convected downstream with the flow



No single frequency is observed but instead, broadband noise is seen. The system is seen to be a **noise amplifier**. Upstream turbulence matters



Simplified base flows

Most important parameter: momentum flux ratio
(or ratio of dynamic pressures)

$$M = \frac{\rho_g u_g^2}{\rho_l u_l^2}$$

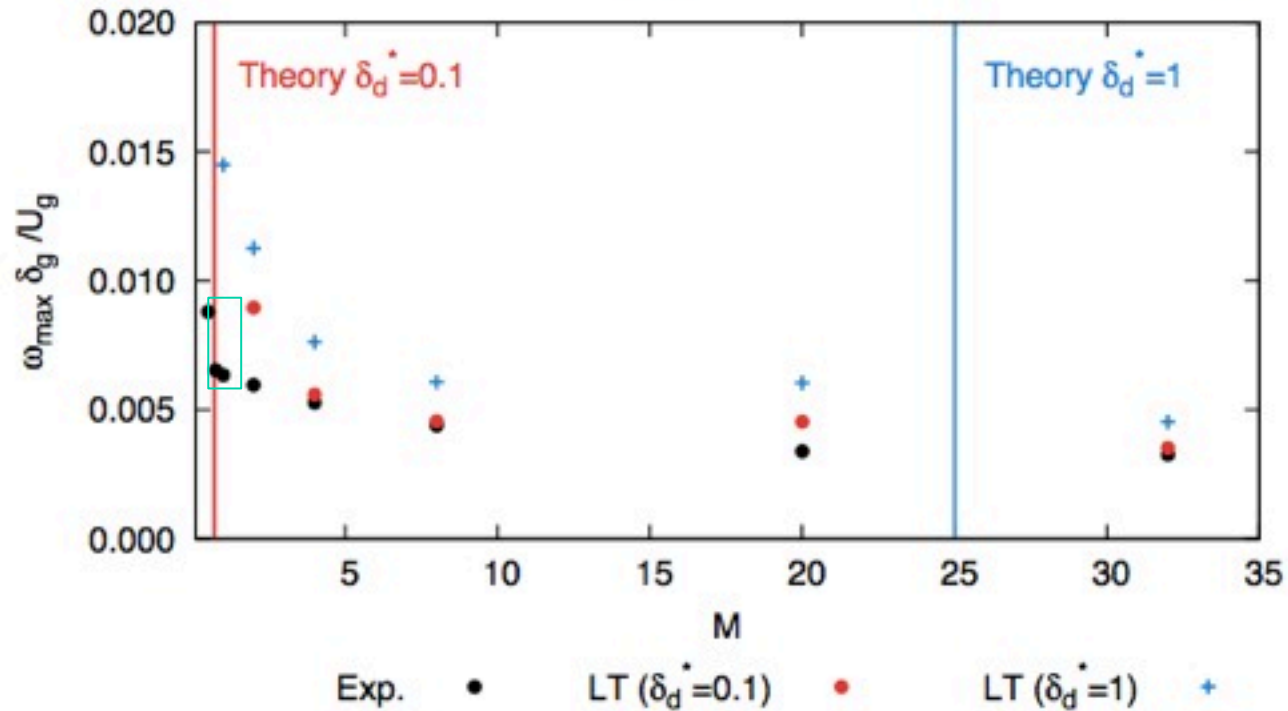
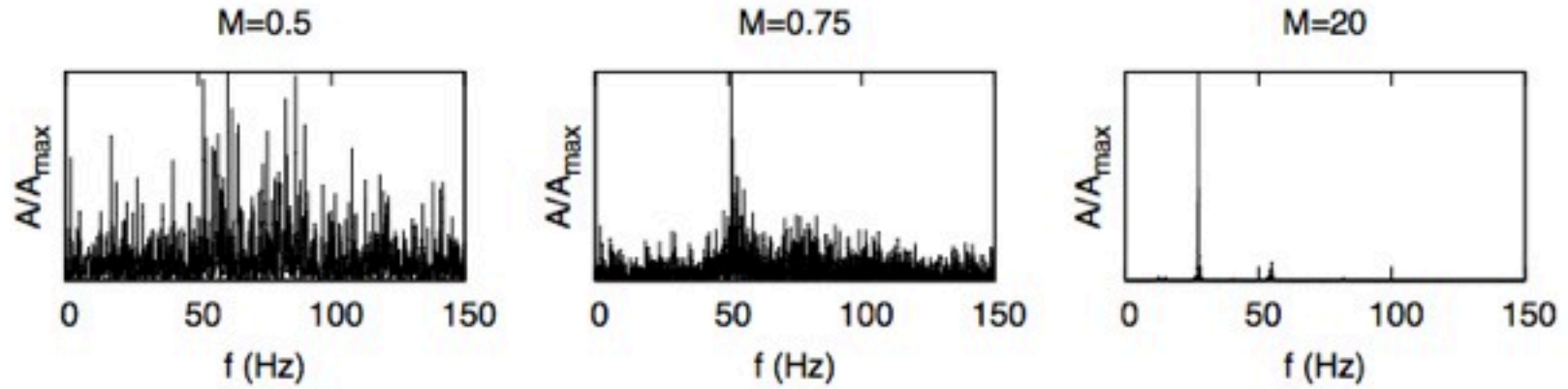


Grenoble experiments: Cartellier, Matas, Marty

convective, noise amplifier

ambiguous

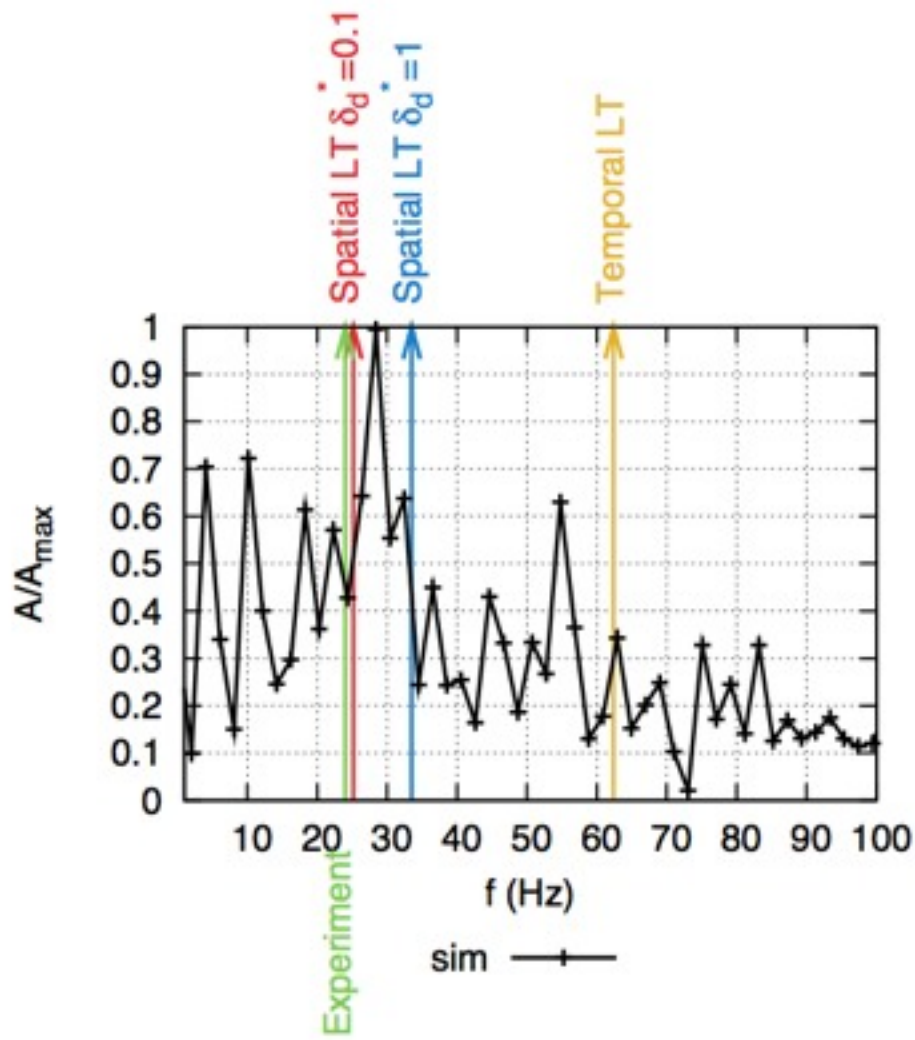
absolute, global mode



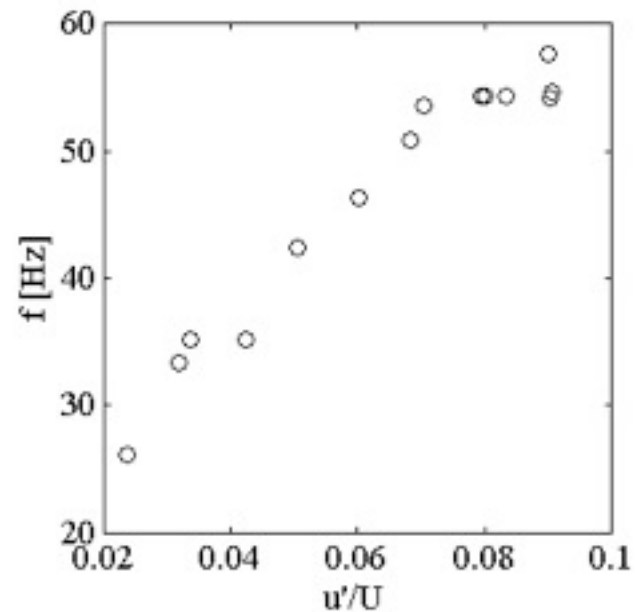
Now **the ultimate test** ! Compare :

- Experiments
- Numerics
- Linear theory





Primary instability of sheared interfaces is still a challenge however.



Strong influence of the turbulence level on the measured frequency.
Figure from Cartellier & Matas (LEGI)

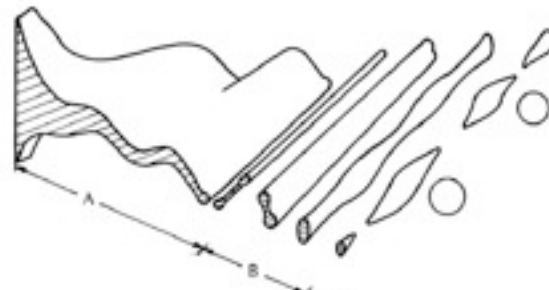
2) 3D: How do 2D sheets break into 3D ligaments and droplets ?



How do 2D sheets break into 3D ligaments and droplets ?

Two universal mechanisms:

1) Cylinder (rim) + Rayleigh-Plateau instability



Dombrowski and Johns (1983)
Zhang, Li V., Brunet, P., Eggers, J. & Deegan, R. D.
2010

2) Hole formation



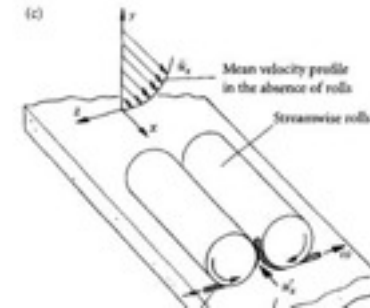
Roisman et al (2006)



Other more specialized mechanisms

for **atomization**

- streamline vortices pre-existing in the upstream bour



- Non-normal instability of two phase mixing layers (Yecko & Zaleski 2005)
(Squire theorem does not apply in two-phase situation, the non-normal instability also leads to streamwise vortices)

for **splashing**

- Richtmyer-Meshkov instability (Gueyffier & Zaleski 1998)

What is observed in atomization ?

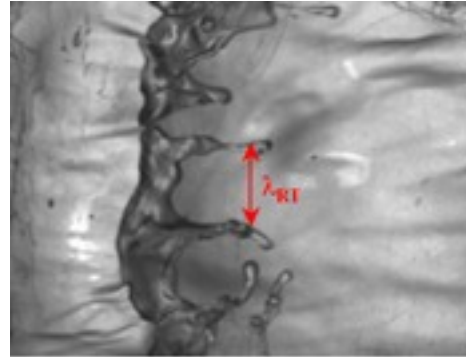
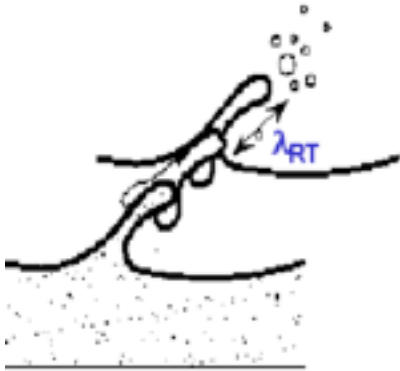


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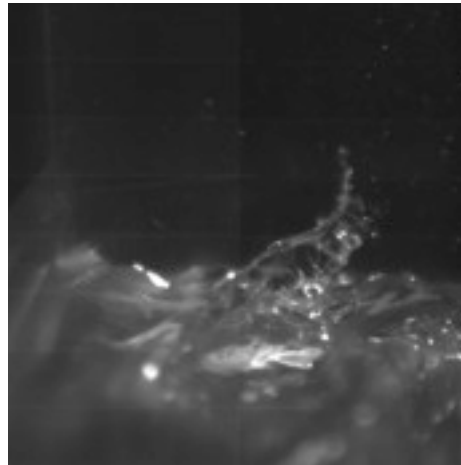
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2D waves + attached ligaments formation

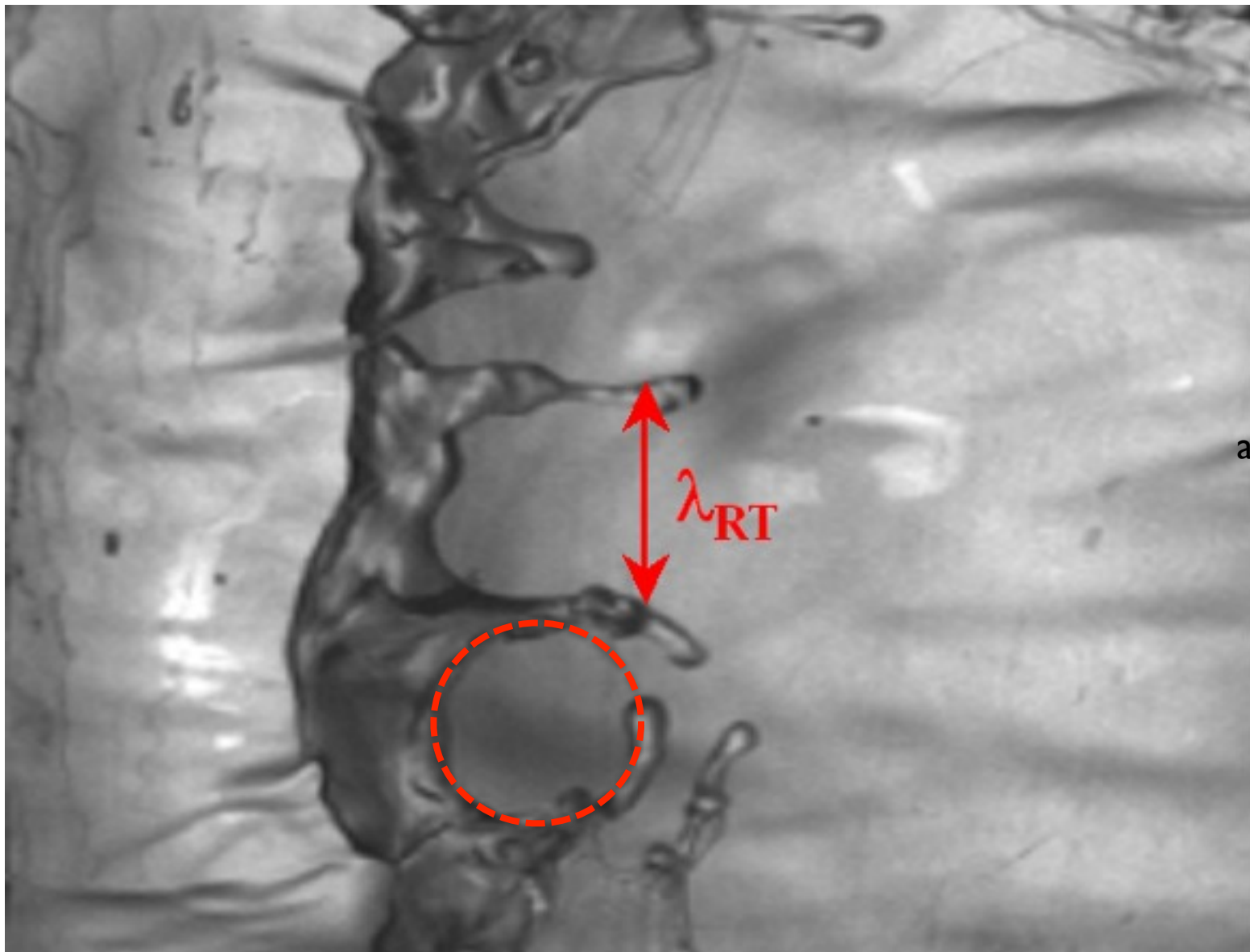


Photograph: Alain Cartellier and Jean-Philippe Matas

Holes + fishbone patterns



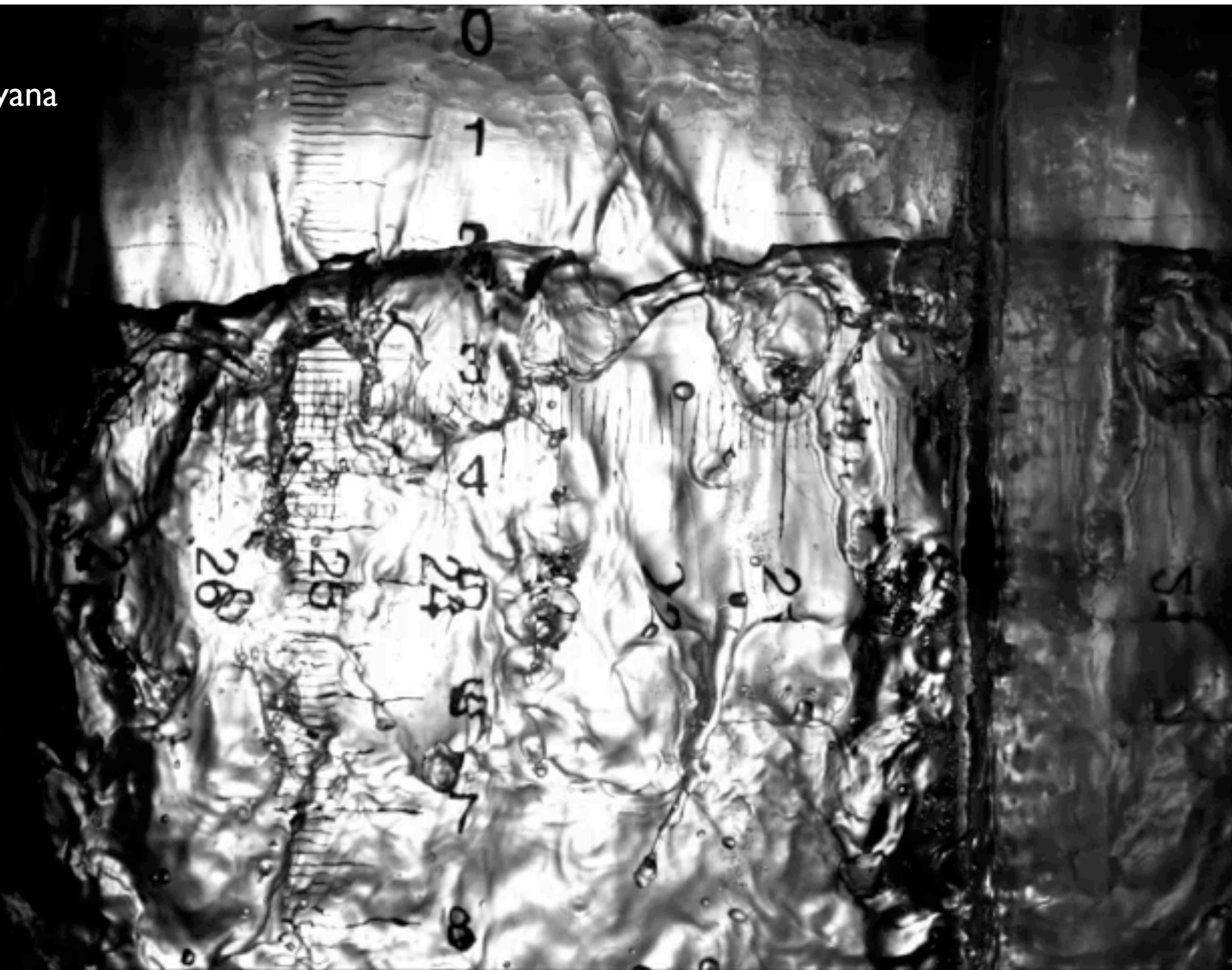
Photograph: Ludovic Raynal



In fact
a) is also b)



Ben Rayana



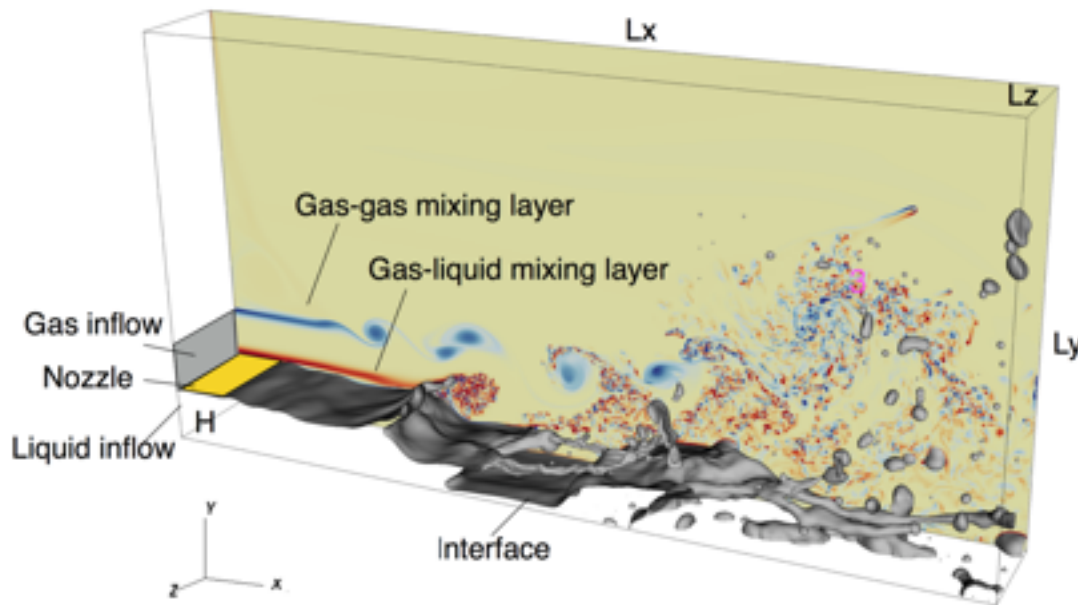


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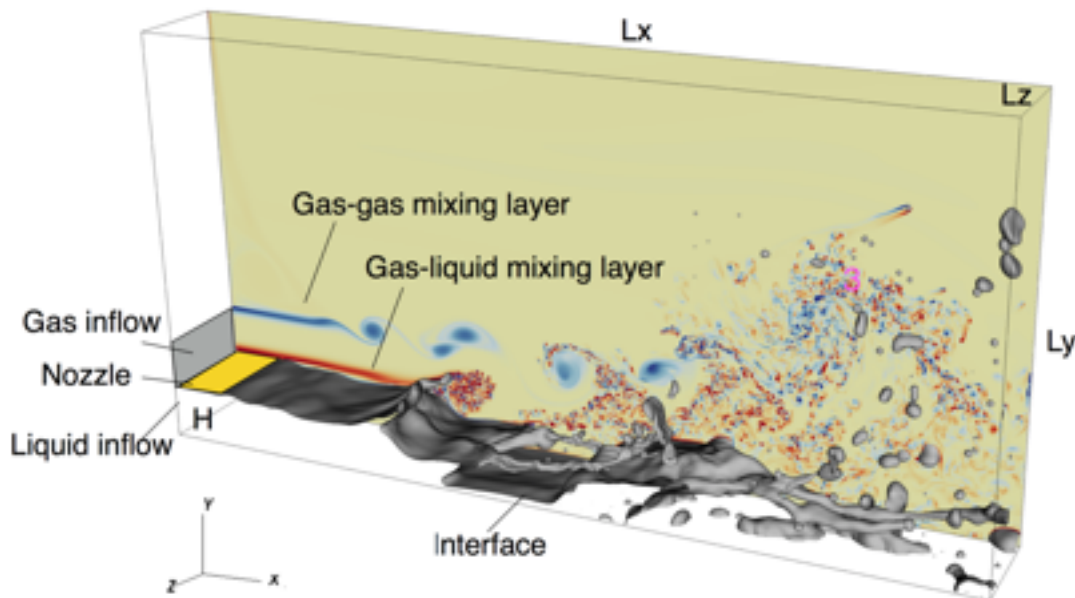
“A20” simplified case (Stanley Yue Ling) dimensional values

	Density (ρ) Kg/m ³	Viscosity (μ) Pa-s	Surface Tension (σ) N/m	Jet Height (H) mm	Boundary Layer (δ) mm	Injection Velocity (U) m/s
Gas	50	5E-05	0.05	0.8	0.1	10
Liquid	1000	1E-03		0.8	0.1	0.5



“A20” Benchmark: dimensionless values

M	$Re_{g,\delta}$	$Re_{g,H}$	$We_{g,\delta}$	r	m	v
$\frac{\rho_g U_g^2}{\rho_l U_l^2}$	$\frac{\rho_g U_g \delta}{\mu_g}$	$\frac{\rho_g U_g H}{\mu_g}$	$\frac{\rho_g U_g^2 \delta}{\sigma}$	$\frac{\rho_l}{\rho_g}$	$\frac{\mu_l}{\mu_g}$	$\frac{U_l}{U_g}$
20	1000	8000	10	20	20	20



- Turbulent gas flow
- Convective instability
Fuster et al. 2013, Otto et al. 2013
- "Strong" atomization

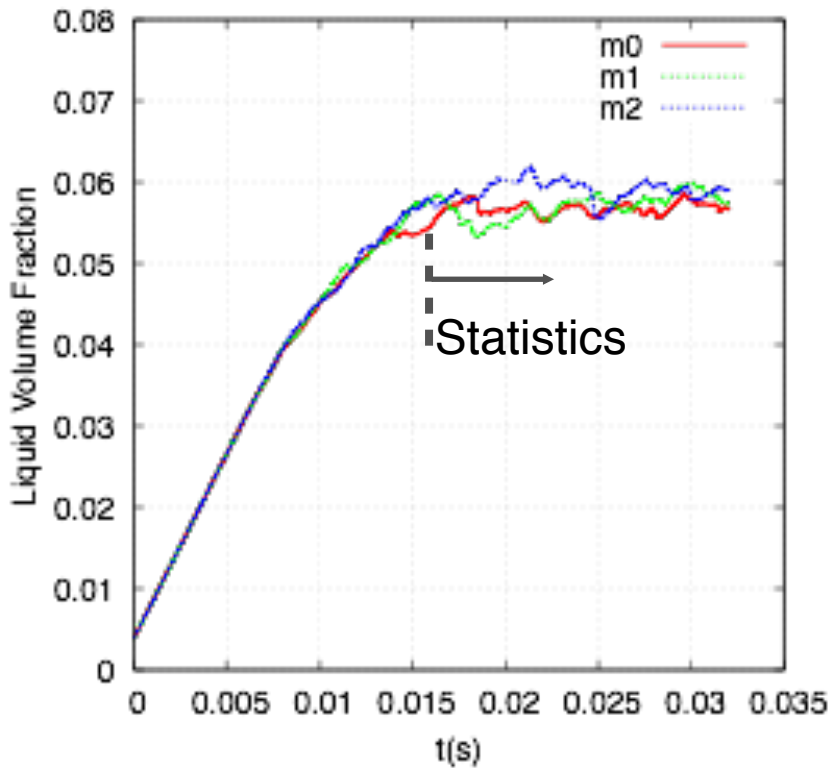
Simulation Cases

Domain: $L_x=16H$, $L_y=8H$, $L_z=2H$; End-Time: $t/(H/U_g)=400$

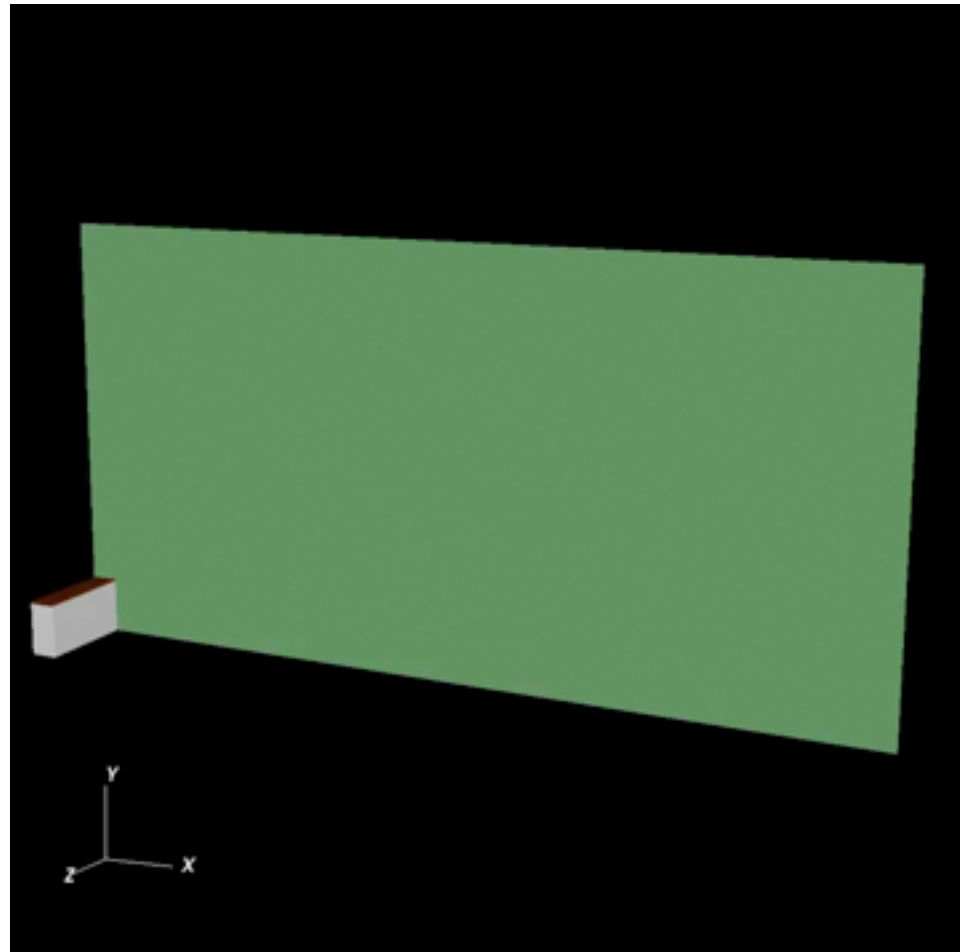
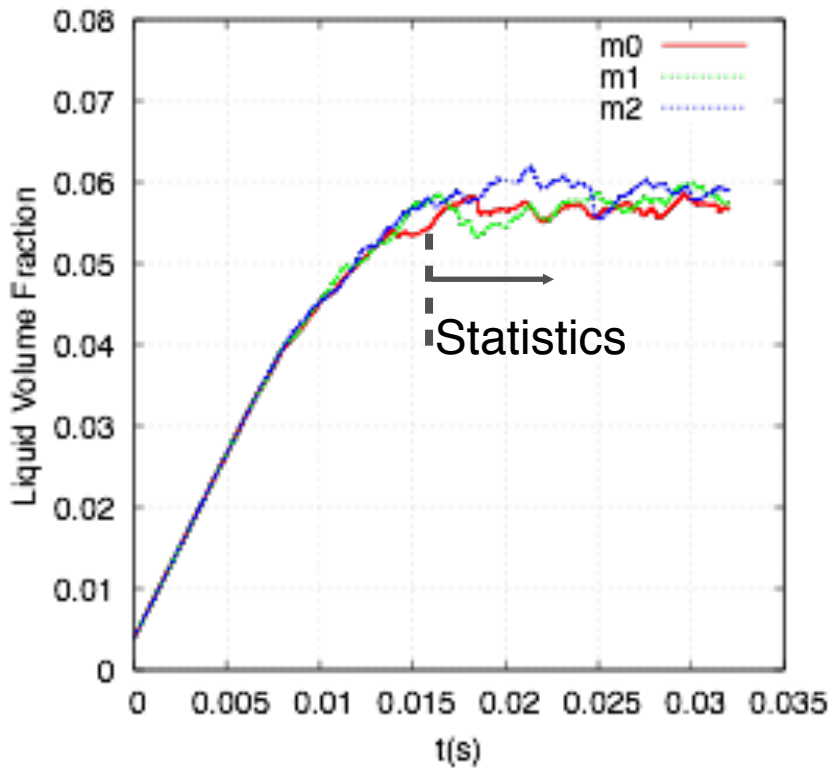
Cases	$h(\mu\text{m})$	H/h	# of cells	# of time steps	Total CPU time (hr)
M0	25	32	8.4 Million	$4.9\text{E}+04$	$2.5\text{E}+03$
M1	12.5	64	67 Million	$1.0\text{E}+05$	$4.3\text{E}+04$
M2	6.25	128	537 Million	$2.2\text{E}+05$	$5.0\text{E}+05$
M3	3125	256	4 Billion	$4.5\text{E}+05$	$8.0\text{E}+06$

CPU time estimate based on performance on TGCC-CURIE machine

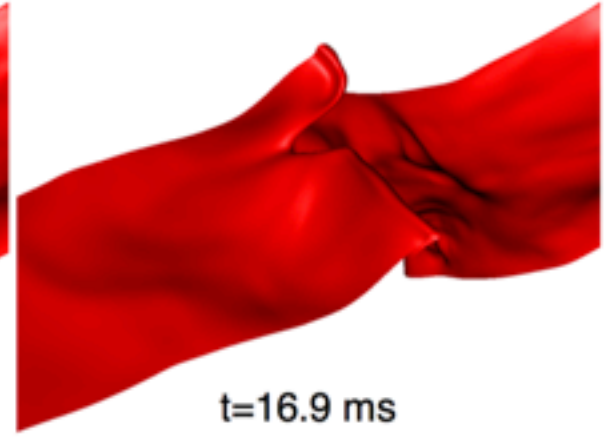
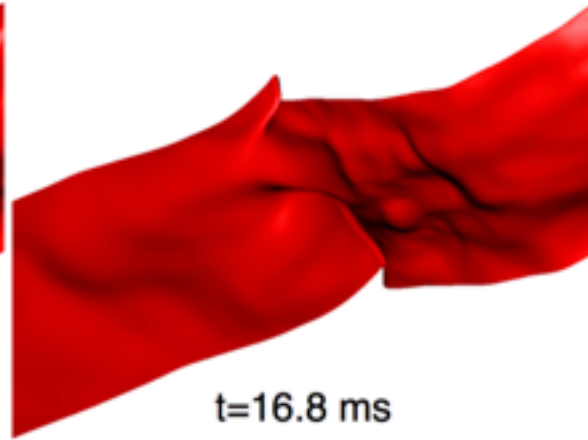
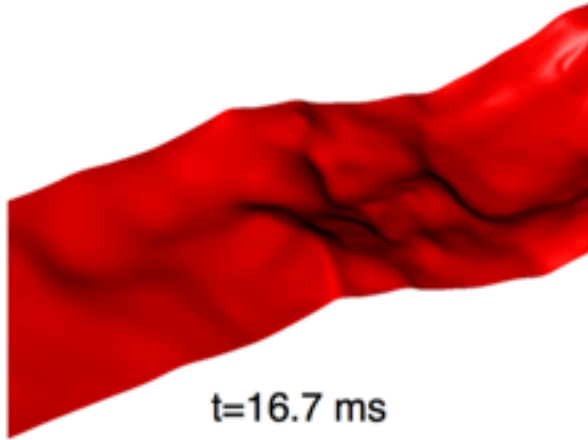
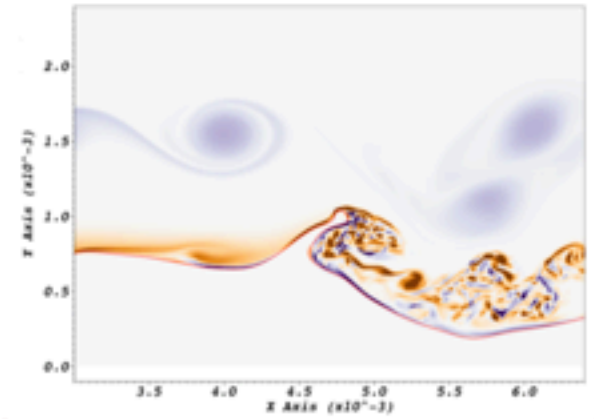
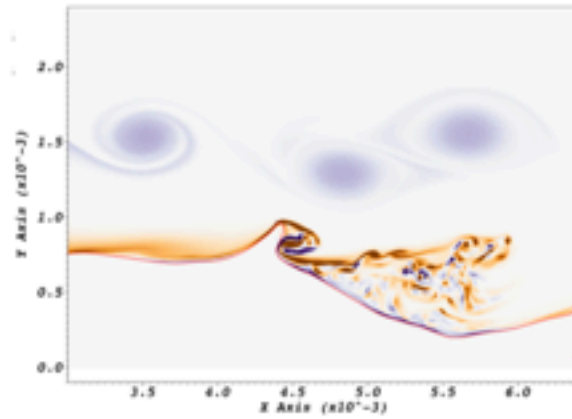
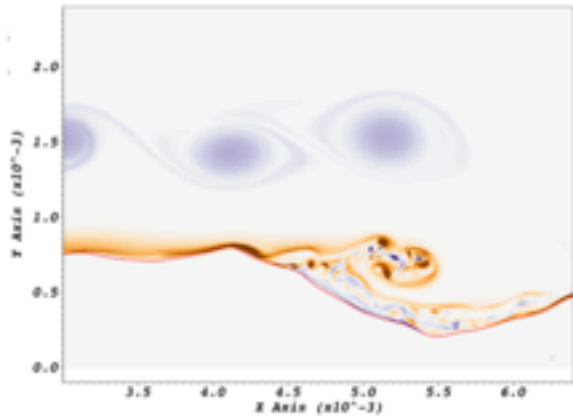
Liquid Volume Fraction



Liquid Volume Fraction

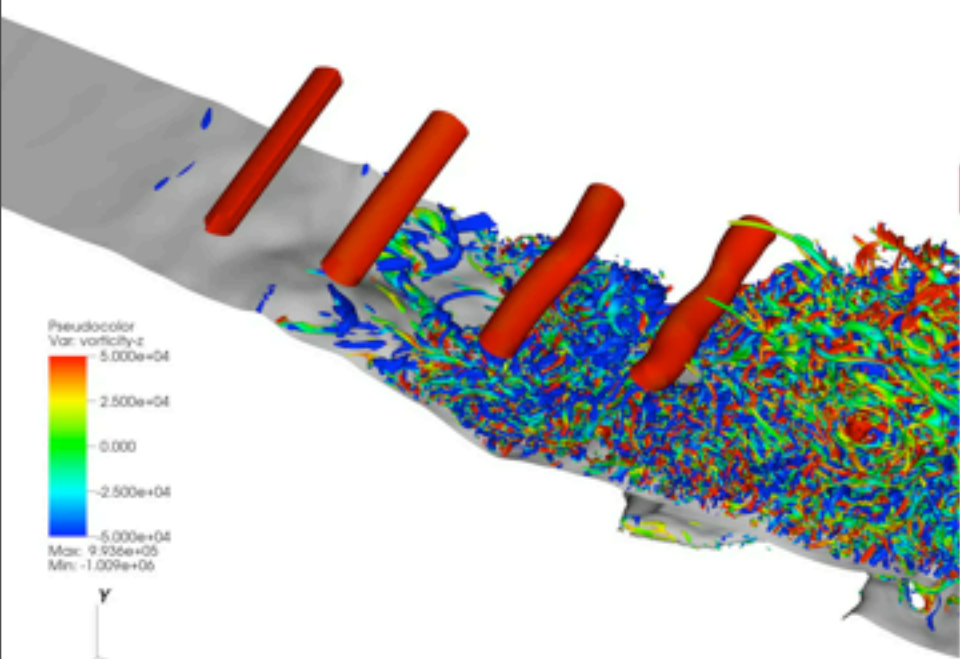


Sheet and rim formation dynamics



DB: multi00160.root
Cycle: 0 Time:0.016

DB: multi00160.root
Cycle: 0 Time:0.016



Pseudocolor
Var: vorticity-z
5.000e+04
2.500e+04
0.000
-2.500e+04
-5.000e+04
Max: 9.936e+05
Min: -1.009e+06



user: d173cos
Wed May 4 19:10:51 2016



user: d173cos
Thu Apr 21 23:29:37 2016



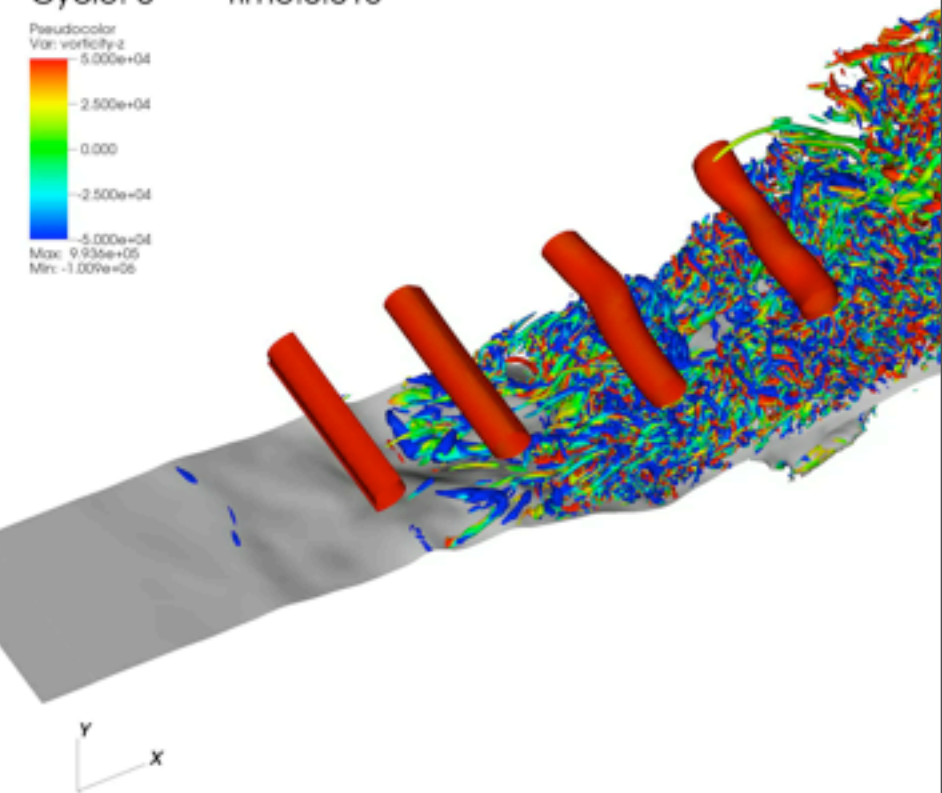
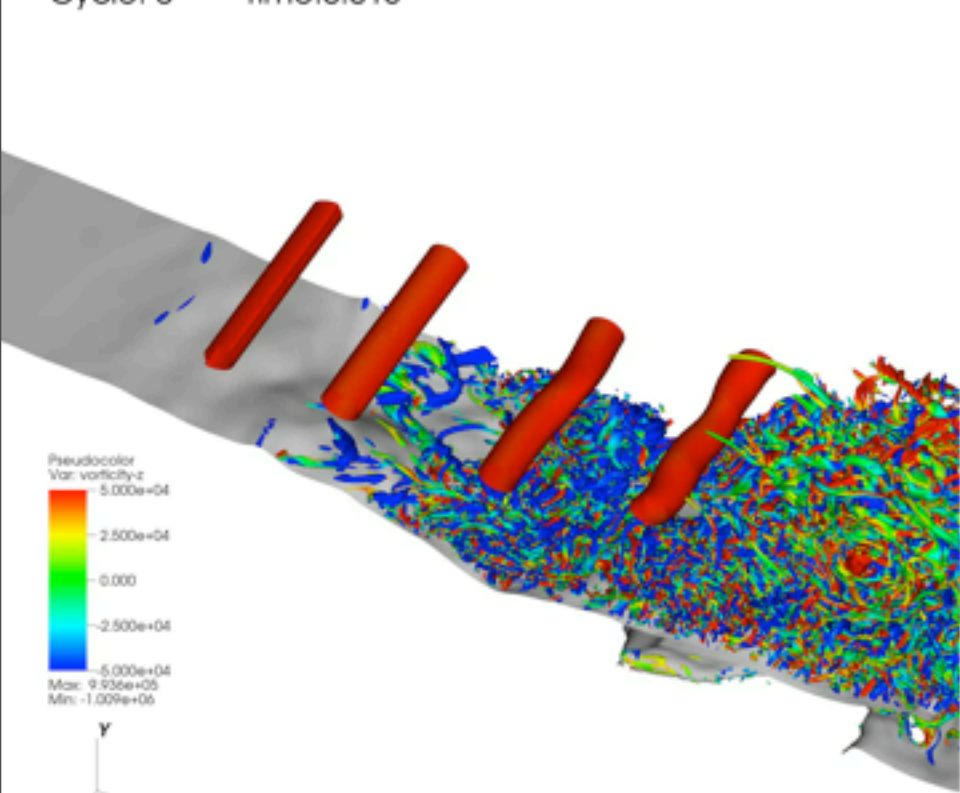


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DB: multi00160.root
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user: d73cos
Wed May 4 19:10:51 2016

user: d73cos
Thu May 5 08:39:14 2016

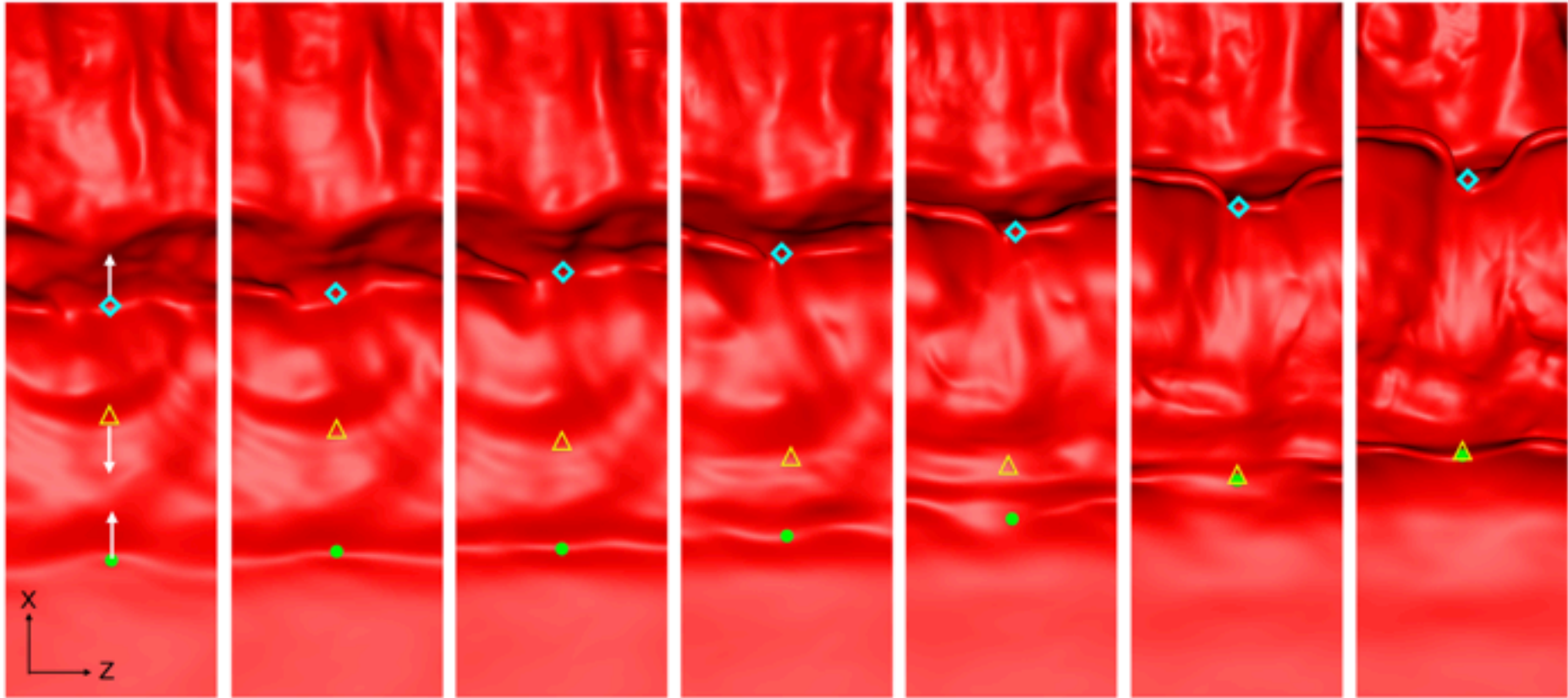


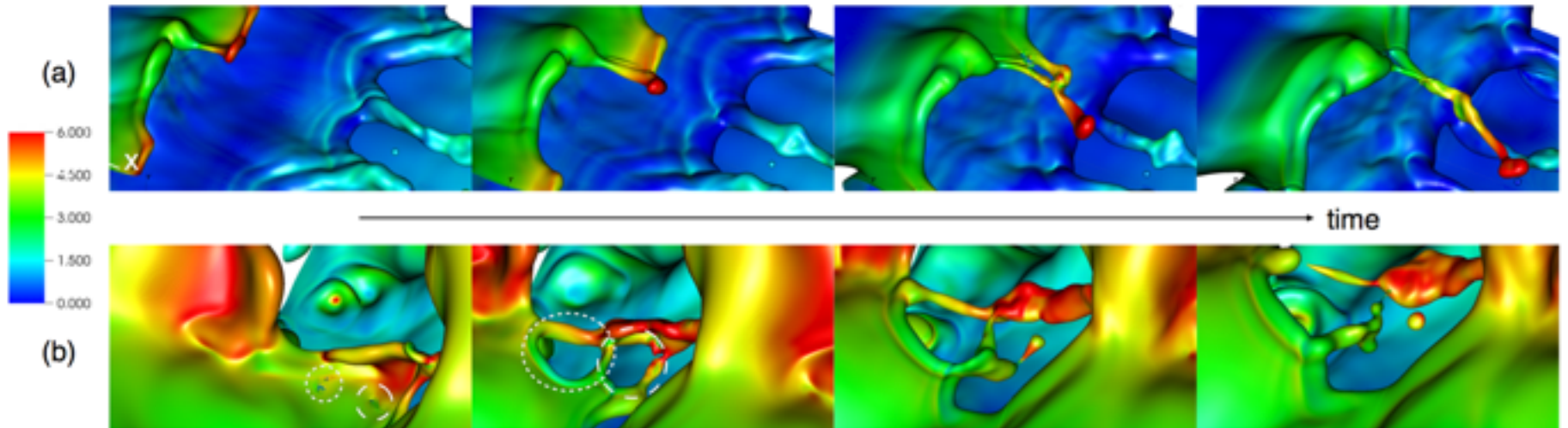


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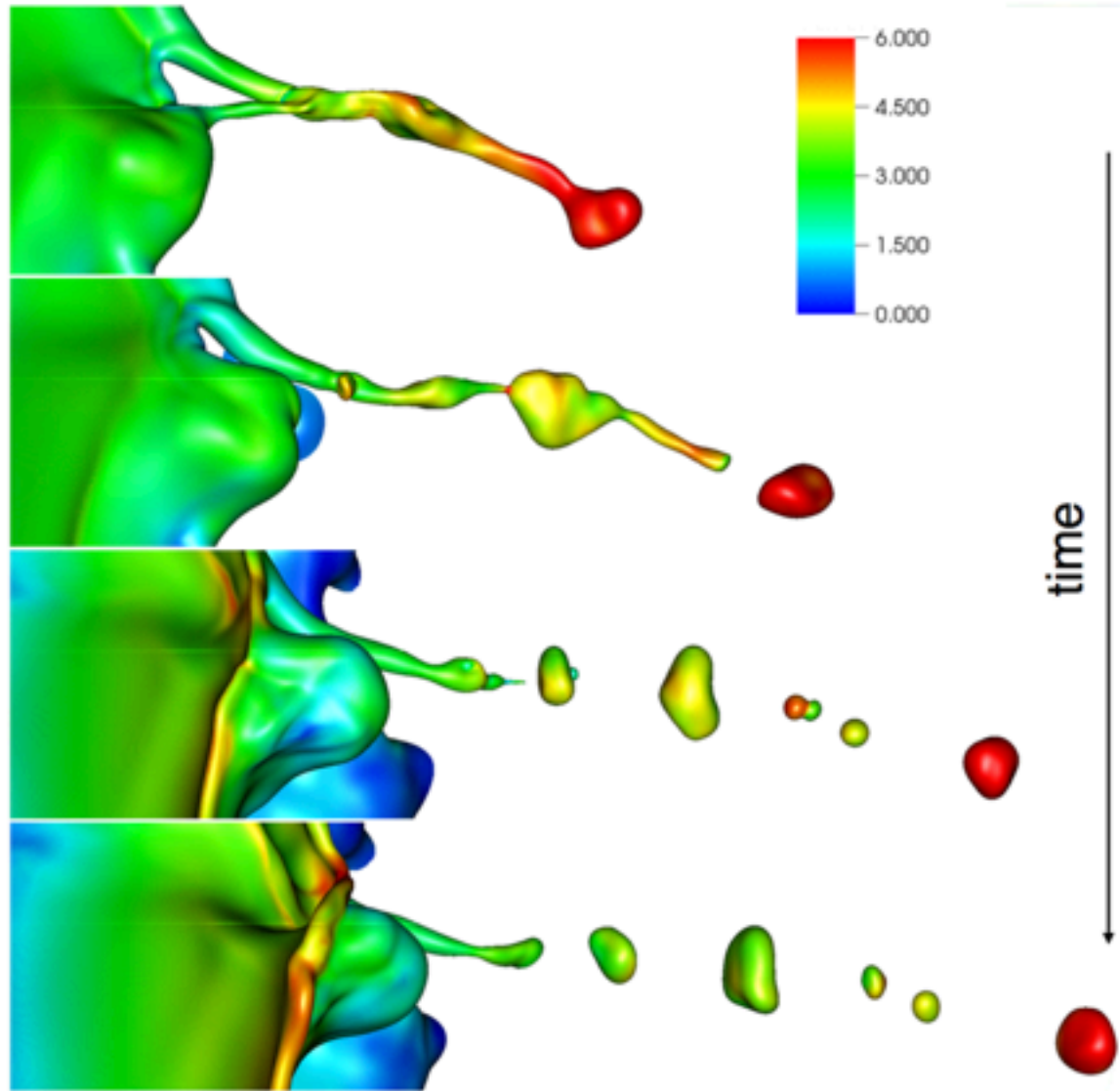


Interfacial wave interaction

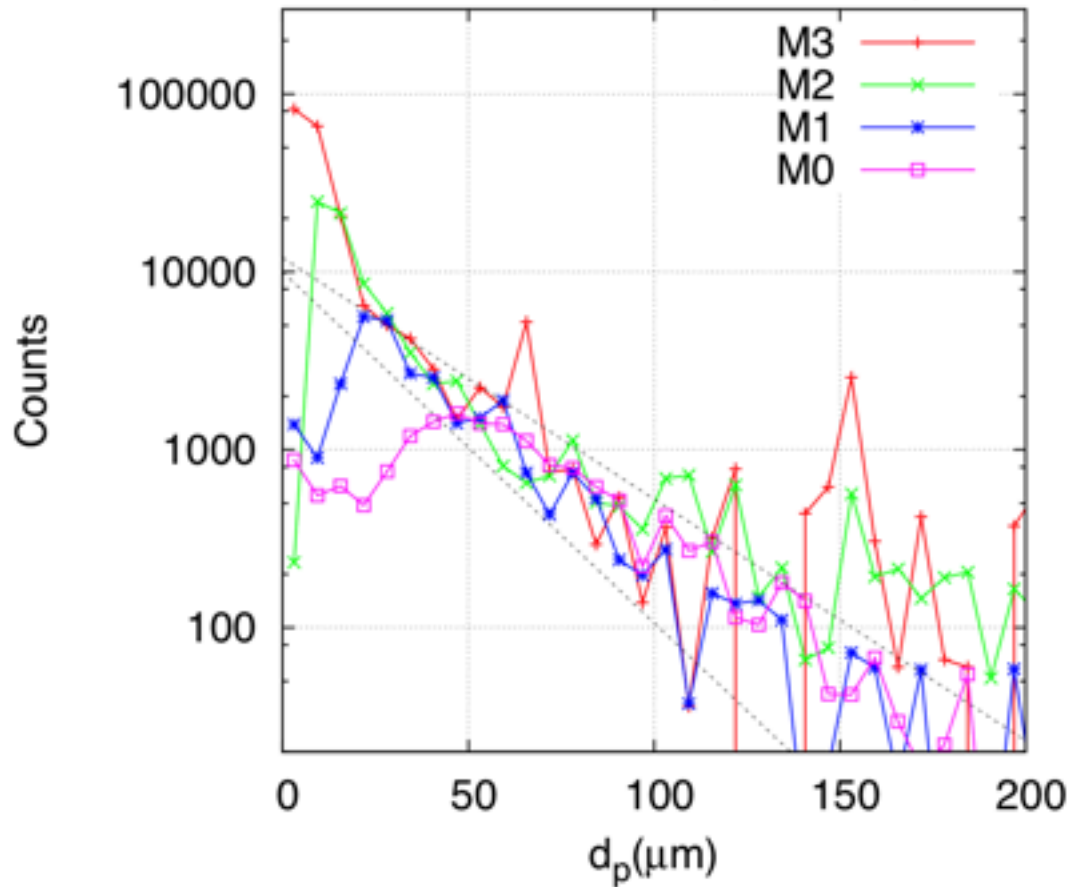




Ligaments formation due to (a) fingering from the tip of liquid sheet and (b) hole formation in the liquid sheet. The color on the interface indicates the streamwise velocity.



Sample region $8H < x < 10H$, $0.5H < y < 2.5H$
Counts are scaled trying to match exponential decay
Bin width = $H/128$ (12.5 μm)



1) Is it possible to do a real Direct Numerical Simulation of atomisation, resolving all the scales ?

Not yet

2) What can we learn from these very detailed simulations ?

How to look at the experiment again
(mechanisms much more complex than expected).



Acknowledgement



Y. Ling, D. Fuster, G. Tryggvason, S. Zaleski
"Spray formation: an inverse cascade",
[*arXiv:1511.04234*](https://arxiv.org/abs/1511.04234)



Thank
you!

Acknowledgement



Y. Ling, D. Fuster, G. Tryggvason, S. Zaleski
"Spray formation: an inverse cascade",
[arXiv:1511.04234](https://arxiv.org/abs/1511.04234)

Backup Slides

This simulation is

- slow
- unstable
- does not parallelize properly
- does not have Lagrangian particles

Challenge: do better.

Two approaches:

- 1) a much more efficient approach to computing on octree: Basilisk by S. Popinet: <http://basilisk.fr>
- 2) or a very simple code on regular grids: Parissimulator by Scardovelli, Ling, Tryggvason, Zaleski
<http://parissimulator.sf.net>



Speed issues



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Add Lagrangian Point Particles (LPP) that obey a point-particle equation

$$\frac{d\mathbf{u}_p}{dt} = \mathbf{F}_p [\mathbf{u}_p, \mathbf{u}_f(\mathbf{x})]$$

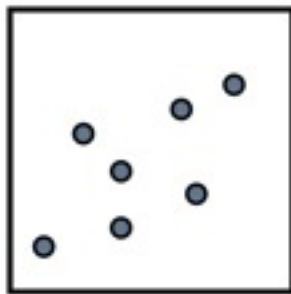
The force is determined by the surrounding carrier fluid velocity field $\mathbf{u}_f(\mathbf{x})$
It reacts on the Navier-Stokes equation through a smoothing Kernel \mathbf{G} :

$$\rho \mathbf{D}\mathbf{u} / Dt = -\nabla p + \nabla \times (2\mu \mathbf{D}) + \sigma \kappa \delta_S \mathbf{n} - \mathbf{F}_p * \mathbf{G}$$

where the strain-rate tensor \mathbf{D} is

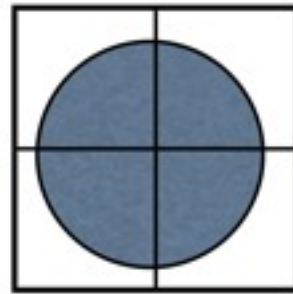
$$D_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \dot{}$$

The choice of resolved interface or LPP modelling depends on the type of simulation and on grid resolution



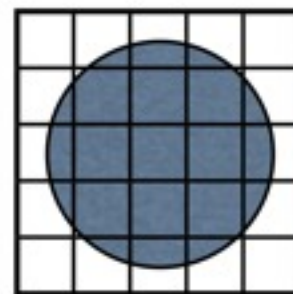
$$dx \gg d_p$$

Conventional
LPP

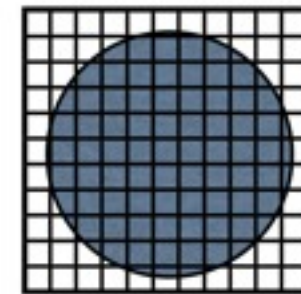


$$dx \approx d_p$$

Poorly Resolved Drop
(Finite-size LPP)



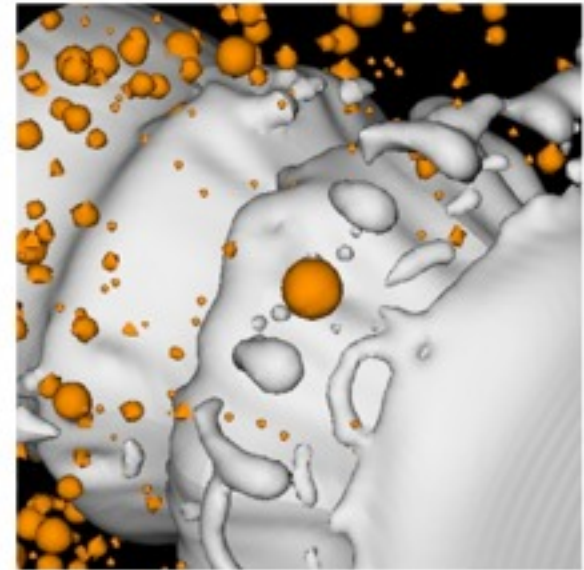
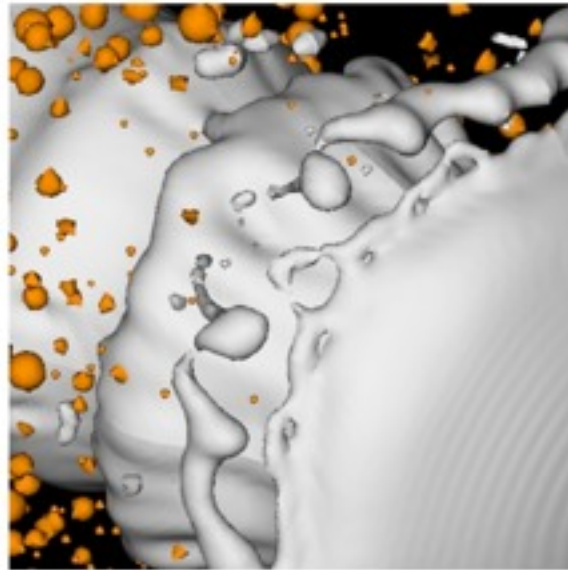
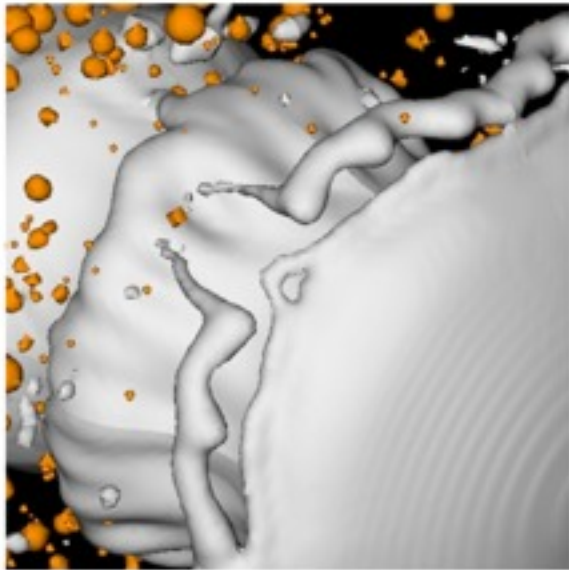
$$dx < d_p$$



$$dx \ll d_p$$

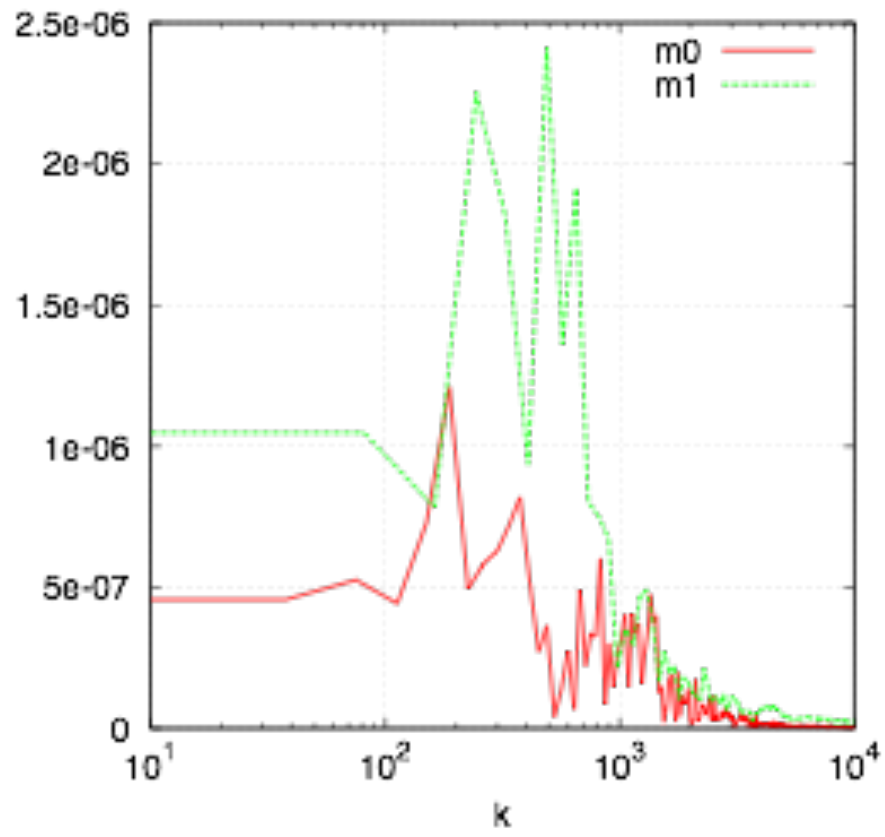
Fully Resolved
Drop

VOF to LPP conversion - High Reynolds – CORIA (Berlemont) jet



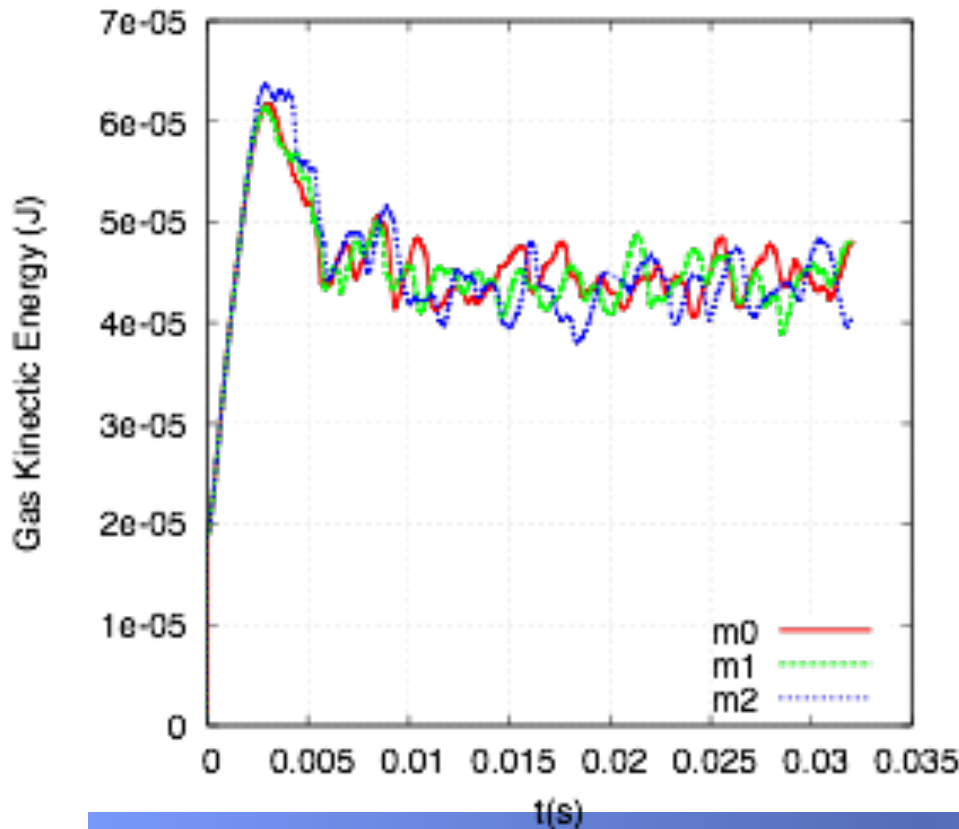
—————→ time



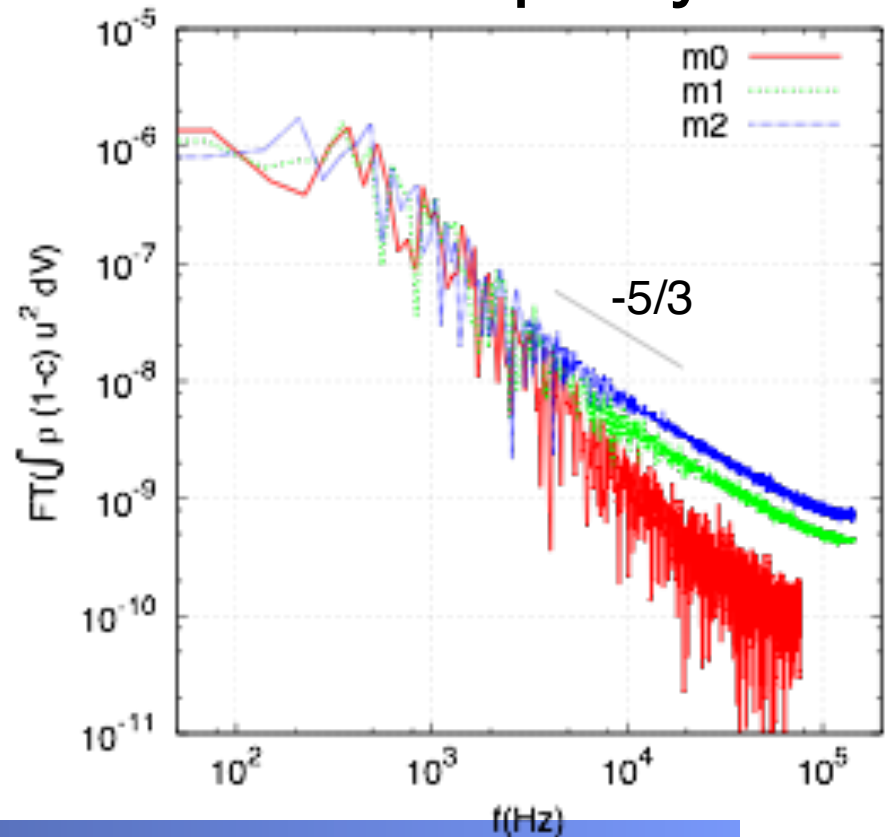


Total Gas Kinetic Energy

Time

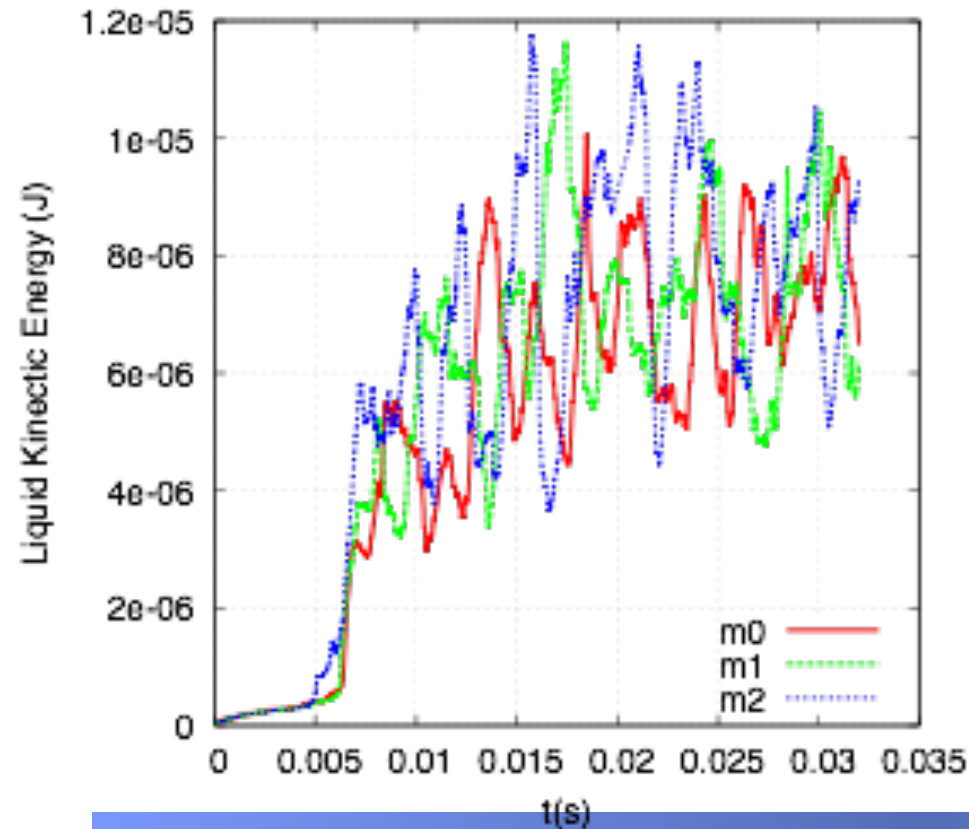


Frequency

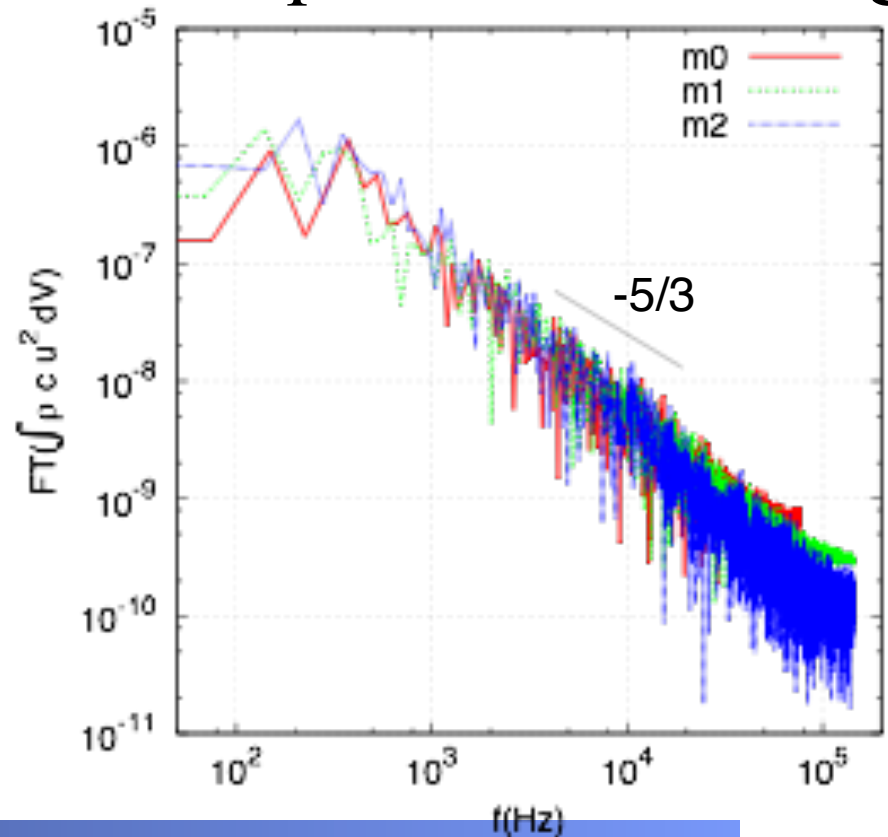


Total Liquid Kinetic Energy

Gas Kinetic Energy

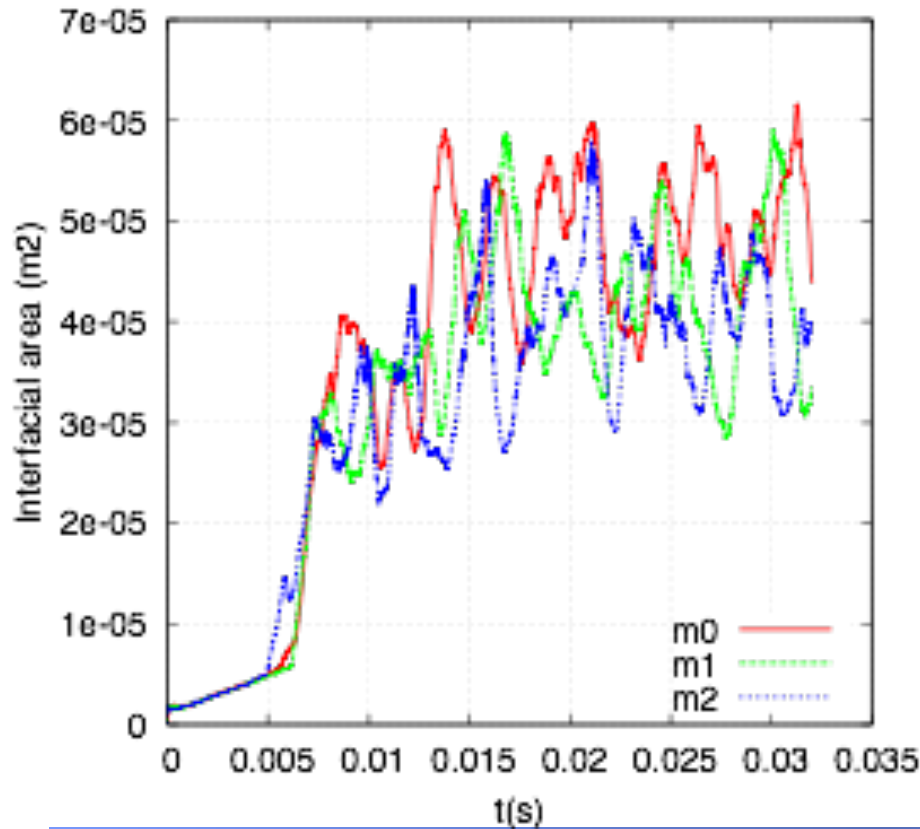


Liquid Kinetic Energy

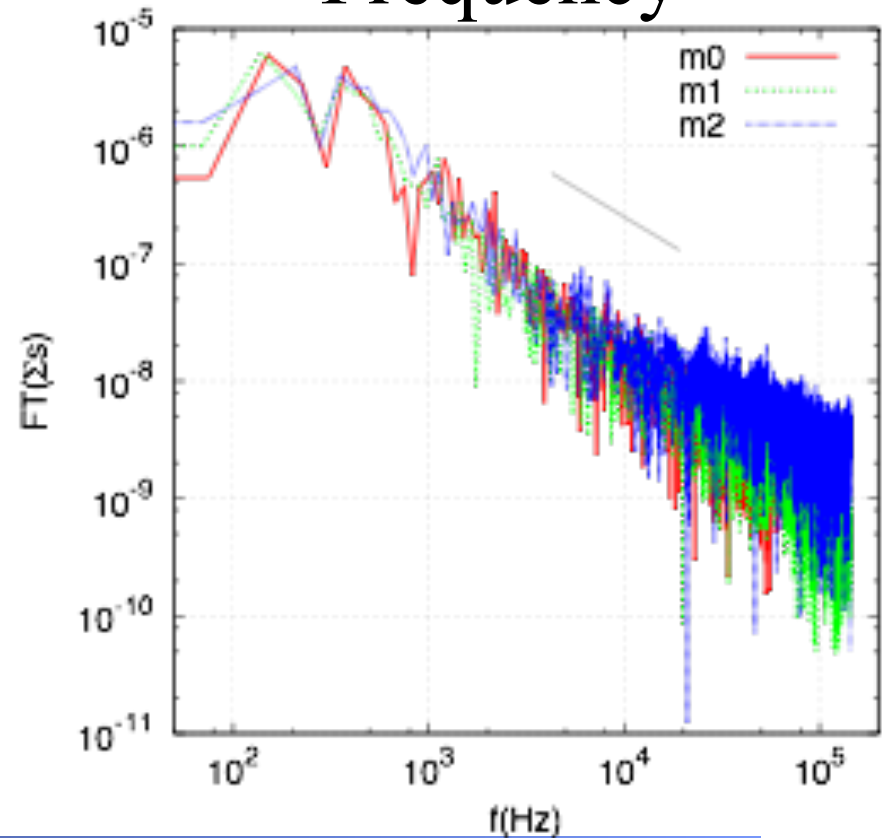


Total Interfacial Area

Time

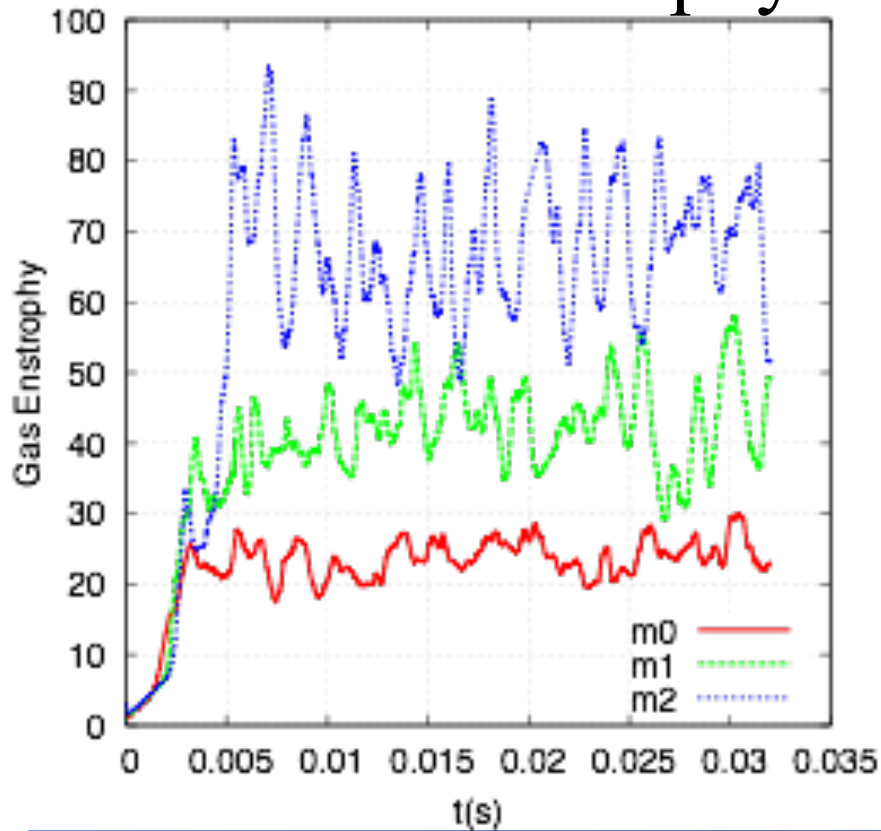


Frequency

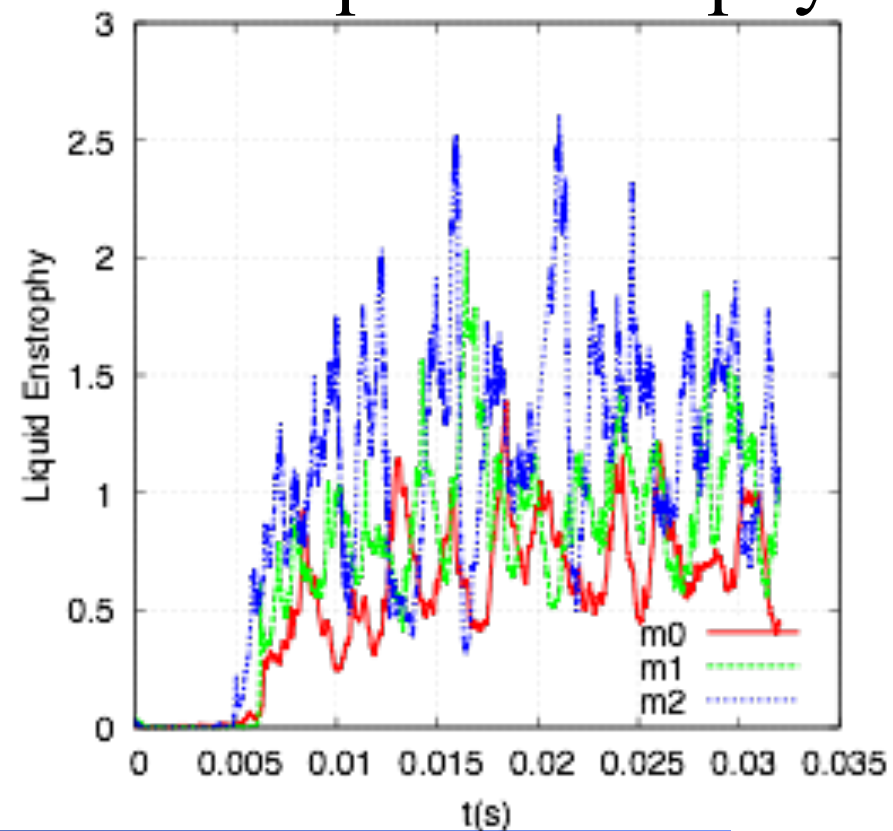


Enstrophy

Gas Enstrophy

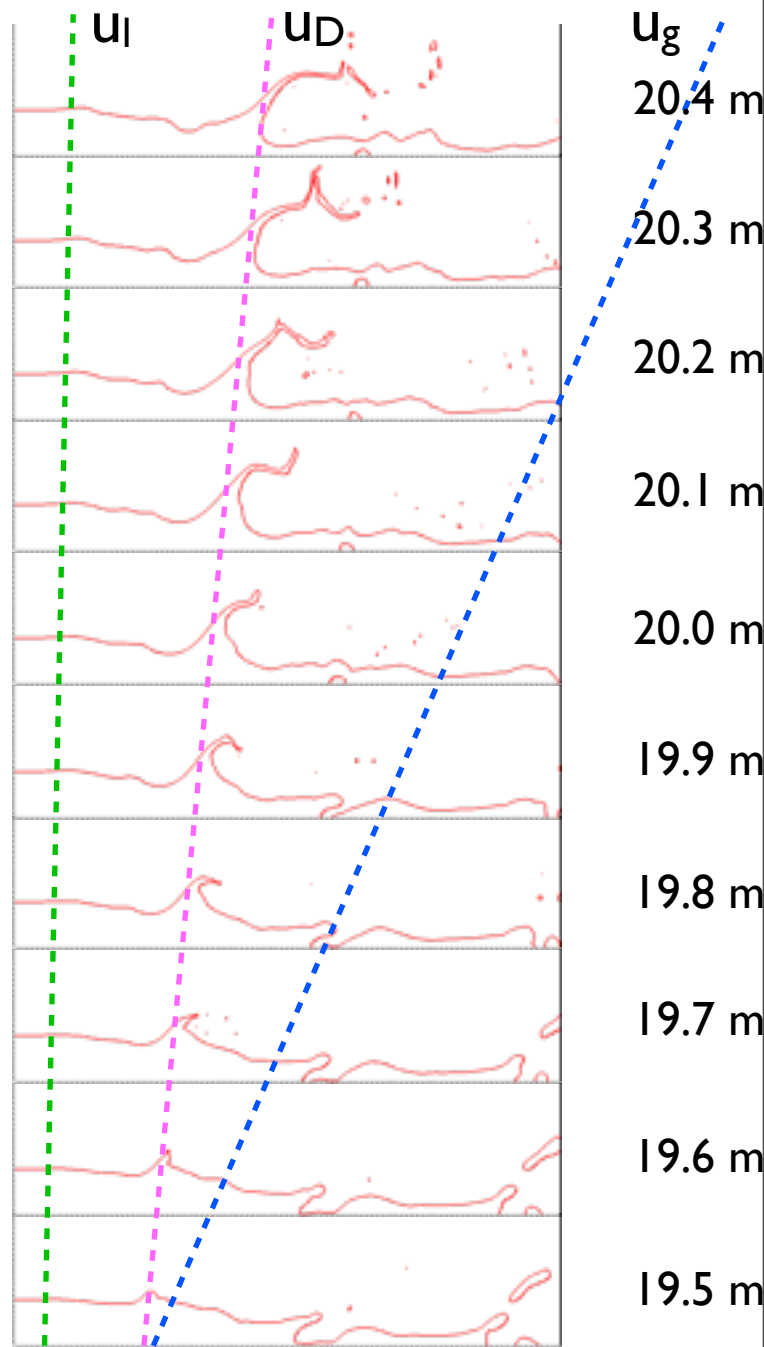
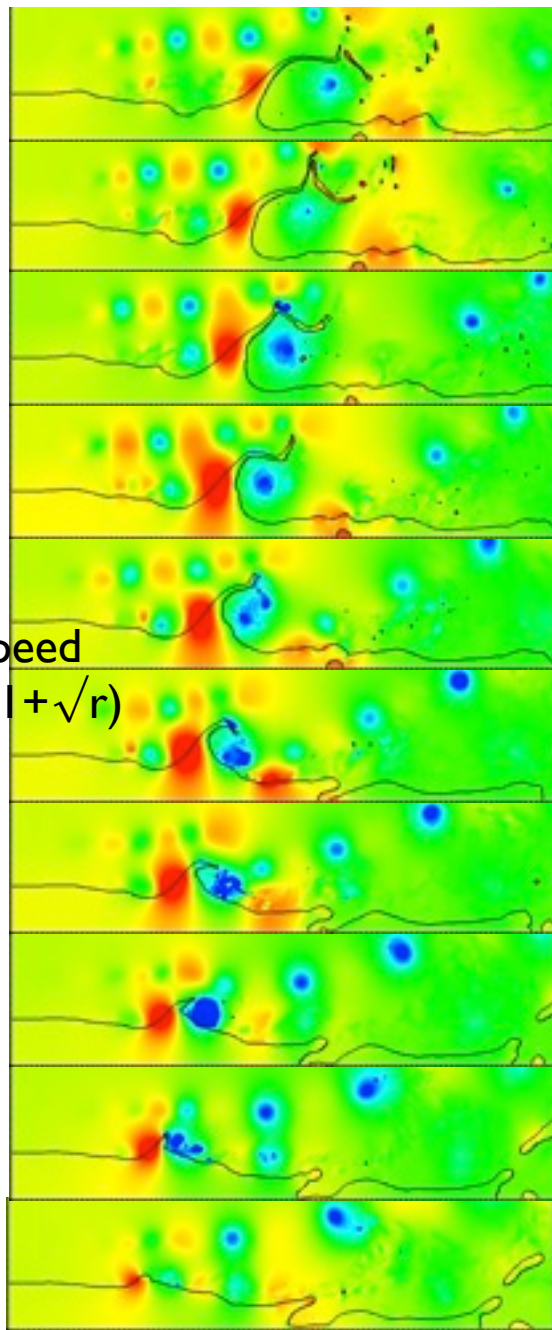


Liquid Enstrophy



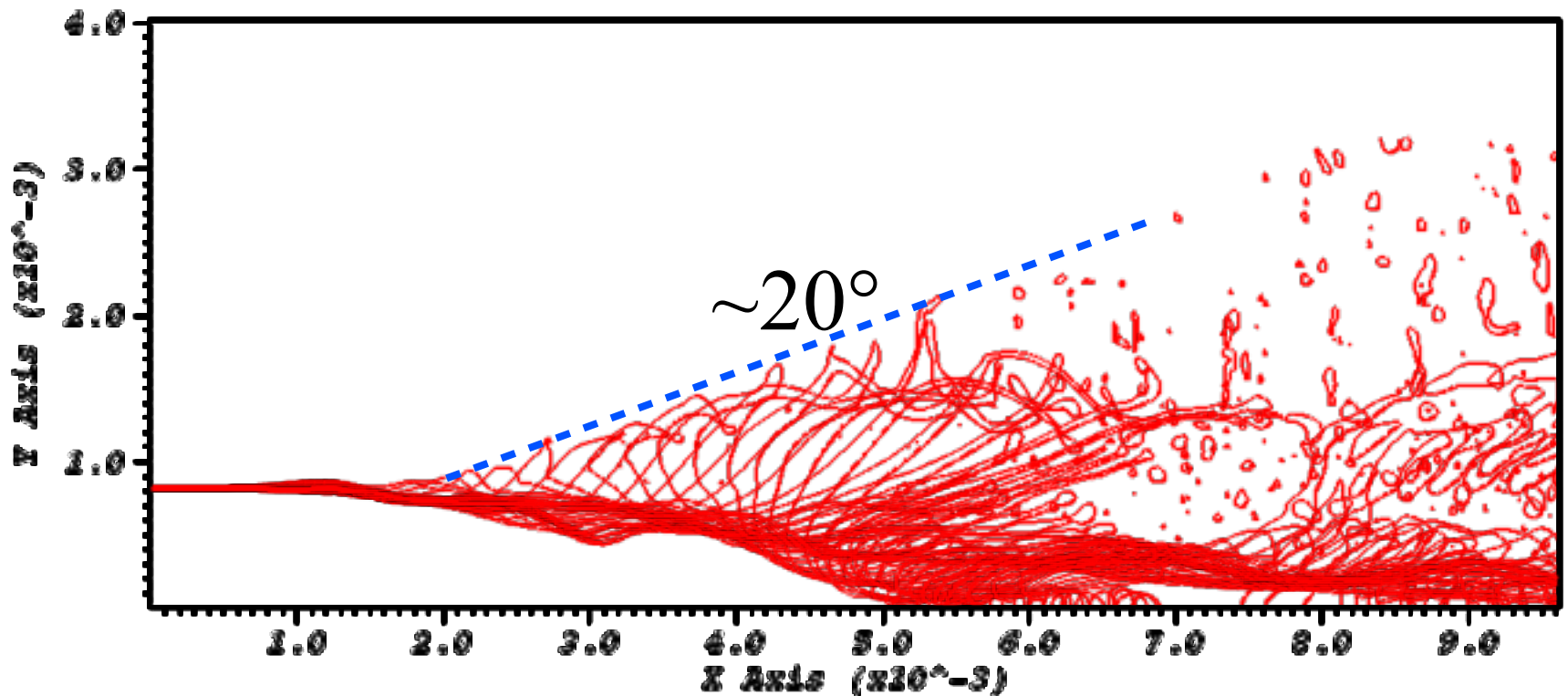
Pressure & Interface Evolution

Dimotakis speed
 $u_D = (u_I + \sqrt{r} u_g) / (1 + \sqrt{r})$



Interfacial Wave Evolution

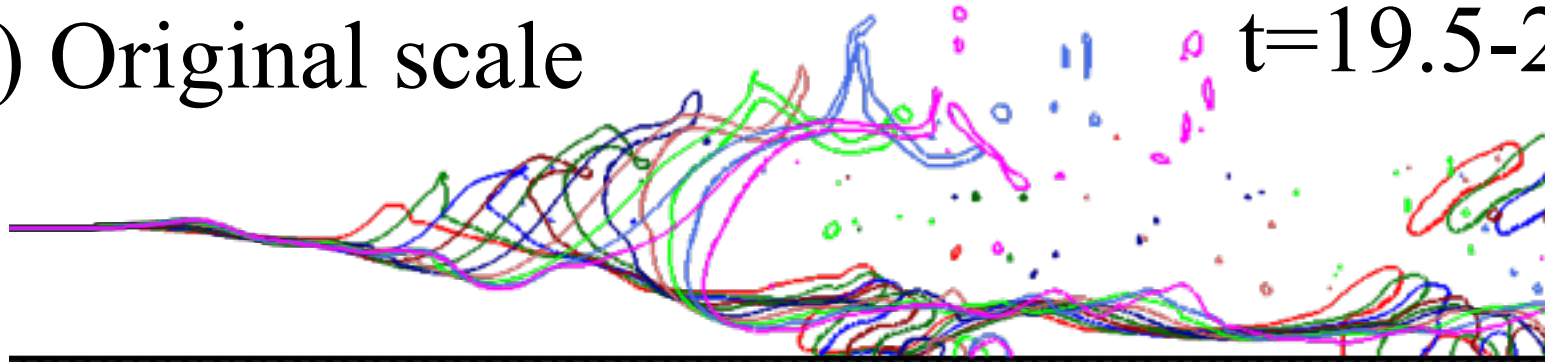
2D Slice of interface from $t=19.0-21.9\text{m}$



Self-Similar Wave

(a) Original scale

$t=19.5-20.4$ ms



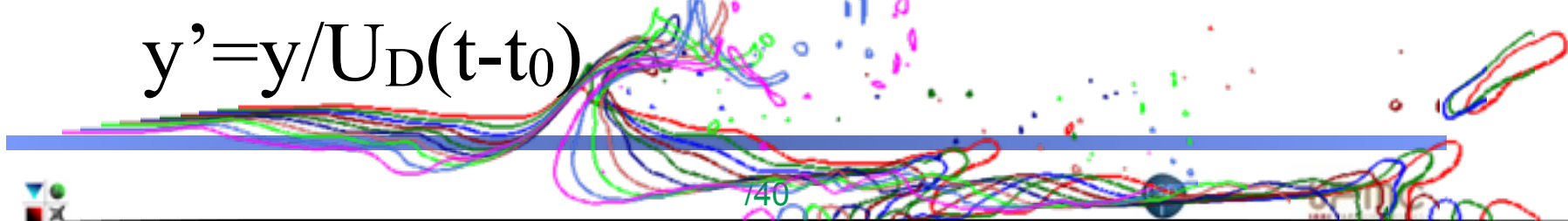
(b) $x' = (x - x_0) / U_D(t - t_0)$

(Hoepffner et al. 2011)



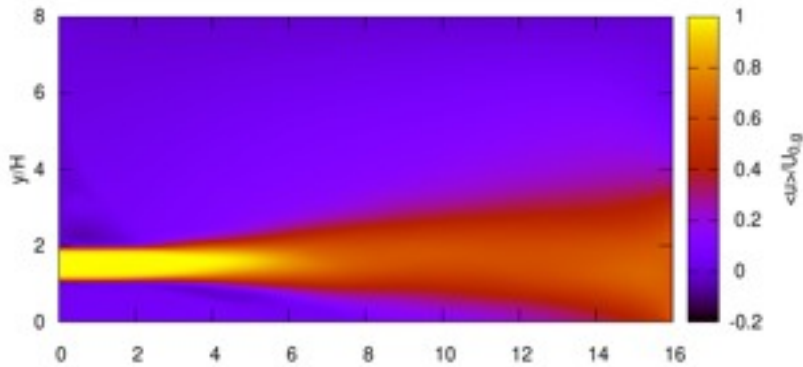
(c) $x' = (x - x_0) / U_D(t - t_0)$

$y' = y / U_D(t - t_0)$

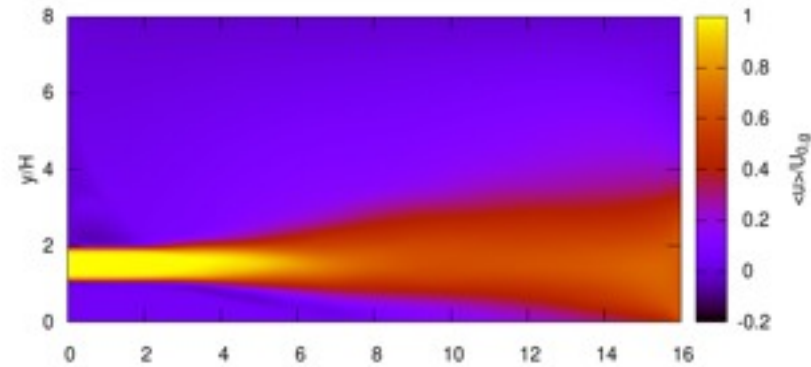


Averaging Velocity

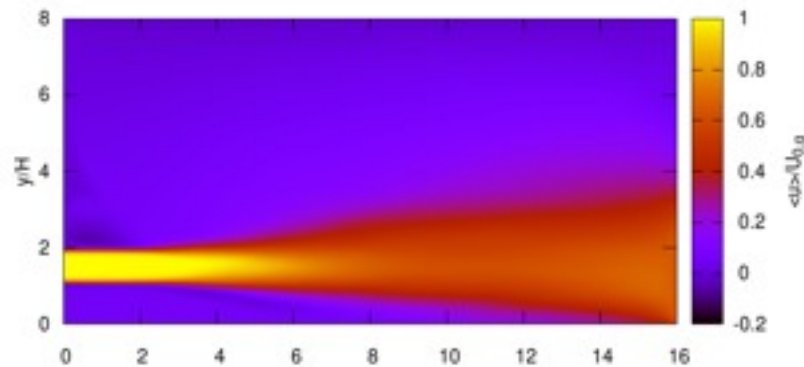
m0



m1



m2

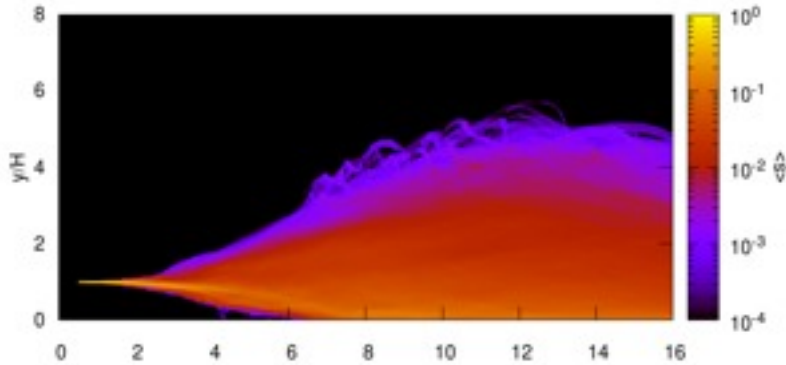


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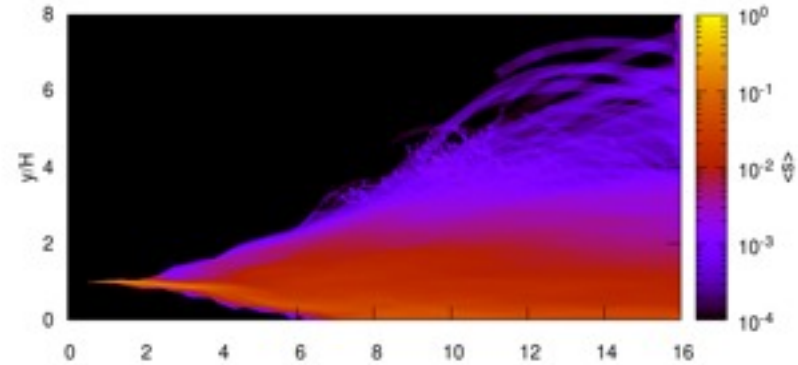


Averaging Interfacial Area

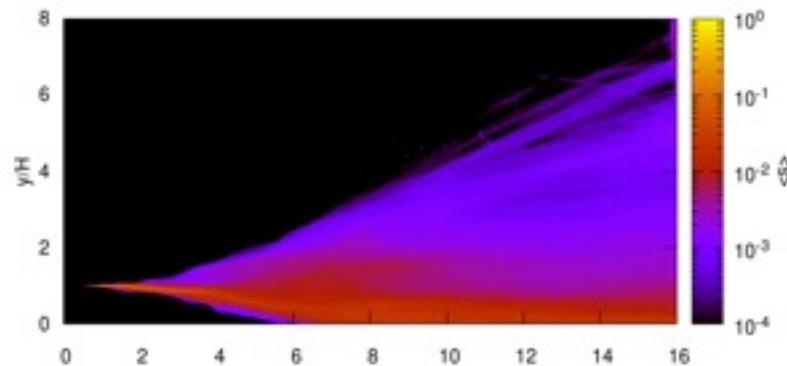
m0



m1



m2

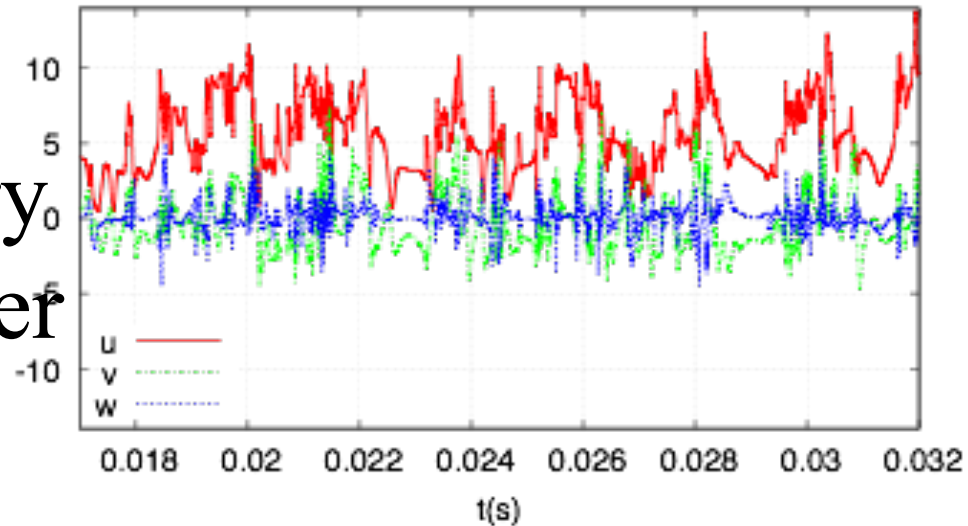


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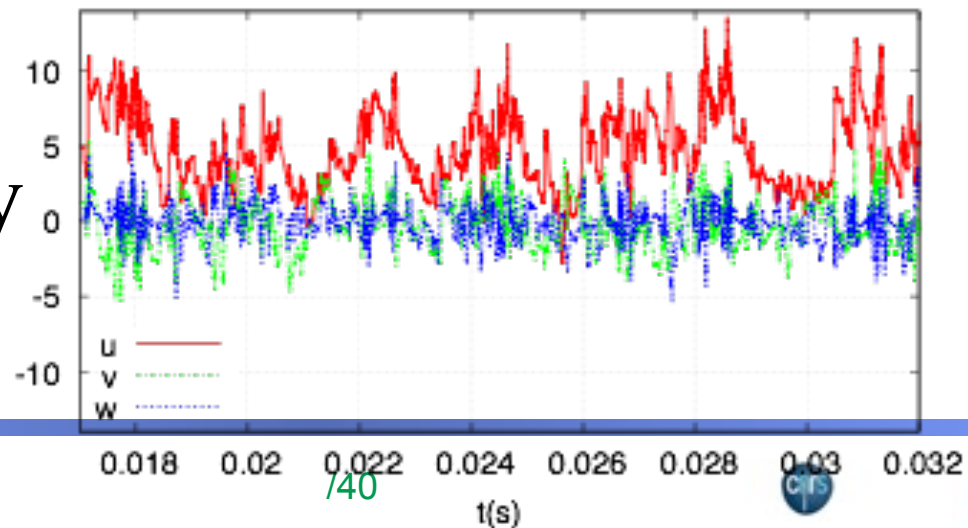


Turbulence Fluctuations

Top jet bdry
Mixing layer



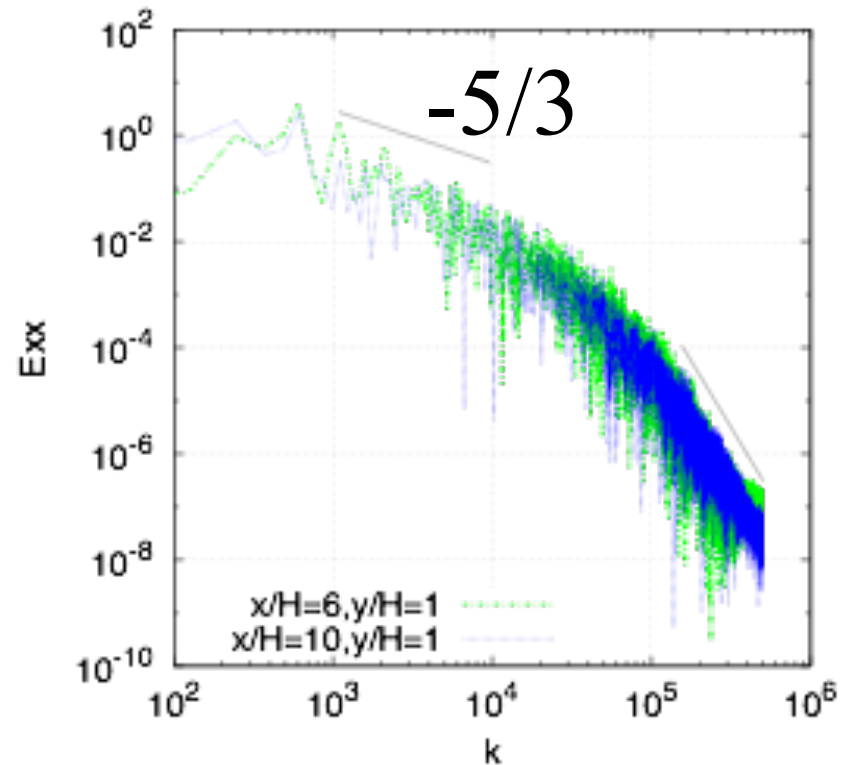
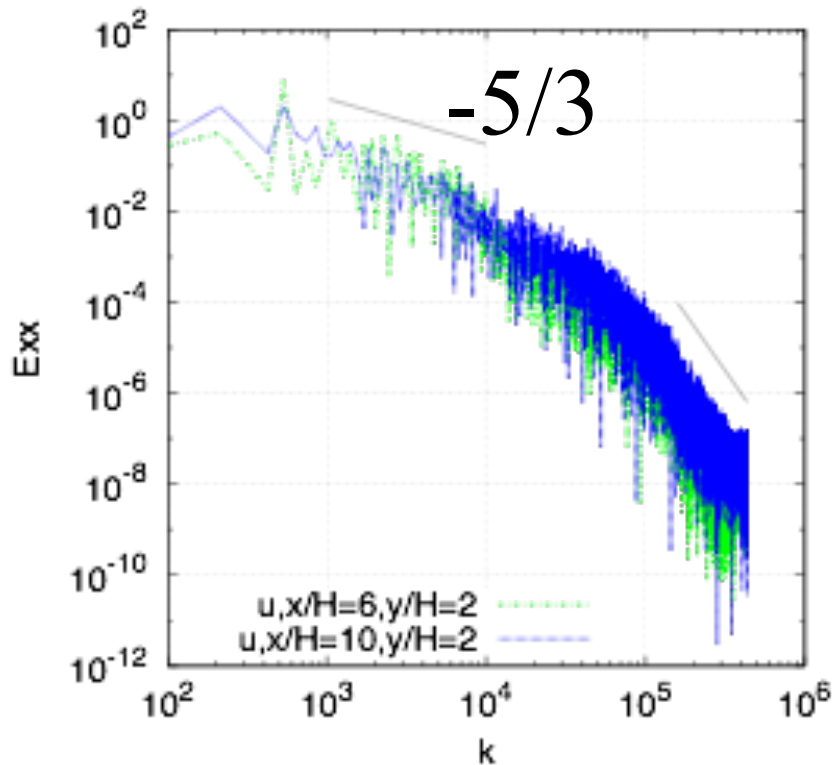
Low jet dry
Interface



Energy Spectra

Gas-gas mixing layer

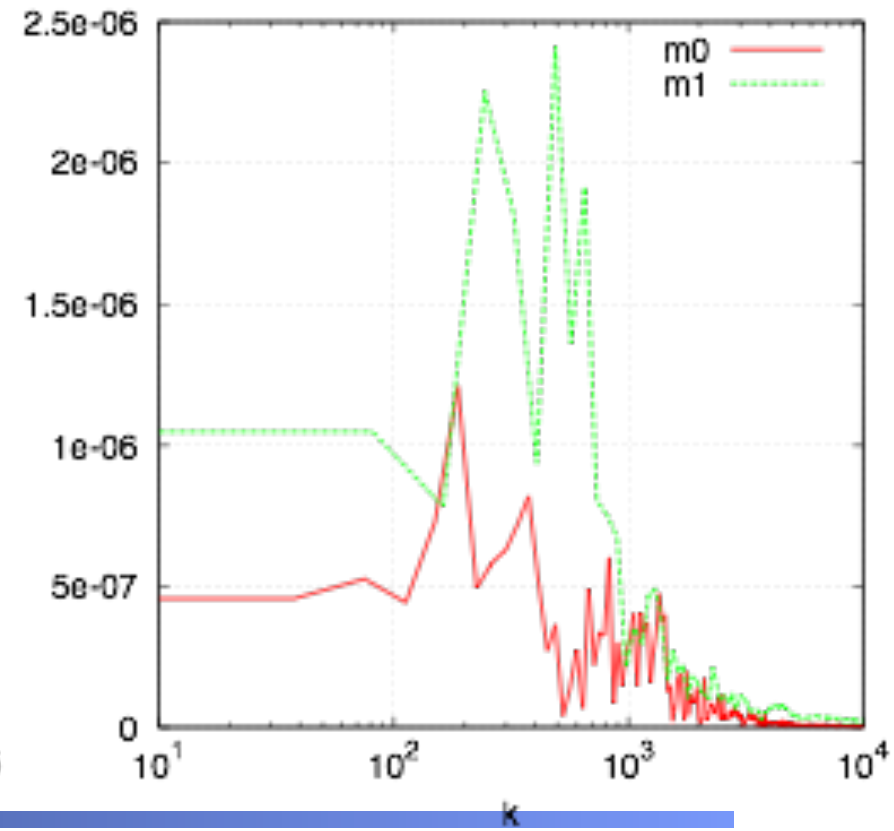
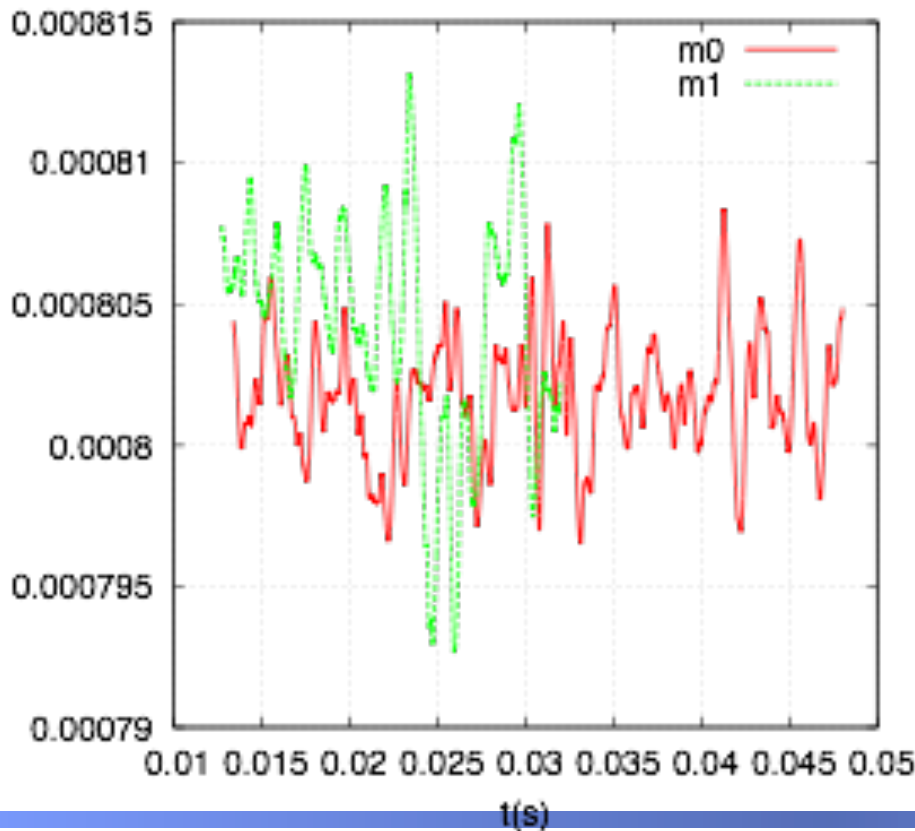
Gas-liquid mixing layer

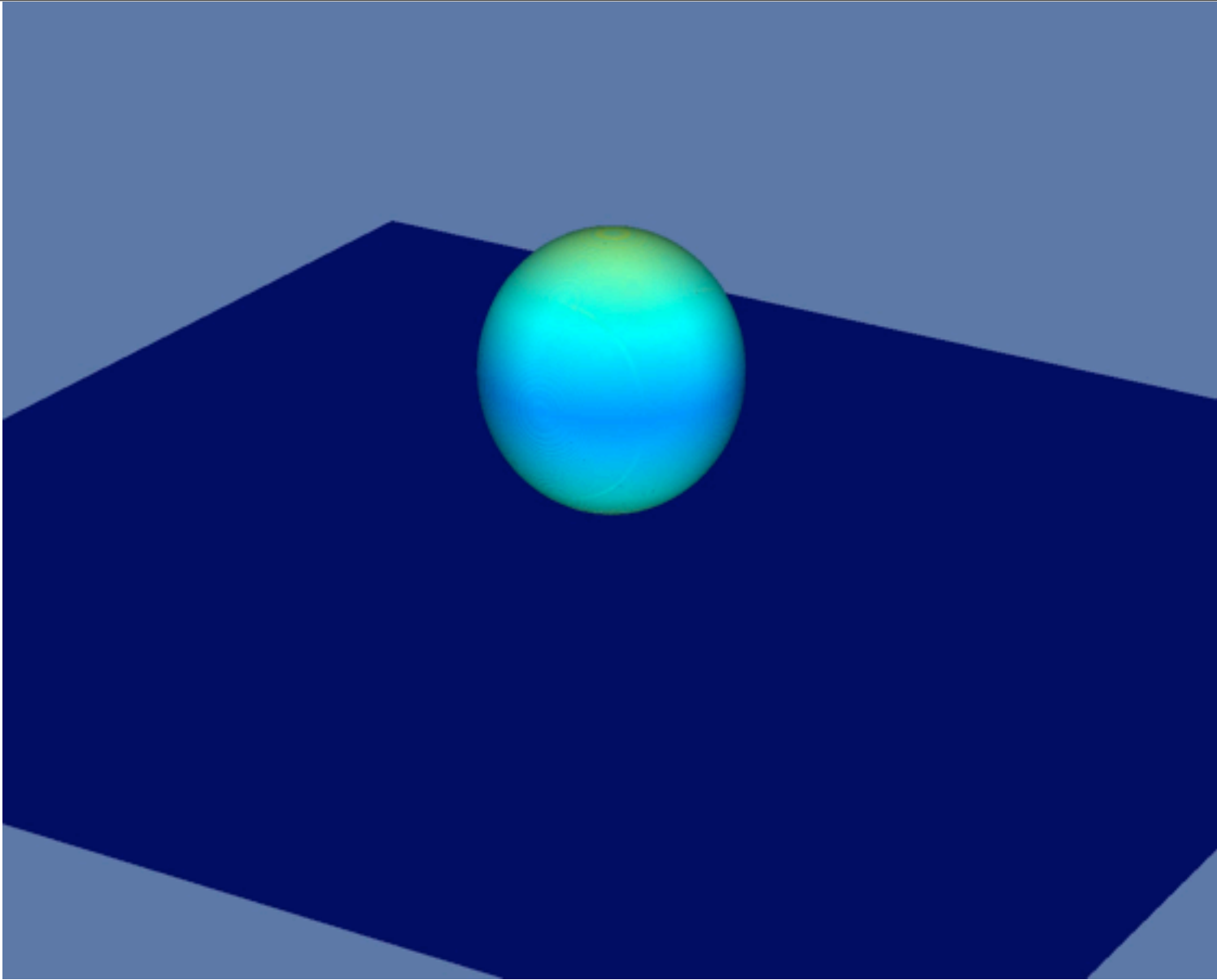


Interfacial Instability

m0

m1





Same as before, higher resolution (Pascal Ray)



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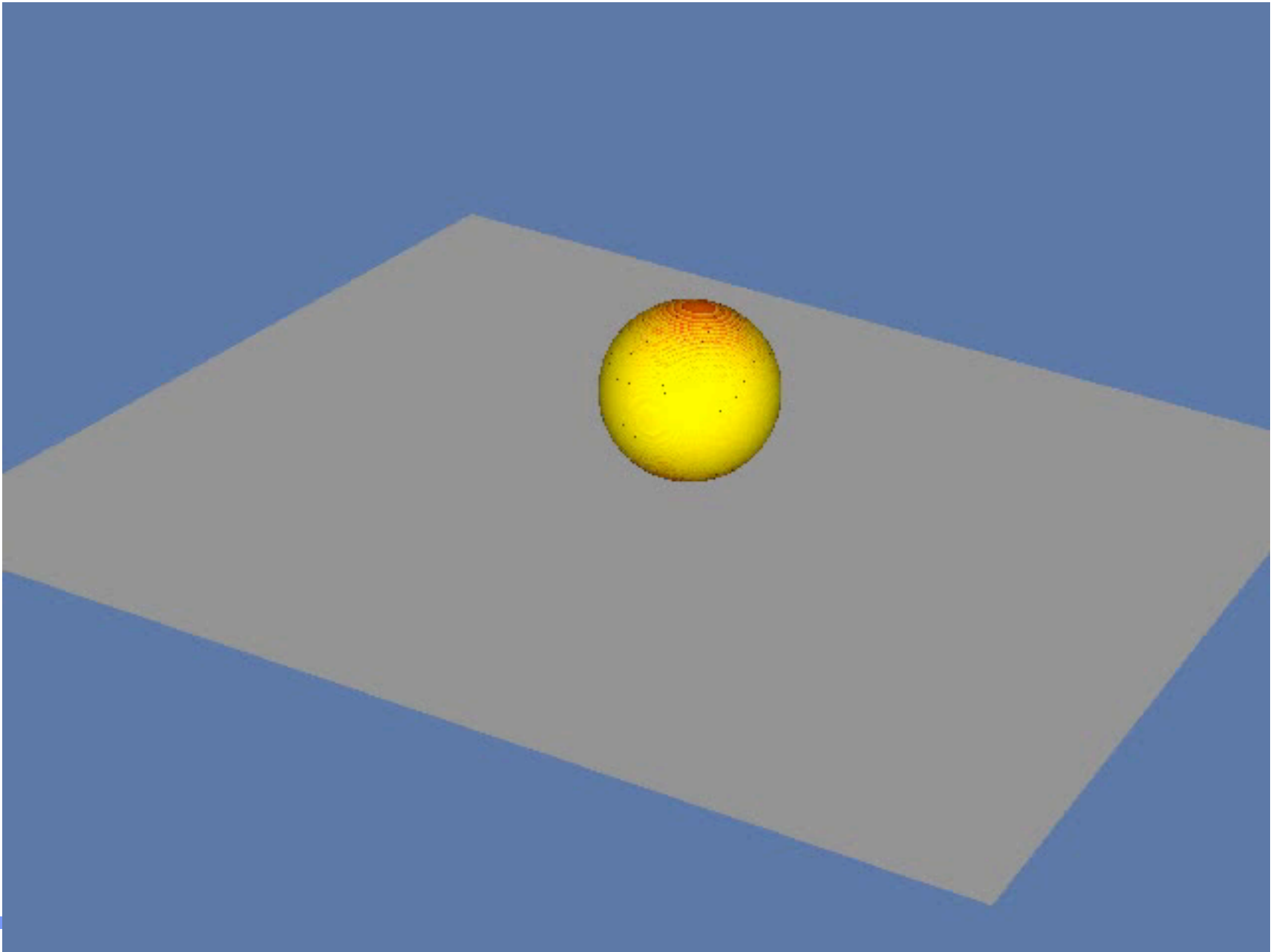
Same as before, higher resolution (Pascal Ray)



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The iconic Marmottant-Villermaux case

Air-Water

$$u_{\text{liq}} = 0.6 \text{ m s}^{-1}, u_{\text{gas}} = 35 \text{ m s}^{-1}$$

injection diameter $D = 7.8 \text{ mm}$



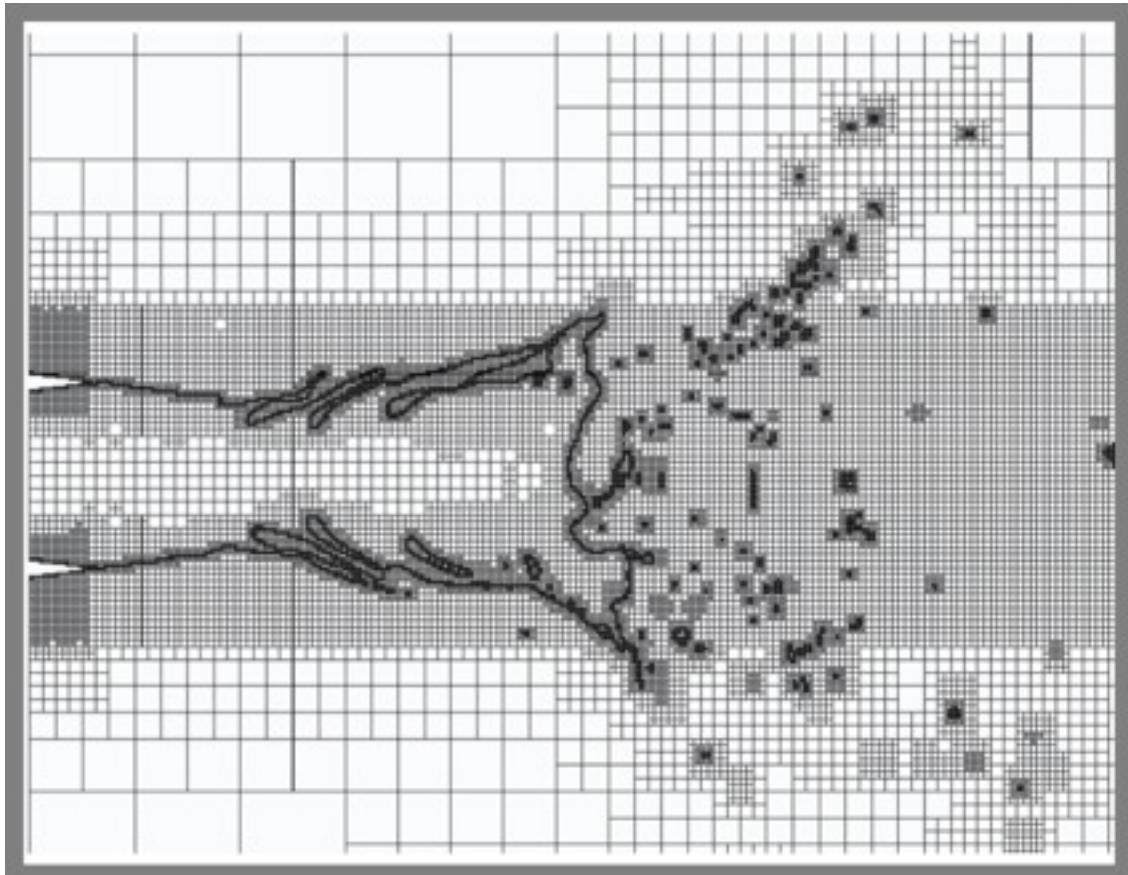
$$\text{Re}_g = 16000, \text{We}_g = 200$$

based on D_1

Simulation : Two months on 64 AMD processors

line of eight 512³ boxes – (equivalent regular mesh but we use octree adaptation)

Difficult to go to higher levels of refinement



Boundary layer size
157 μm

Injector thickness
comparable.



Simulation: Gilles Agbaglah



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0 0



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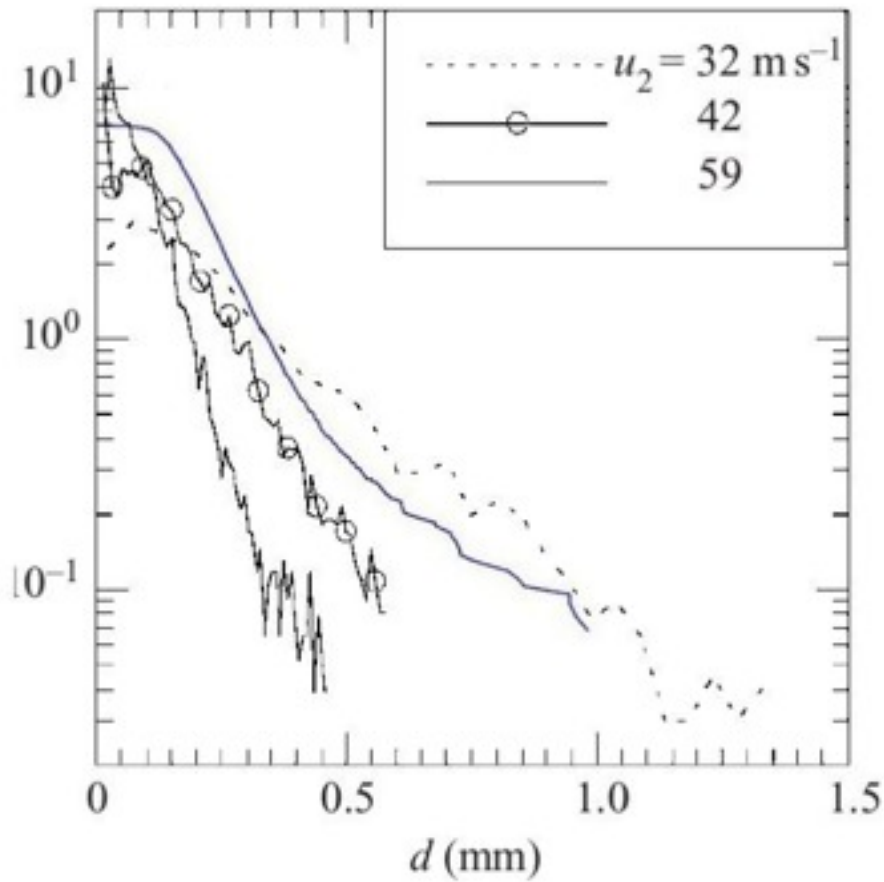
Simulation: Gilles Agbaglah



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Particle size distributions
 experimental and computed
 at UPMC

$u_2 = 35 \text{ m / s}$



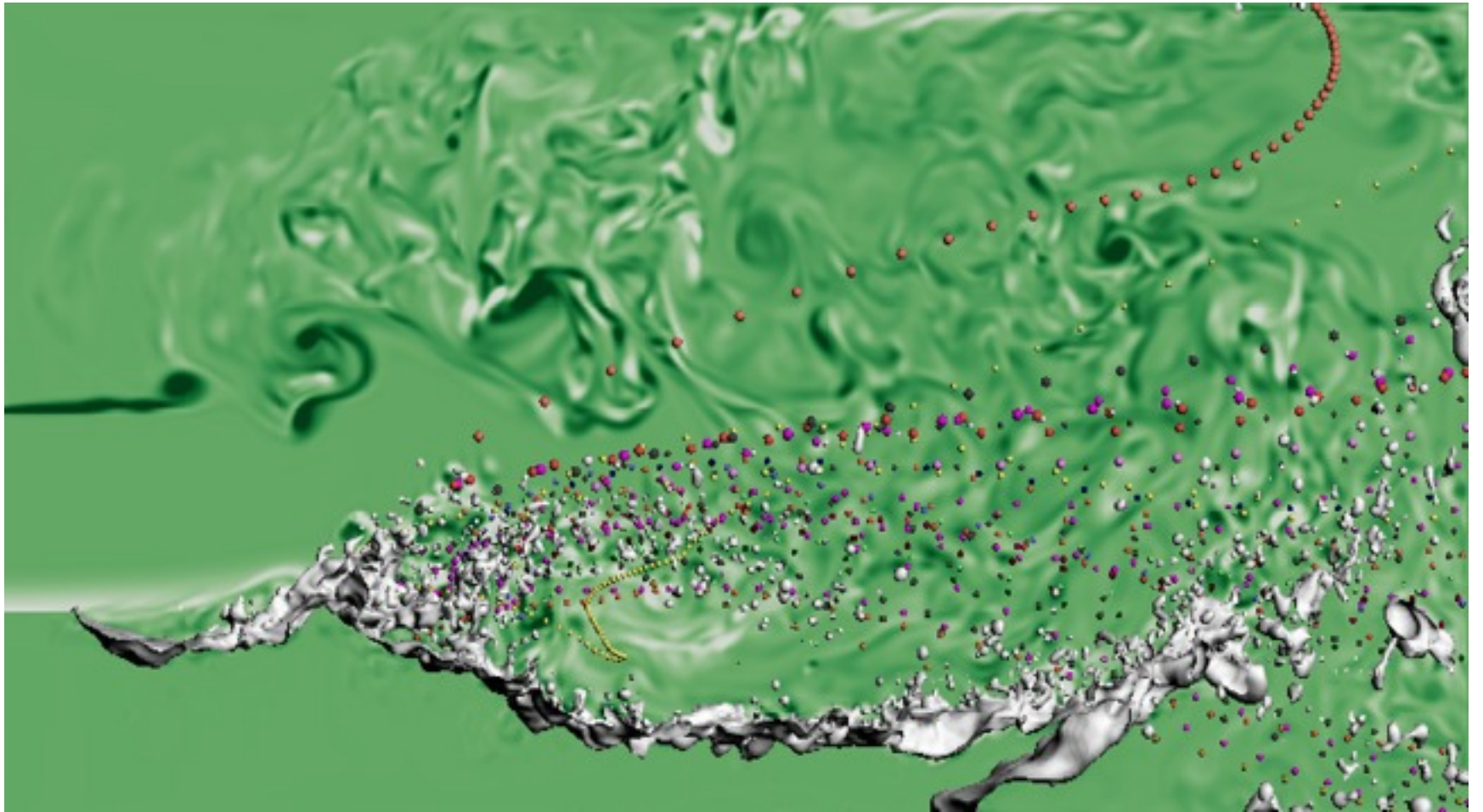
Planar shear flow of Descamps, Matas & Cartellier.
2nd colloque INCA, 2008.

Particle trajectories are measured.

$$\text{Re}_\delta = 1000$$

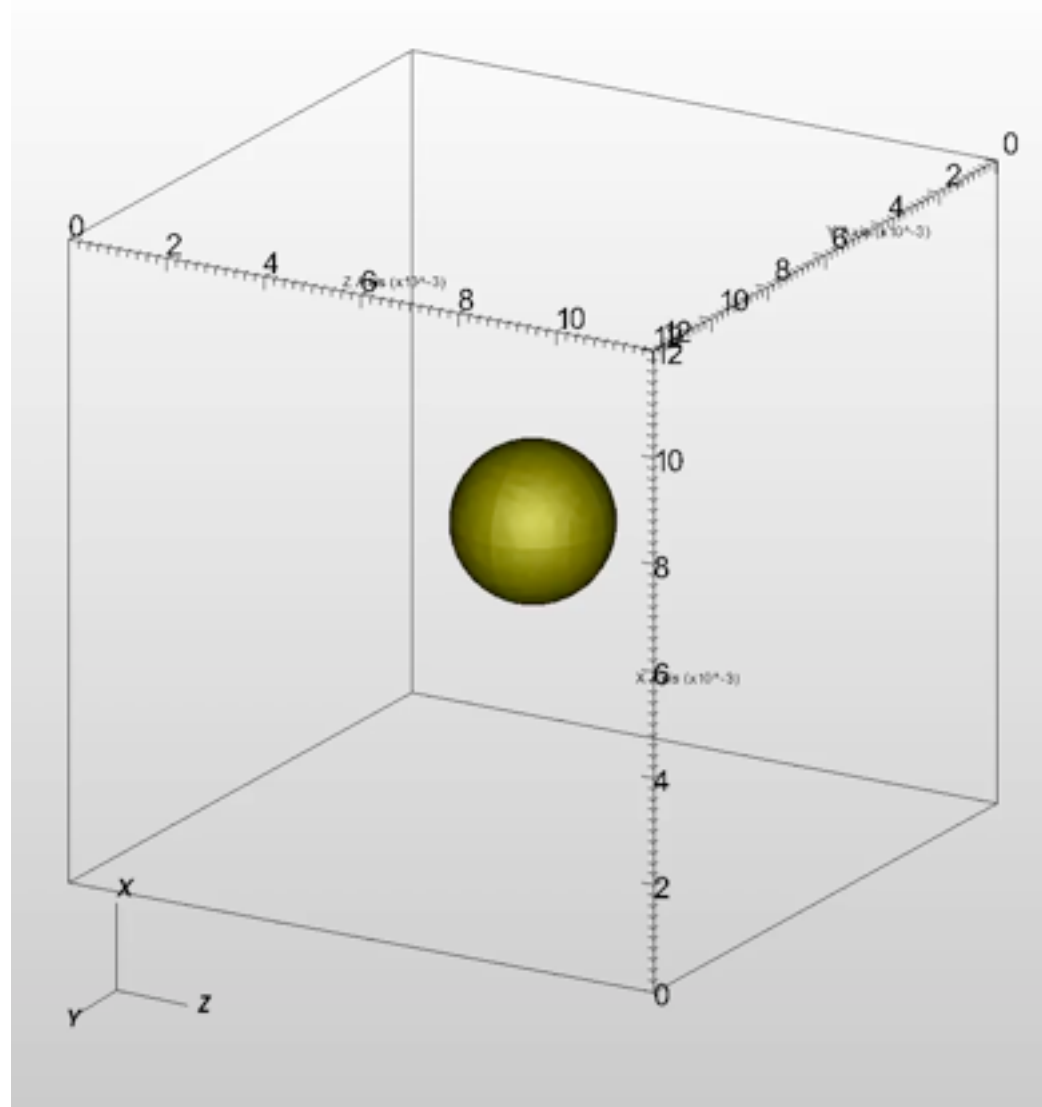
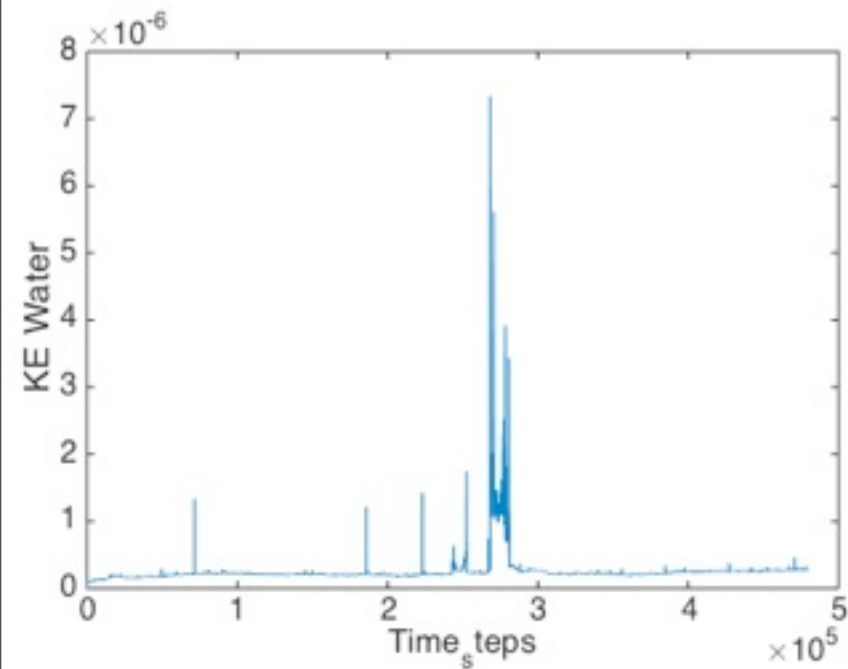
Simulation $64 \times 256 \times 512$





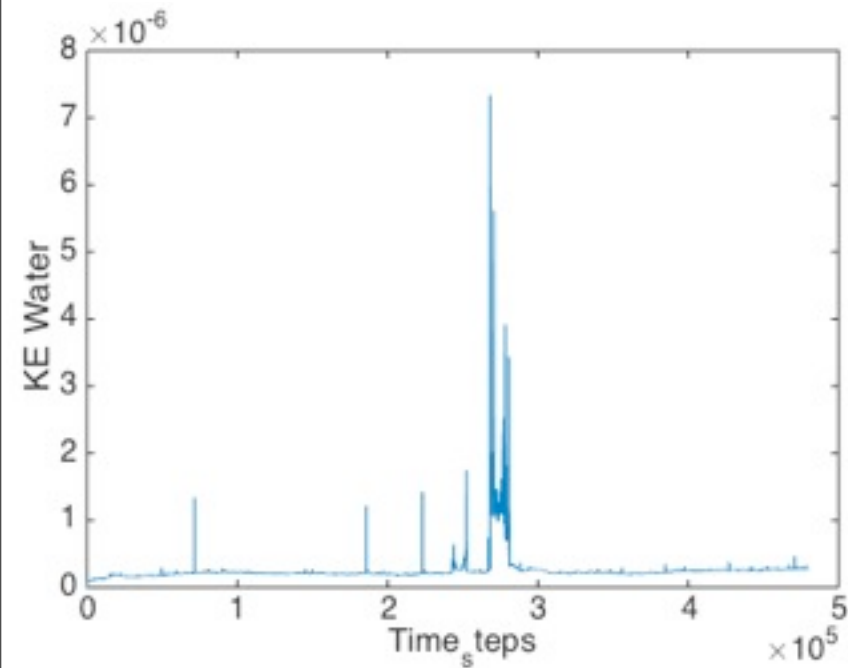
Refinement level $1.D/\Delta x=15$.
Spurious currents observed.

Kinetic energy of the droplet

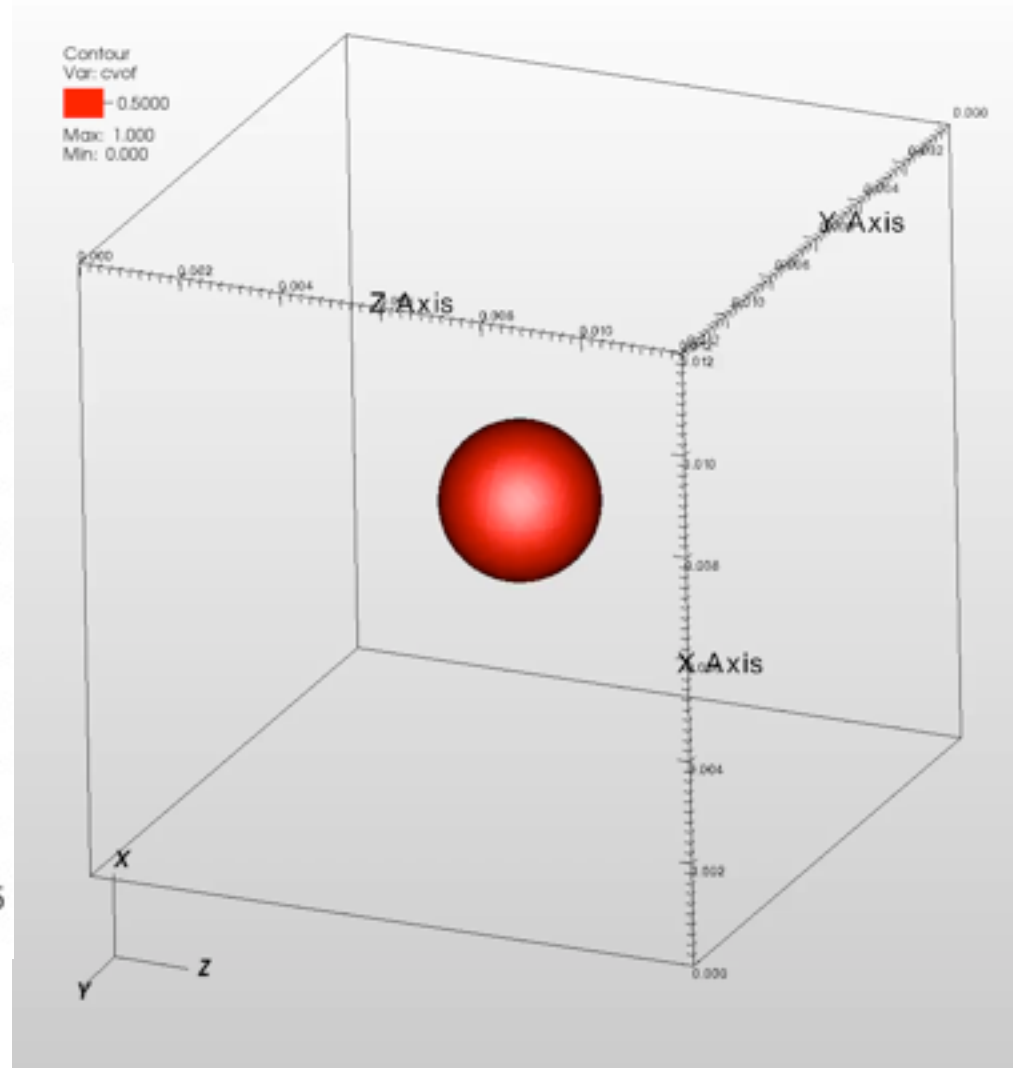
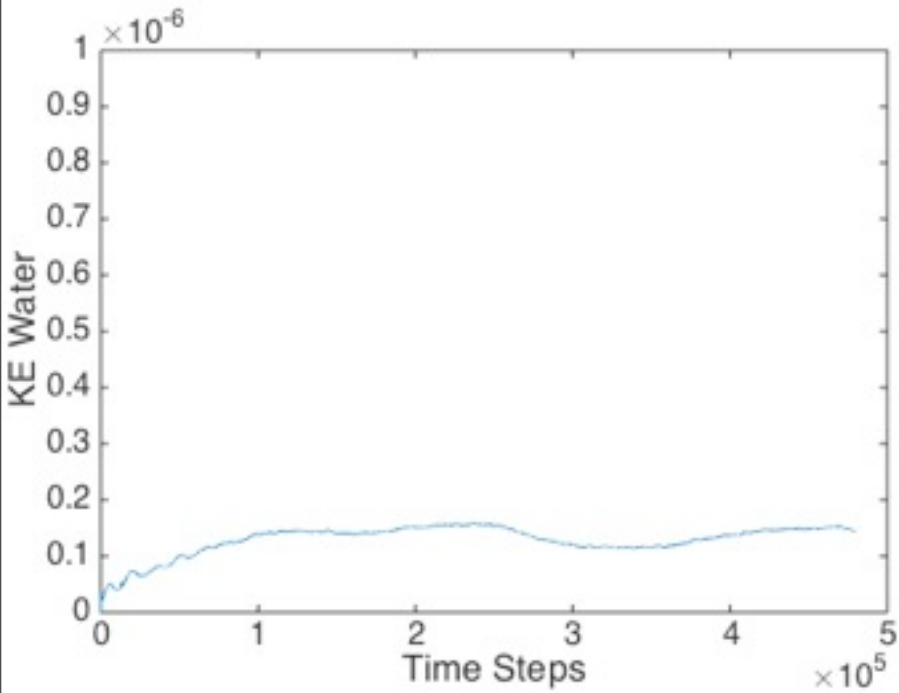


Refinement level $l.D/\Delta x=15$.
Spurious currents observed.

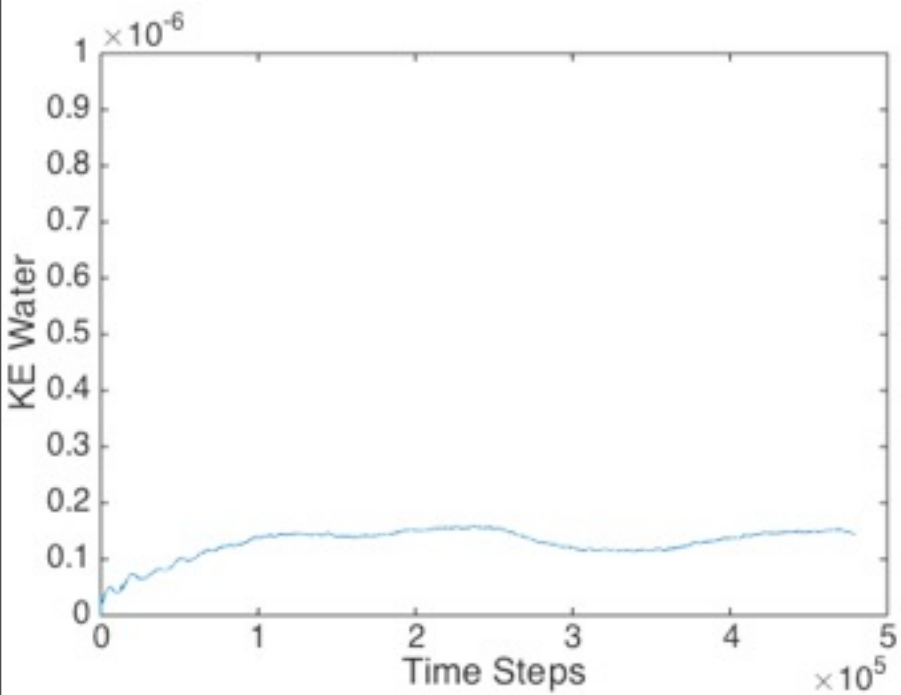
Kinetic energy of the droplet



Refinement level 2. $D/\Delta x=30$.
Kinetic energy

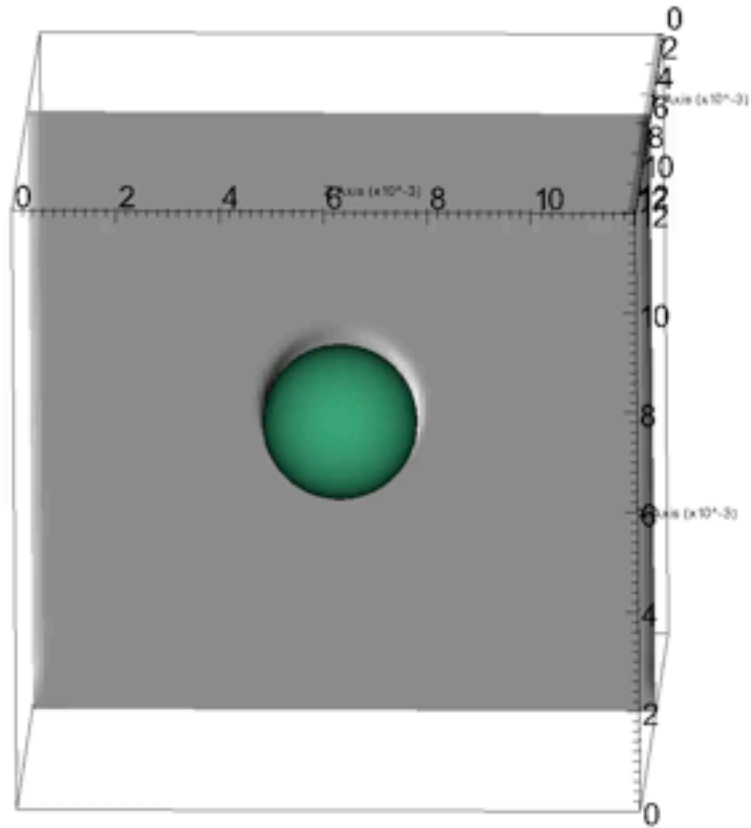
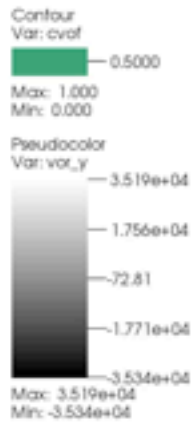


Refinement level 2. $D/\Delta x=30$.
Kinetic energy of the droplet



diameter $d=8$ mm

DB: multi00001.root
Cycle: 0 Time:0.0002



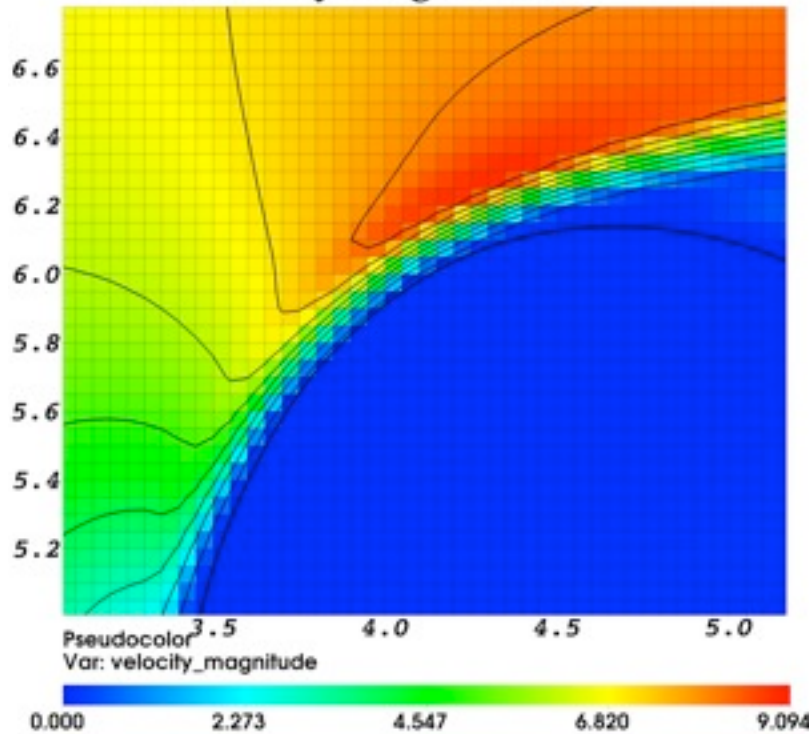
user: tomasarrufat
Mon Mar 9 14:43:12 2015



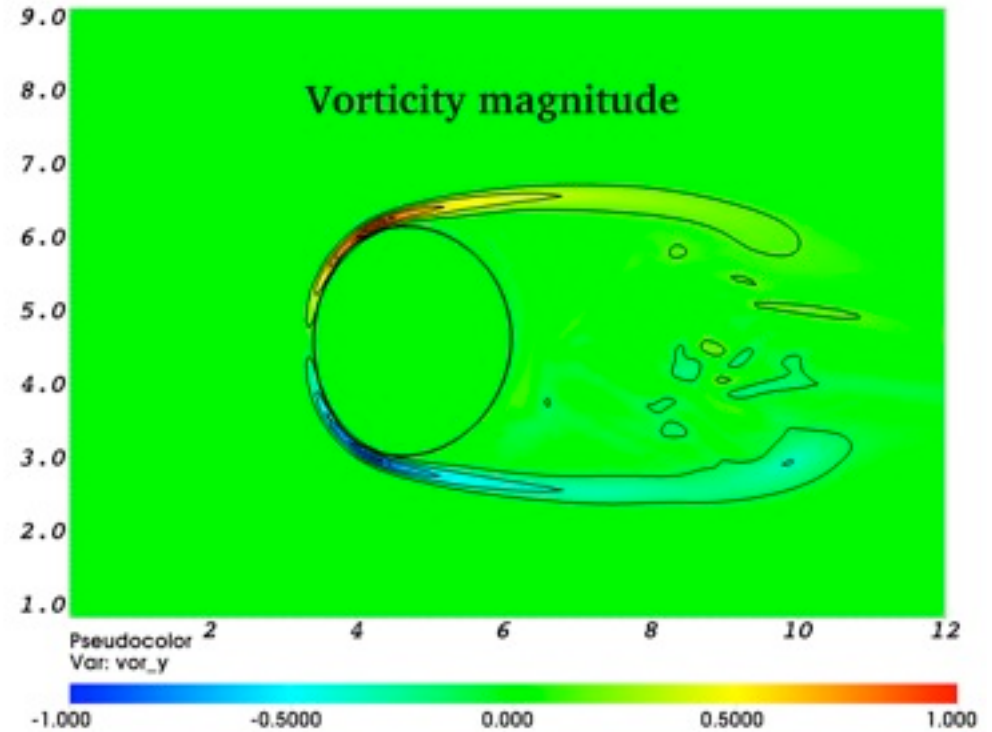
diameter $d=8$ mm



Velocity magnitude



Vorticity magnitude



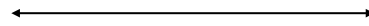
- Even for $D/\Delta x = 60$ the boundary layer is only covered by 5 cells.
- The boundary layer is very small relative to the droplet diameter.
- Such results suggest that the accurate solution of air flow with water droplets can be extremely challenging.

D'Alembert 



DROPLET IMPACT

D



Liquid

Simulation setup

U

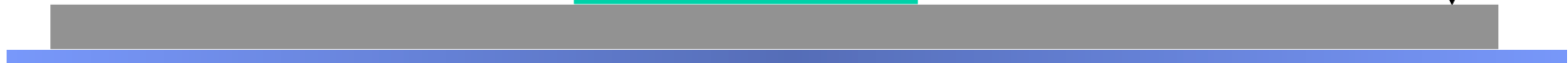


gas



Same liquid

h

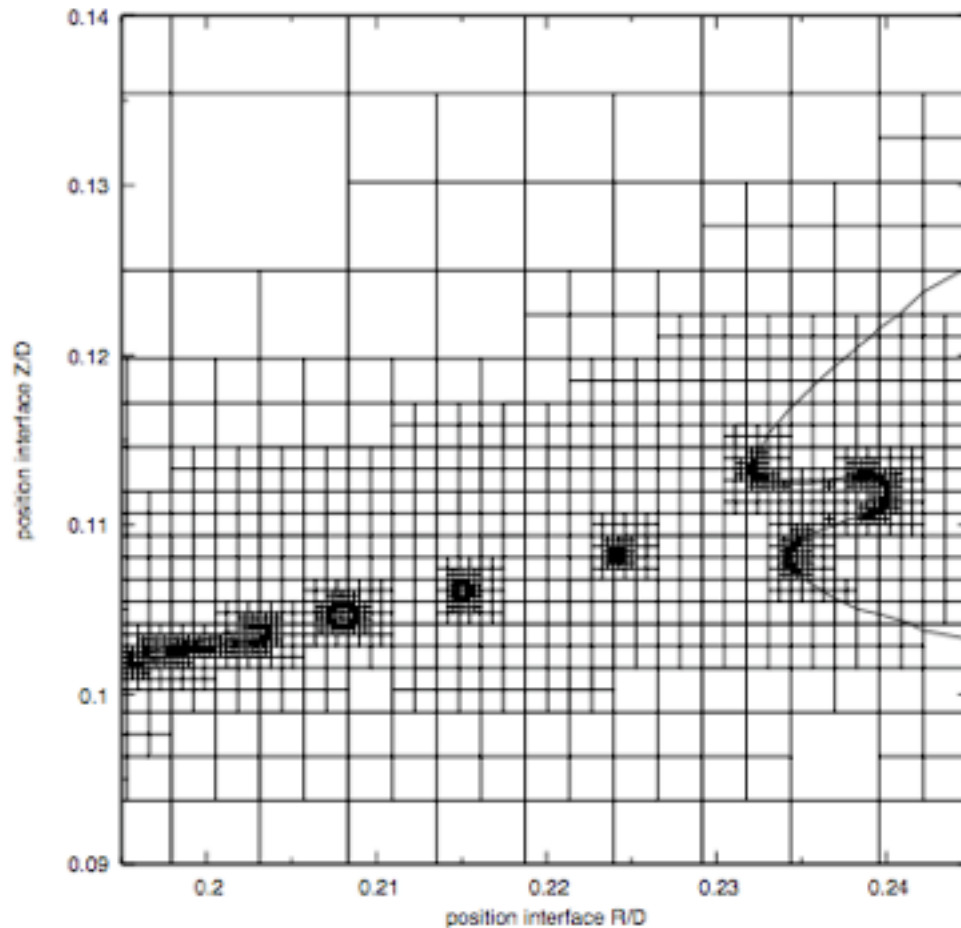




experiments by Thoroddsen



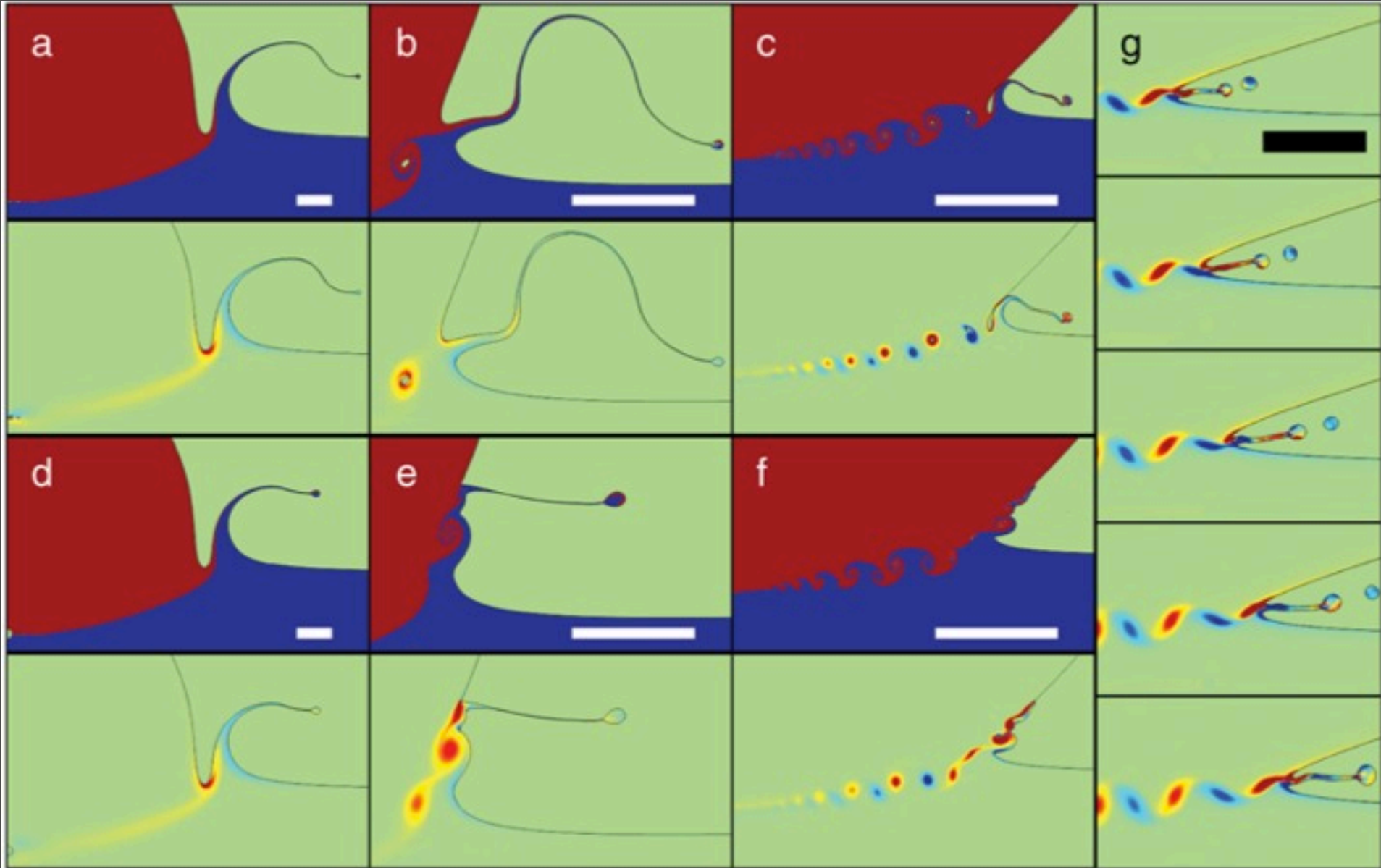
Even higher resolutions, with octree-AMR, up to $D/h \sim 6000$.



From Josserand, Ray and
SZ, ICMF2010

Simulation Pascal Ray
Gerris code

Adapting on curvature and (less strongly) on vorticity



Thoroddsen, Thoraval & others + Gerris, KAUST, Phys. Rev. Lett. (2012)

Figure 4f



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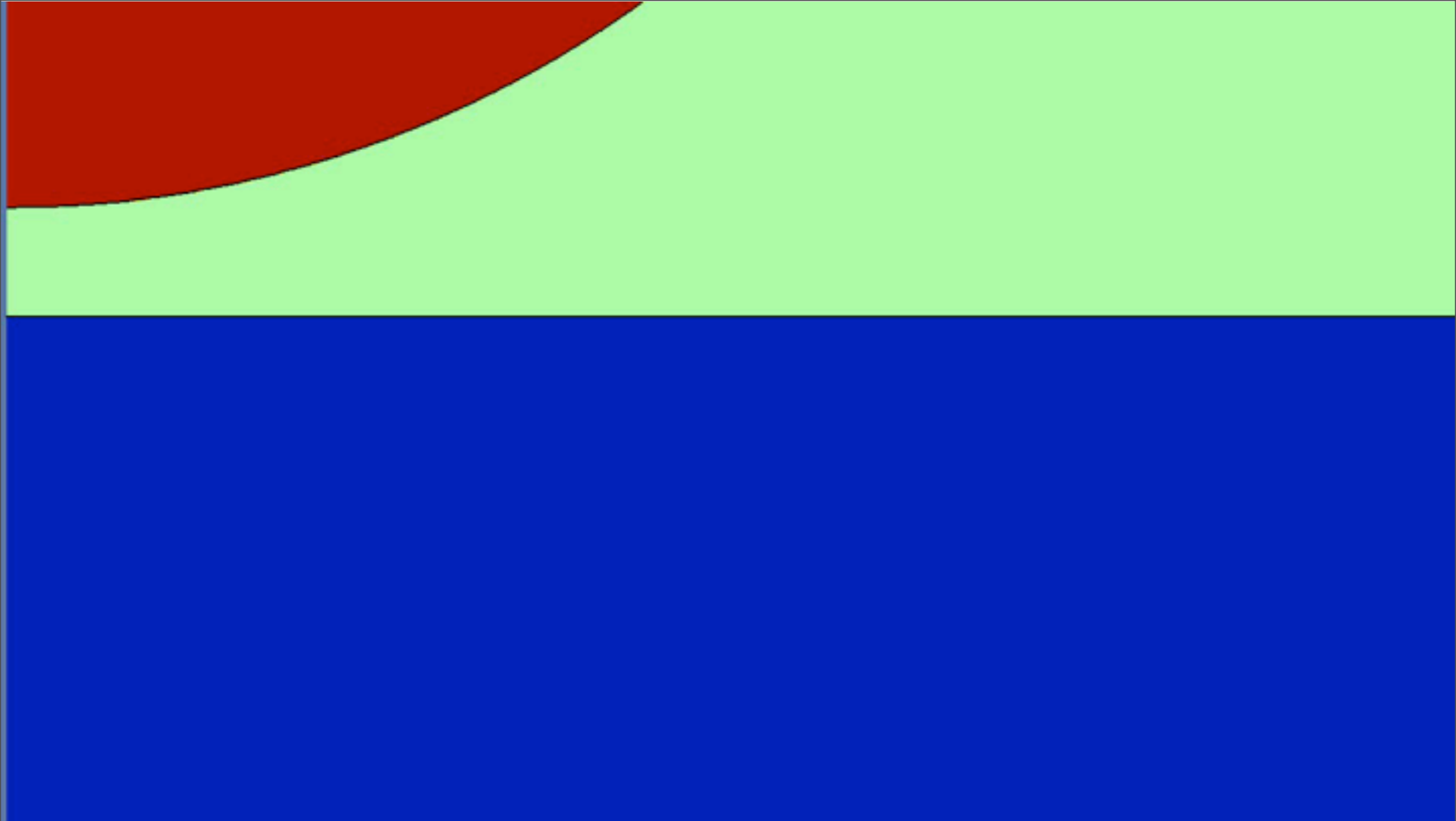


Figure 4f

