

Gouttes et bulles, un univers fascinant à l'intérieur des solutions des équations de Navier-Stokes

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Collaborators in the past ten years on atomisation.

Ruben Scardovelli, Stephane Popinet, **Daniel Fuster**, Tomas Arrufat, Peng Cheng, Gretar Tryggvason, Leon Malan, Yue Stanley Ling, Alexandre Guion, Subin Tomas, Taraneh Sayadi, Florence Marcotte, Wojciech Aniszewski, Sagar Pal, Nelson Joubert, Marco Crialesi, Youssef Saadeh, Alexandre Limare, Raphael Villiers.

Current students and postdocs

Tomas Fullana, **Mandeep Saini**, Saeed Bidi, Ahmed Basil K., Cesar Pairetti, Jacob Maarek, Leonardo Chirco, **Yash Kulkarni**, Xiangbin Chen, Désir-André Koffi-Bi, Damien Thomas, Tobias Bauer, Elena Batzella, Jieyun Pan, Tian Long.



The Navier-Stokes equations (incompressible, single phase)

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

$$\rho(\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}) = -\nabla p + \mu \Delta \mathbf{u} + \rho \mathbf{g}$$

Henri Navier





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Henri Navier



the view in this talk

$$\rho(\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u}) = -\nabla p + \mu \Delta \mathbf{u} + \phi \nabla C + \rho \mathbf{g}$$

C : phase characteristic function ϕ : surface tension. Constant viscosity (for simplification).
Incompressible, no coupling with thermal effects (pandora box).

Claude Louis Marie Henri Navier, « Mémoire sur les lois du mouvement des fluides » (lu à l'Académie royale des sciences le 18 mars 1822), *Mémoires de l'Académie royale des Sciences de l'Institut de France*, Paris, vol. 6, 1827, p. 389-440

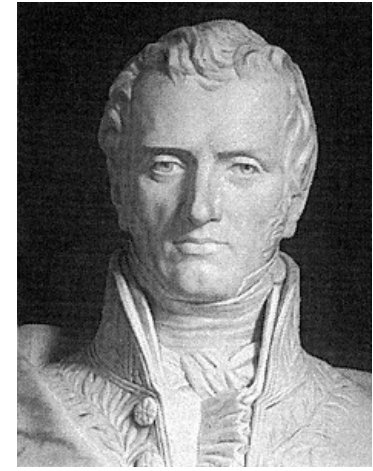
George Gabriel Stokes, *Transactions of Cambridge Philosophical Society*, vol. 8, 1845, p. 287–305.

Boundary conditions

$$\mathbf{u} = \mathbf{u}_{\text{solid}}$$

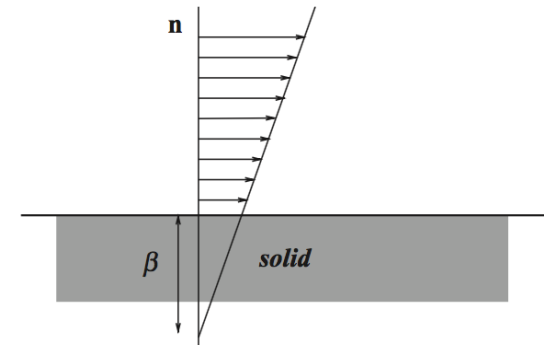
lead to severe singularities with two phase flow with contact lines.

Henri Navier



- A Navier Boundary Condition (NBC) is often used as a regularization

$$u = \lambda \frac{\partial u}{\partial y}$$



- λ is called the **slip length**, and is **measured** to be of the order of a nanometer or less.

Applications, motivations



420



Ten times the number 42 ?



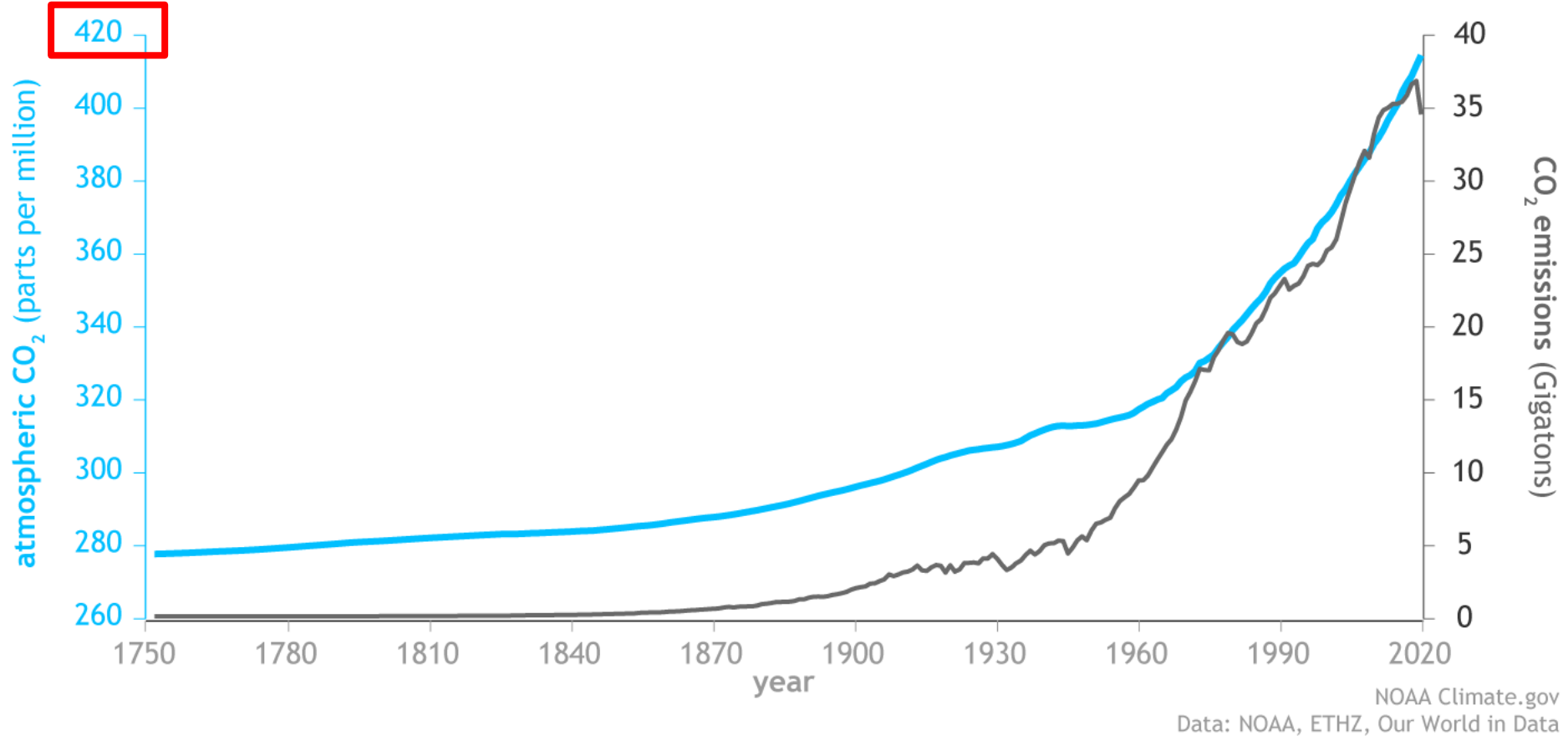
42 | ppm is the current CO₂ level in earth's atmosphere



If you measure more than 421 ppm in a room, it is a sign that aeration is not sufficient and you are at risk of contamination by a respiratory disease such as SARS, MERS, Covid-19, the flu or a common cold.

The 420 CO₂ level is also the result of 150 years of fossil fuel burning

Carbon dioxide emissions and atmospheric concentration (1750-2020)



ipcc

INTERGOVERNMENTAL PANEL ON climate change

Climate Change 2022

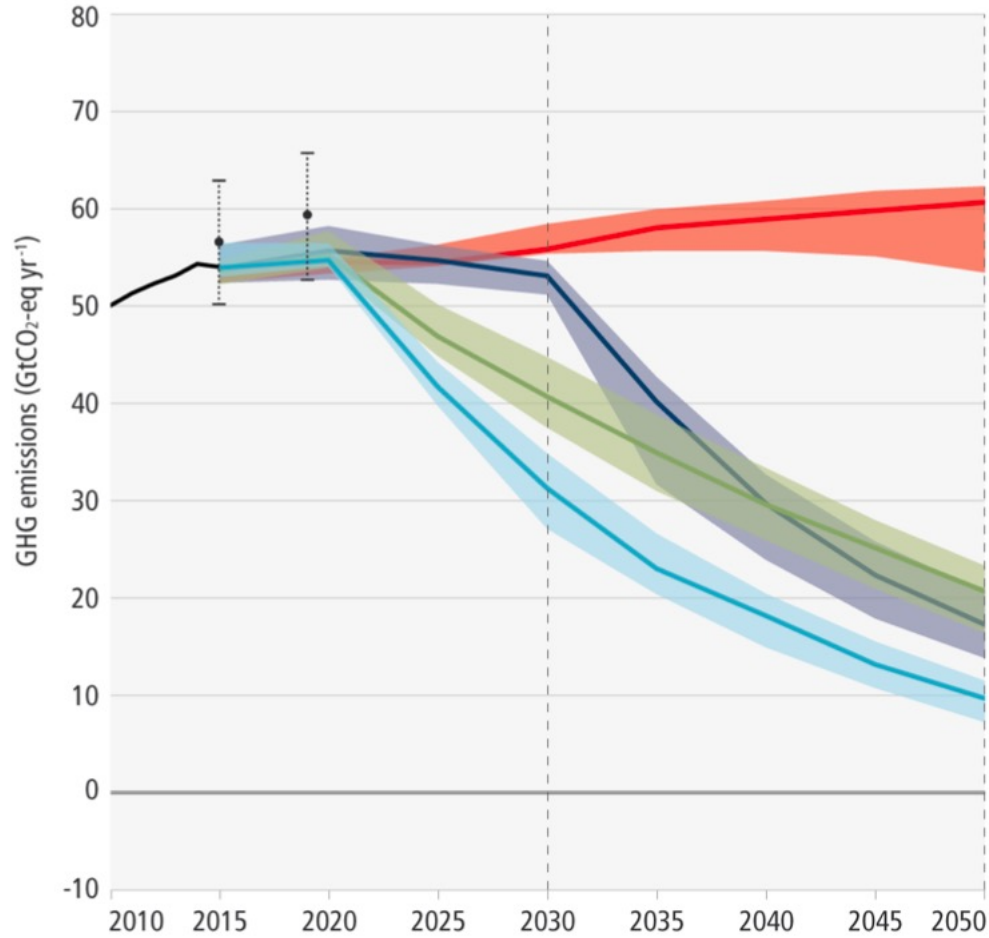
Mitigation of Climate Change

Summary for Policymakers



pathways

a. Global GHG emissions

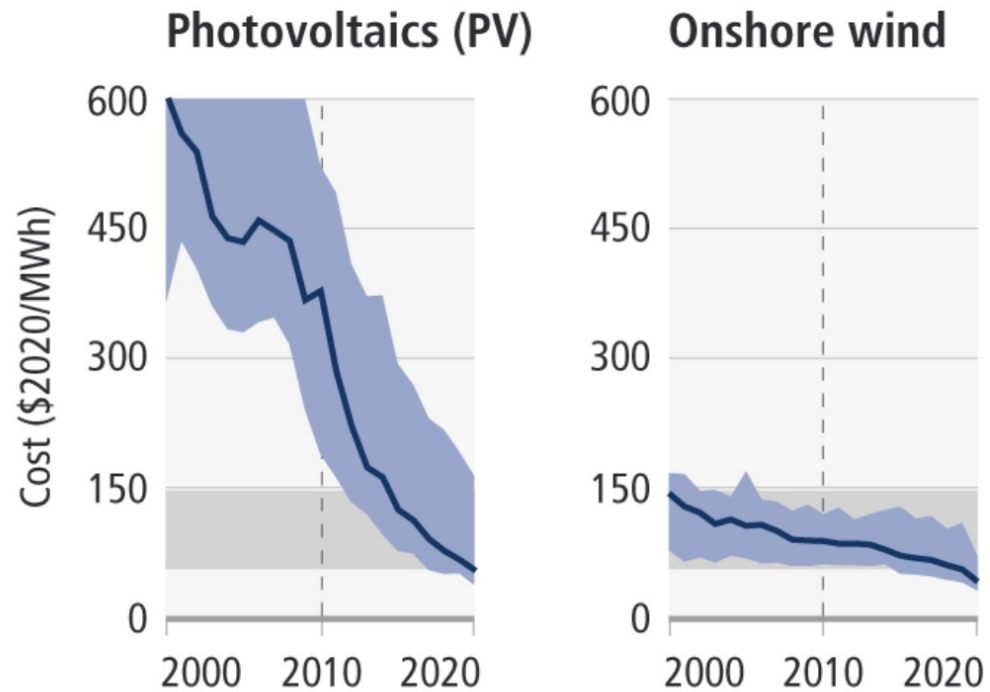


Modelled pathways:

- Trend from implemented policies
- Limit warming to 2°C (>67%) or return warming to 1.5°C (>50%) after a high overshoot, NDCs until 2030
- Limit warming to 2°C (>67%)
- Limit warming to 1.5°C (>50%) with no or limited overshoot
- Past GHG emissions and uncertainty for 2015 and 2019 (dot indicates the median)

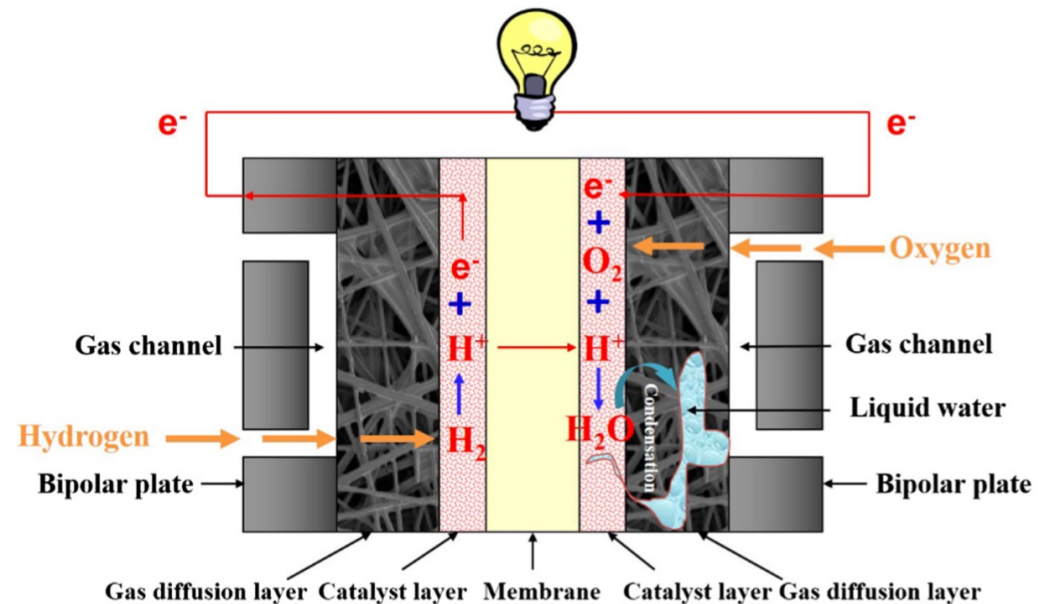
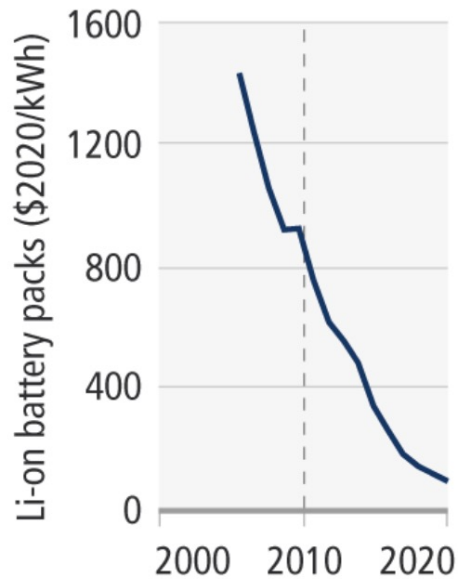
NDC : National Determined Contributions

Solutions are available: wind and solar have become much cheaper



But energy storage remains a big issue. To compensate for the intermittency and annual oscillation of wind and solar power, about six months of storage of a country's energy consumption is needed. Sadly, although now **cheaper to produce**, batteries last only a **few hours**...

Batteries for passenger electric vehicles (EVs)



Fuel cell

The number 42 | is thus connected to two of the main issues discussed in this lecture:

- Energy and climate : production, storage, usage, ocean-atmosphere interactions
- Respiratory disease transmission by aerosols.

Climate change and the emission reductions necessary to mitigate it are related to many natural phenomena and technologies.

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An essential phenomenon is the ocean-atmosphere interface.





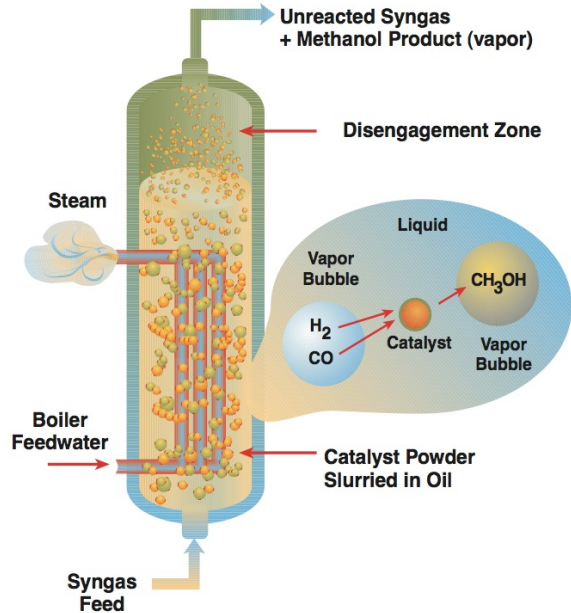
From Véron, ocean spray, 2015

Chemical and process engineering



Bubble Columns

From: <http://p2pays.org/ref/16/15865.pdf>



Liquid Phase Methanol (LPMEOH™) Process

Examples of Applications of Bubble Columns

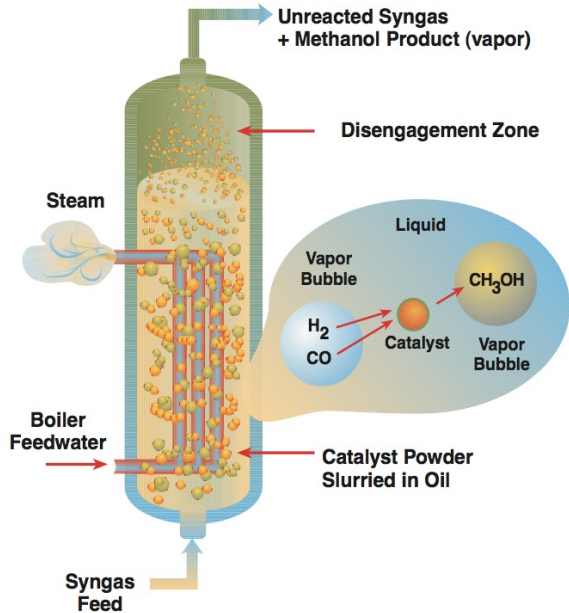
Process	Methods and/or Reactants
Acetone	Oxidation of cumene
Acetic acid	Oxidation of acetaldehyde
	Oxidation of sec-butanol
	Carbonylation of methanol
	Oxidation of acetaldehyde
Acetic anhydride	Partial oxidation of ethylene
Acetaldehyde	Oxidation of ethylbenzene
Acetophenone	Barium sulfide and chlorine
Barium chloride	Oxidation of toluene
Benzoic acid	Aqueous calcium oxide and chlorine
Bleaching powder	Aqueous sodium bromide and chlorine
Bromine	Absorption in aqueous solutions of sulfuric acid
Butene	Absorption in ammoniated brine
Carbon Dioxide	Carbon disulphide and chlorine
Carbone tetrachloride	Oxidation of cuprous chloride
Copper oxychloride	Oxidation of phenol
Cumene	Copper and cupric acid or hydrochloric acid
Cupric chloride	Oxychlorination of ethylene
Dichlorination	Benzene and ethylene
Ethyl benzene	Benzene and chlorine
Hexachlorobenzene	Oxidation of hydroquinone
Hydrogen peroxide	Absorption in aqueous solutions of sulfuric acid
Isobutylene	Oxidation of xylene
Phtalic acid	Oxidation of cumene
Phenol	Aqueous potassium carbonate
Potassium bicarbonate	Aqueous sodium carbonate
Sodium bicarbonate	Carbon dioxide, aqueous sodium carbonate, and sulfur dioxide
Sodium metabisulphides	Dithiocarbamates, chlorine, and air
Thiuram disulphides	Oxidation of ethylene in acetic acid solutions
Vinyl acetate	Wet oxidation of waste water
Water	



After: S. Furusaki, L.-S. Fan, J. Garside. **The Expanding World of Chemical Engineering** (2nd ed), Taylor & Francis 2001

Bubble Columns

From: <http://p2pays.org/ref/16/15865.pdf>



Liquid Phase
Methanol
(LPMEOH™)
Process

Transform back
CO into fuel

Examples of Applications of Bubble Columns

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Acetone	Oxidation of cumene
Acetic acid	Oxidation of acetaldehyde
	Oxidation of sec-butanol
	Carbonylation of methanol
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Copper oxychloride	Oxidation of phenol
Cumene	Copper and cupric acid or hydrochloric acid
Cupric chloride	Oxychlorination of ethylene
Dichlorination	Benzene and ethylene
Ethyl benzene	Benzene and chlorine
Hexachlorobenzene	Oxidation of hydroquinone
Hydrogen peroxide	Absorption in aqueous solutions of sulfuric acid
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Water	

capture CO₂

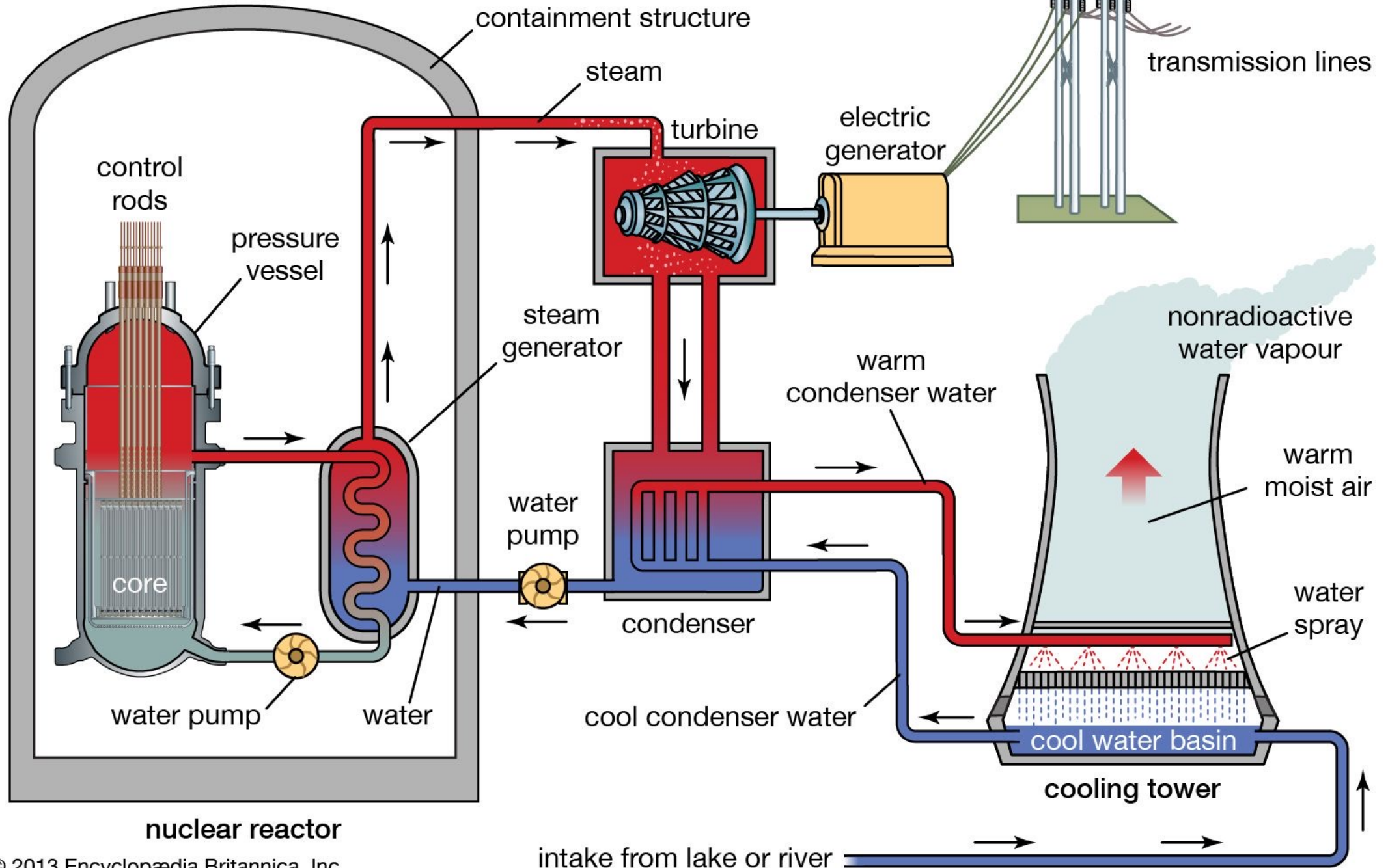


After: S. Furusaki, L.-S. Fan, J. Garside. **The Expanding World of Chemical Engineering** (2nd ed), Taylor & Francis 2001

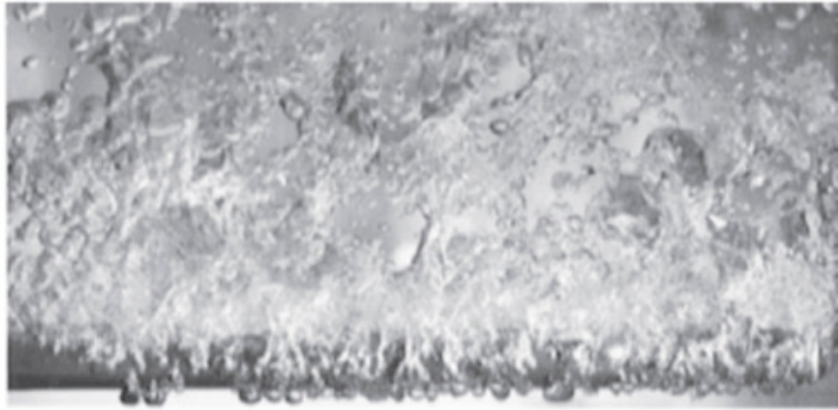
Boiling



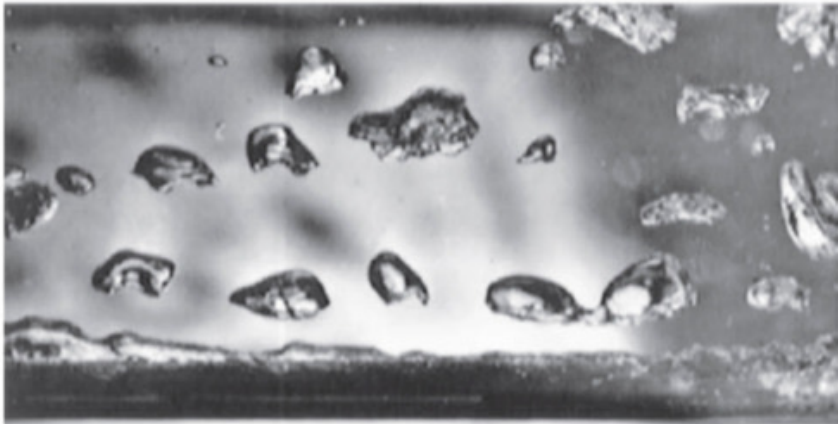
Nuclear power plant



Boiling



(a)



(b)



Bergman, T.L.; Incropera, F.P.; DeWitt, D.P.; Lavine, A.S. *Fundamentals of Heat and Mass Transfer*, John Wiley & Sons: Hoboken, NJ, USA, 2011.

Covid and atomization



Recent motivation: respiratory disease transmission

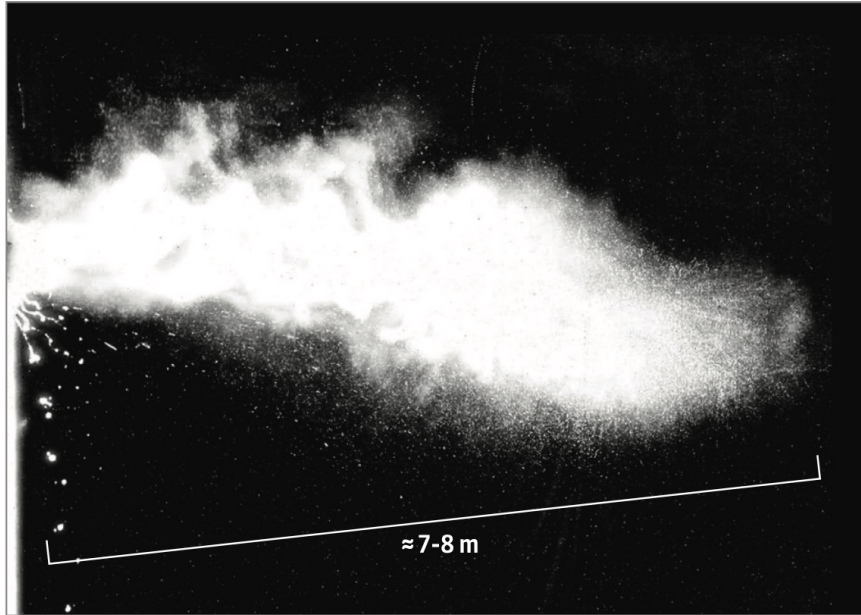
A short history of epidemiology and droplets

- Pasteur thought that pathogens were transmitted by dust particles. (Hence vacuum cleaners, waxing floors etc.)
- Paradox: why mandatory masks and no mandatory vacuuming ?
- No paradox: masks and waxing floors at time 1918 influenza epidemic
- In 1930 Wells introduces the distinction between « droplets » and « aerosols » or « droplet nuclei ». Studies tuberculosis. Makes assumptions about the droplet size distribution. Introduces arbitrary 5 micron limit.



turbulent puff.

From *Bourouiba L. Turbulent gas clouds and respiratory pathogen emissions: potential implications for reducing transmission of COVID-19. Jama. 2020 Mar 26.*

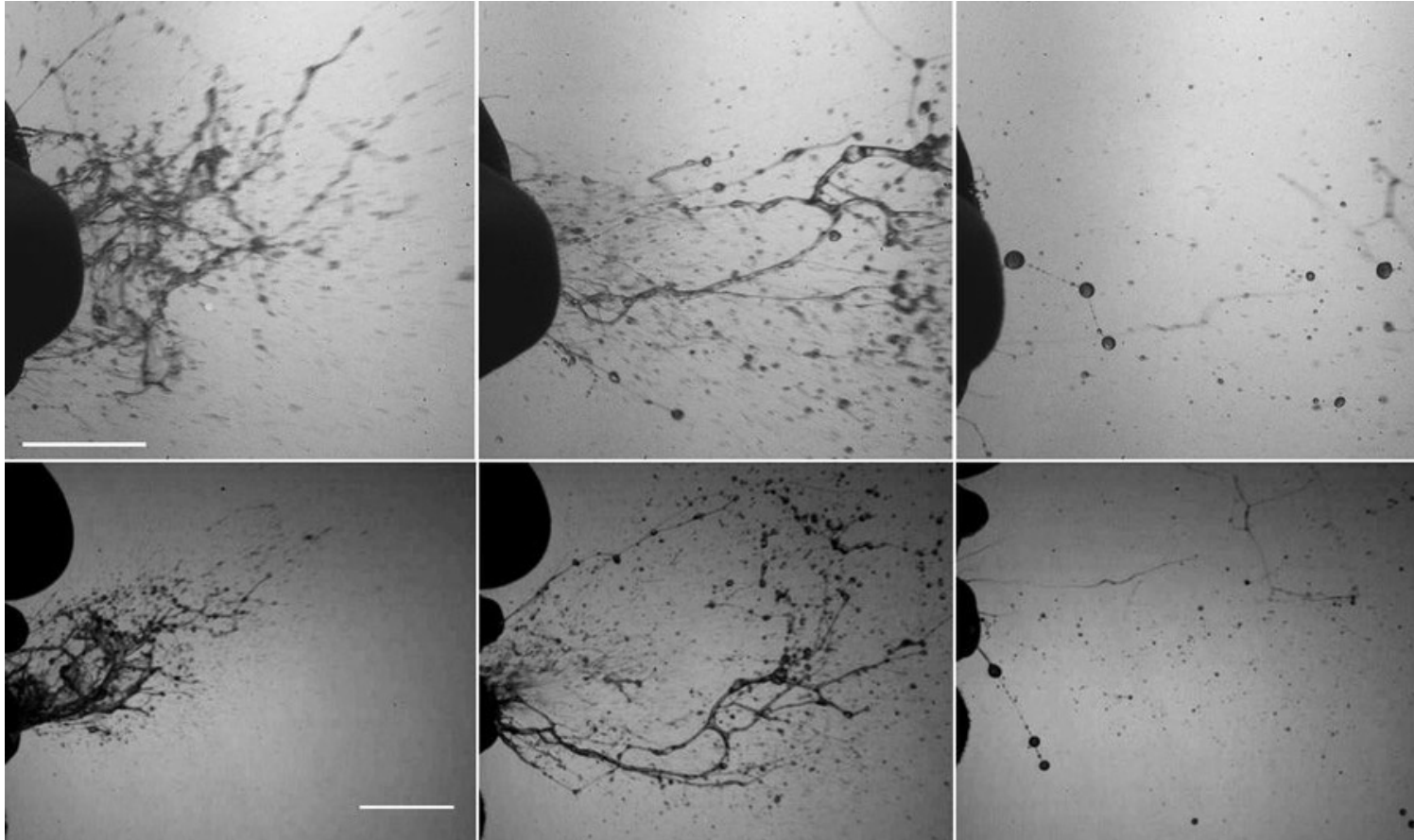


A turbulent puff created by a sneeze. The larger droplets (approx > 100 microns) fall to the ground in less than a meter. Smaller droplets are entrained into the turbulent puff. The image is from *Bourouiba L. Turbulent gas clouds and respiratory pathogen emissions: potential implications for reducing transmission of COVID-19. Jama. 2020 Mar 26.*

[vidéo](#)

The hotter turbulent puff can rise by natural convection and either stagnate near the ceiling or be entrained into the HVAC system and spread to other rooms.

Disease Transmission via Bioaerosols



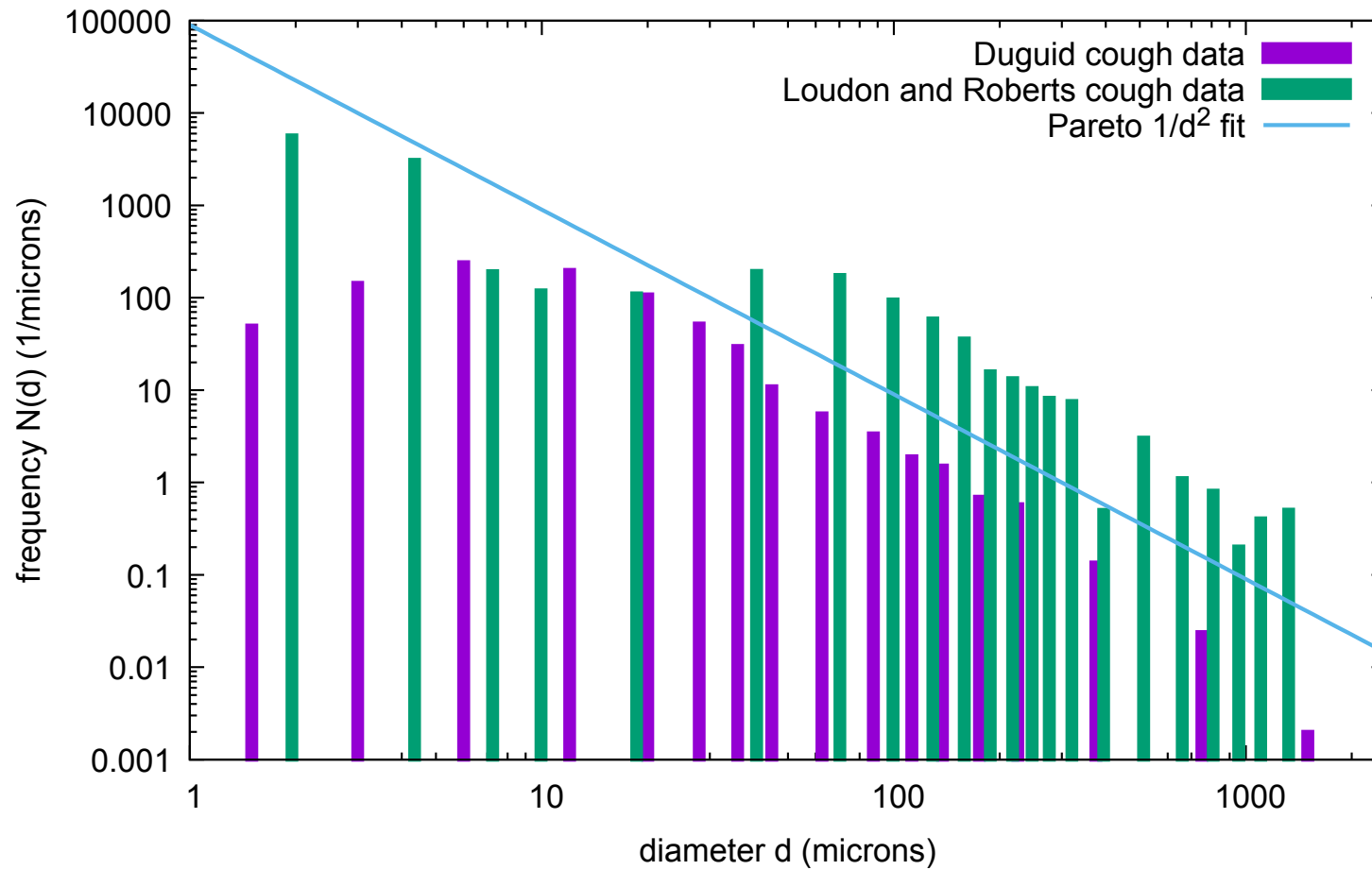
- Wide range of d !
- Viscoelastic !

Scharfman, et al. *Experiments in Fluids* (2016)

Question: what is the size of the droplets in the atomisation process ?

First **experimental** answer from Duguid (1946) ... Hard to do better since

Pareto $N(d) \sim 1/d^2$ fit



Cough Machine (with D. Lohse, P. Kant)

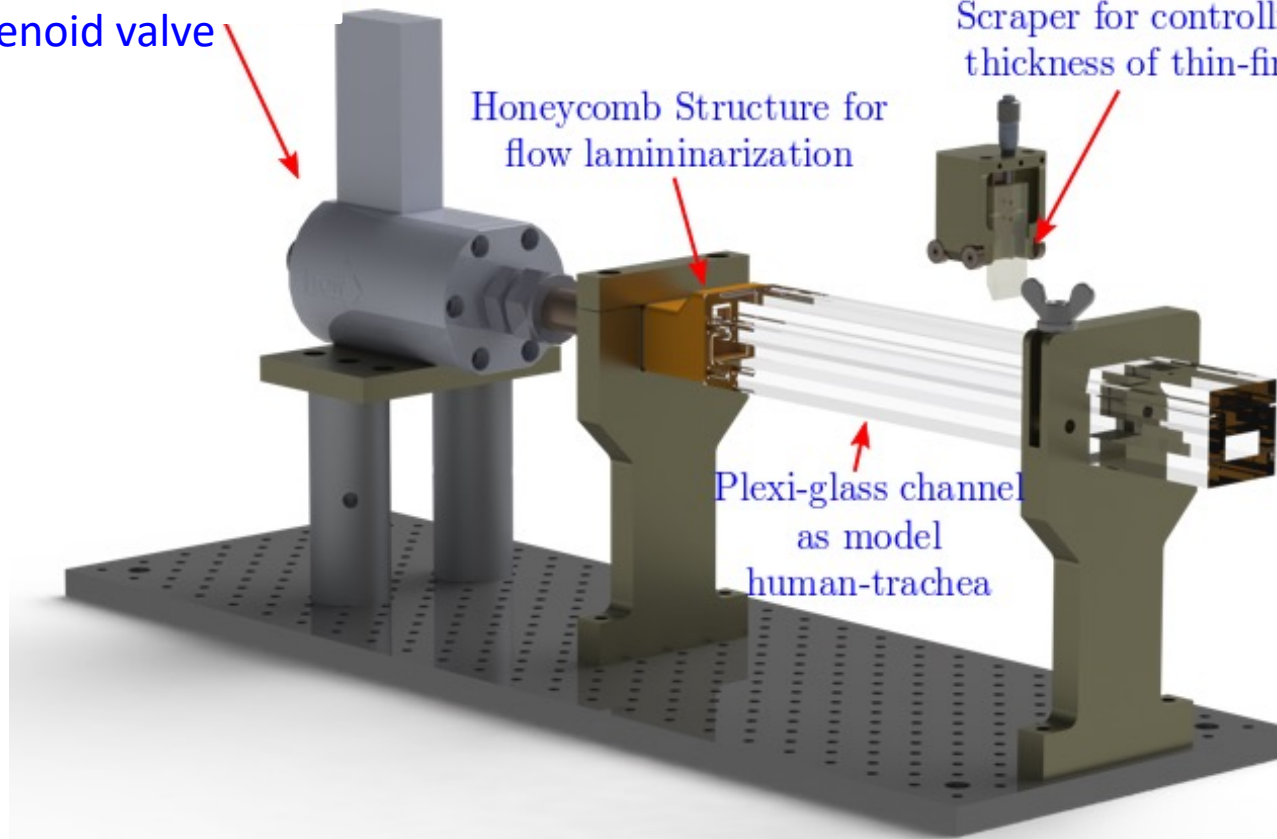
Flow meter connected to
pressurized vessel via a
solenoid valve

Honeycomb Structure for
flow laminarization

Scraper for controlling
thickness of thin-fims

Plexi-glass channel
as model
human-trachea

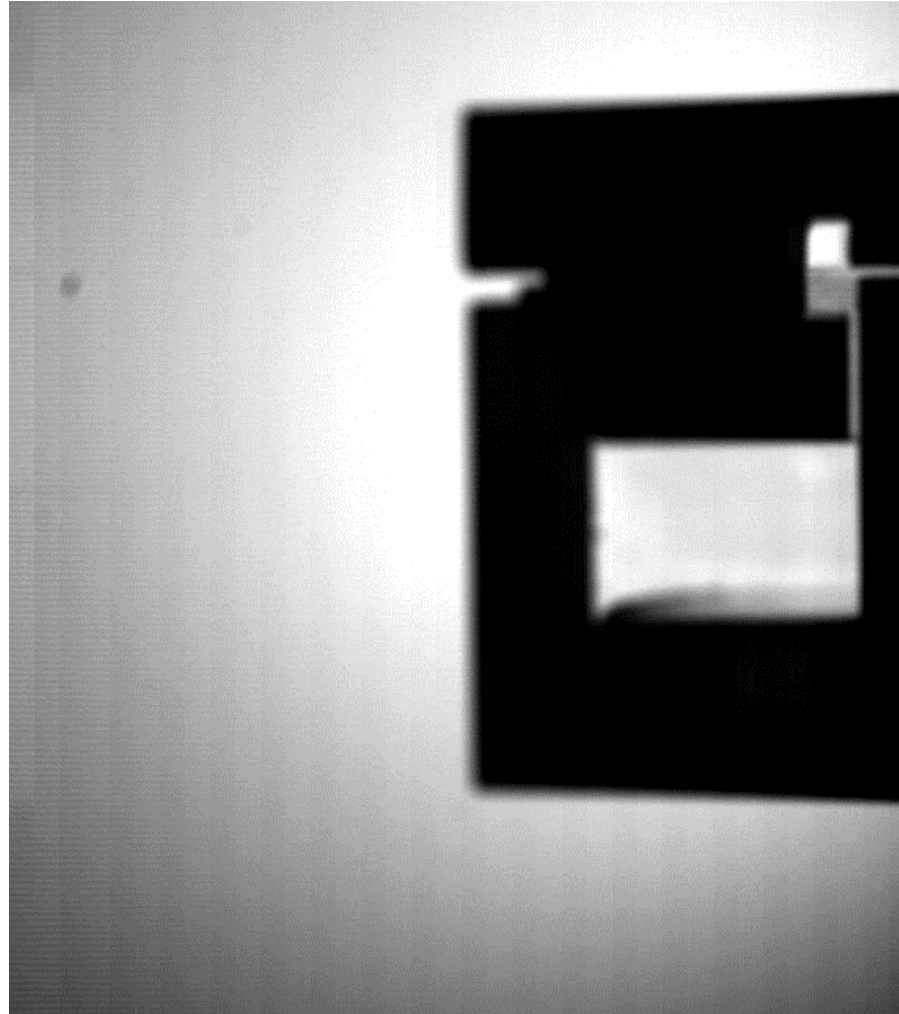
Cross-section
2 cm x 1cm



Experimental Parameters

- Liquid film : water-glycerol mixture
- Liquid viscosity : $2 - 100 \cdot 10^{-3} \text{ kg m}^{-1} \text{ s}^{-1}$
- Surface tension : $62 - 72 \text{ mN/m}$
- Flow velocity : $10 - 30 \text{ m/s}$

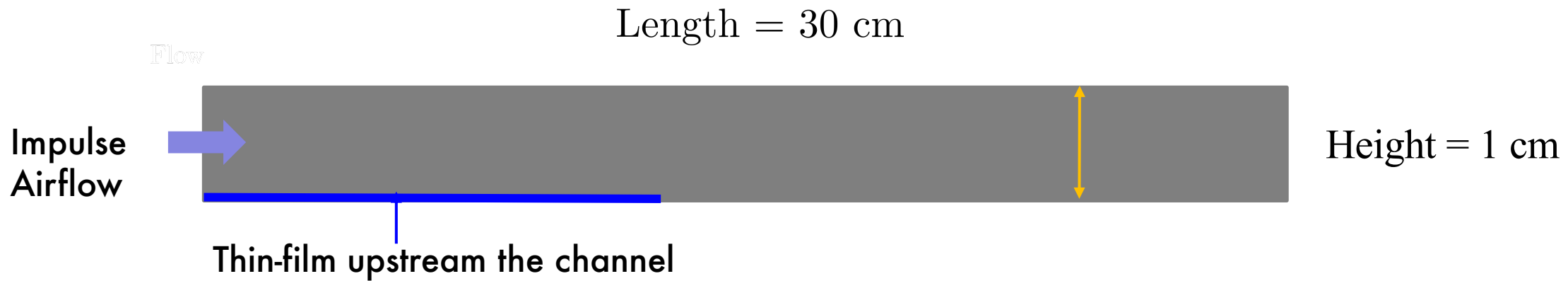
Droplet Generation



- Fine droplets are produced deeper in the channel
- Larger droplets form at the exit

Film Thickness $\mathcal{H}_f = 1 \text{ mm}$
Mean Flow Velocity $U \sim 29 \text{ m/s}$

Experimental configuration



Bag rupture mechanism

Example - 1

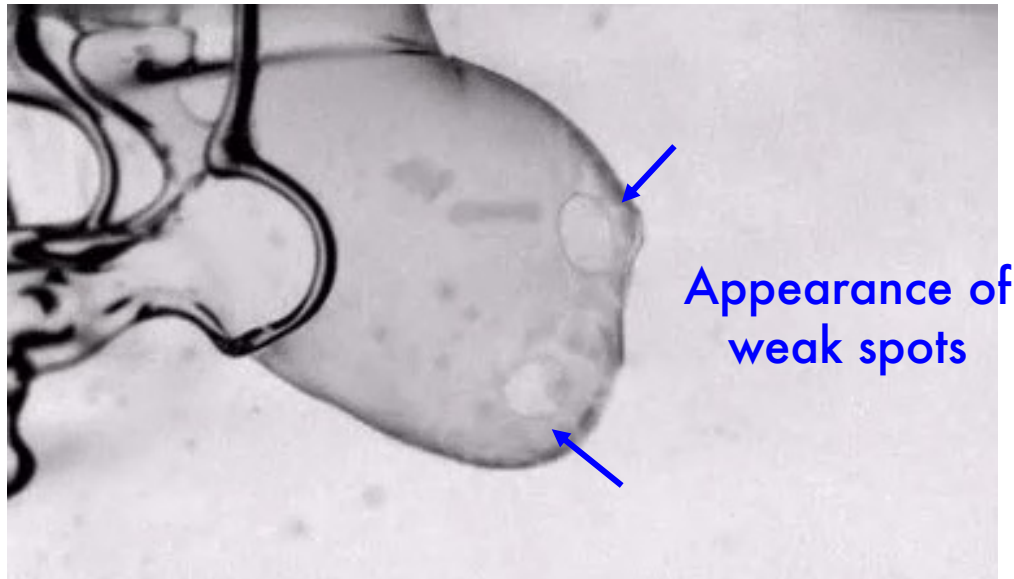


Example - 2

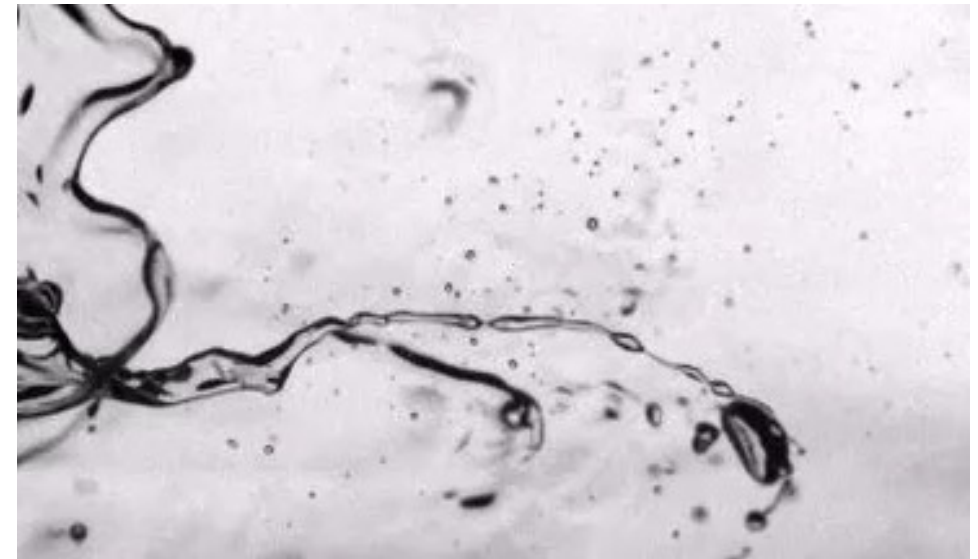


Bag rupture mechanism: Weak Spots

Example - 1



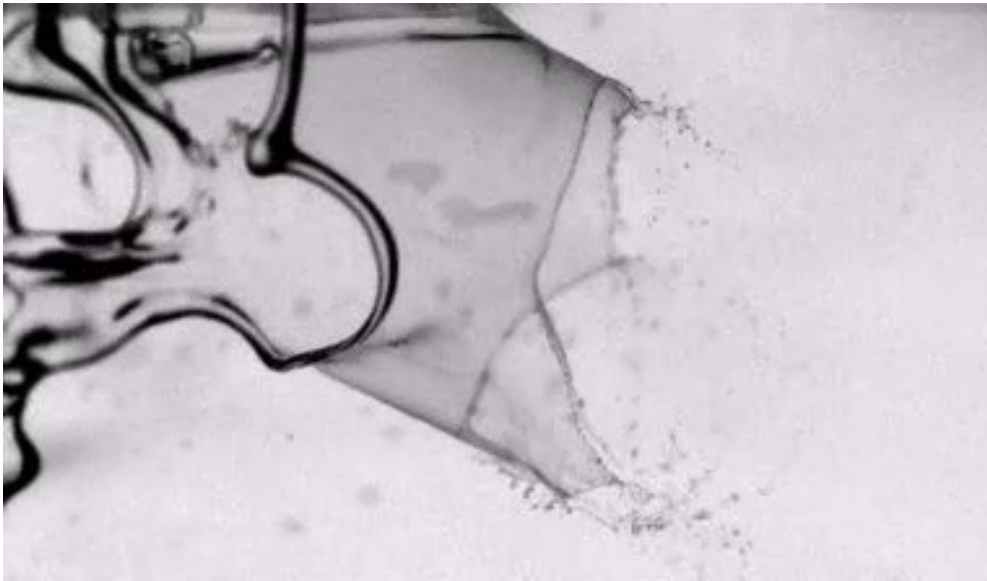
Example - 2



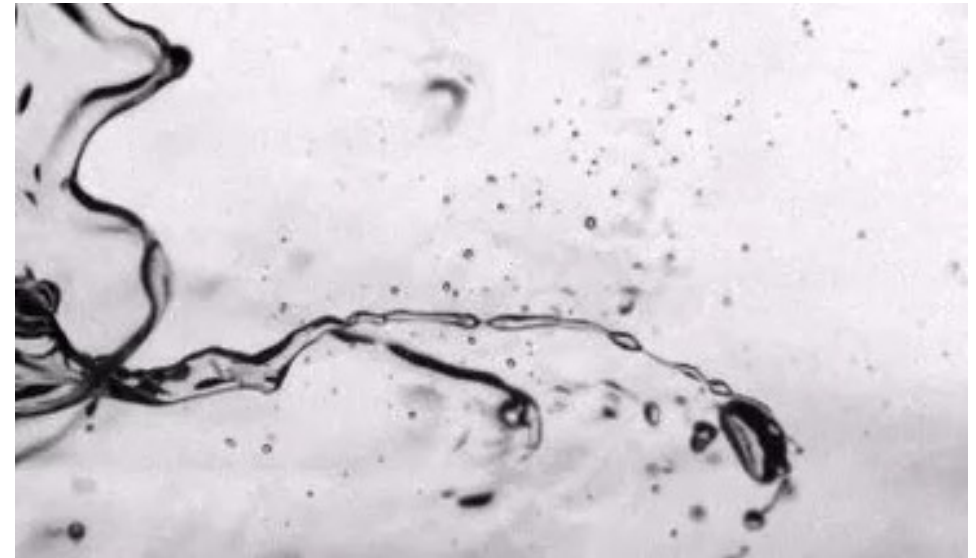
Unstable motion of retracting sheet generates small droplets $d \leq 50 \mu\text{m}$

Bag rupture: Appearance of Weak Spots

Example - 1



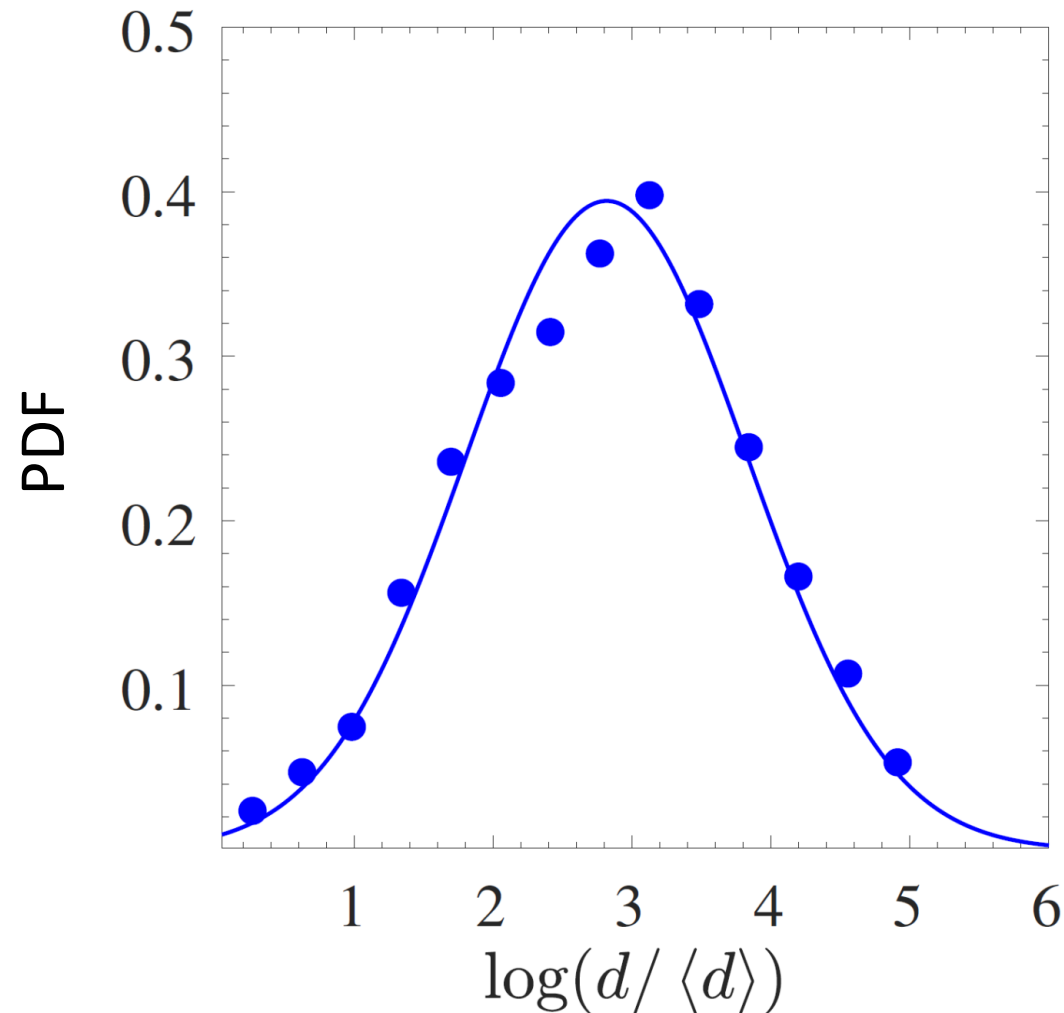
Example - 2



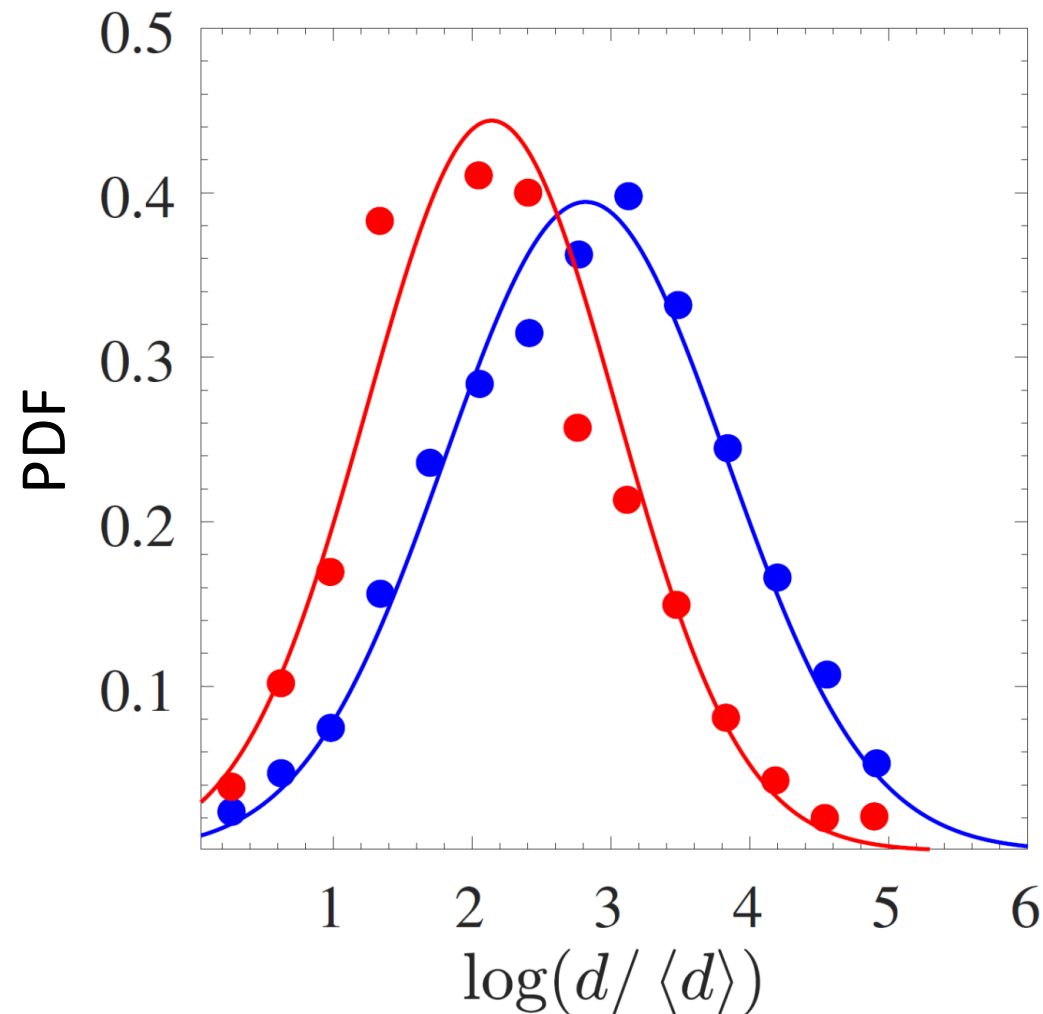
Finally the breakup of rim
creates larger droplets $d > 200 \mu\text{m}$

Droplet size distribution : Log-normal

$\nu = 5 \text{ cst}$



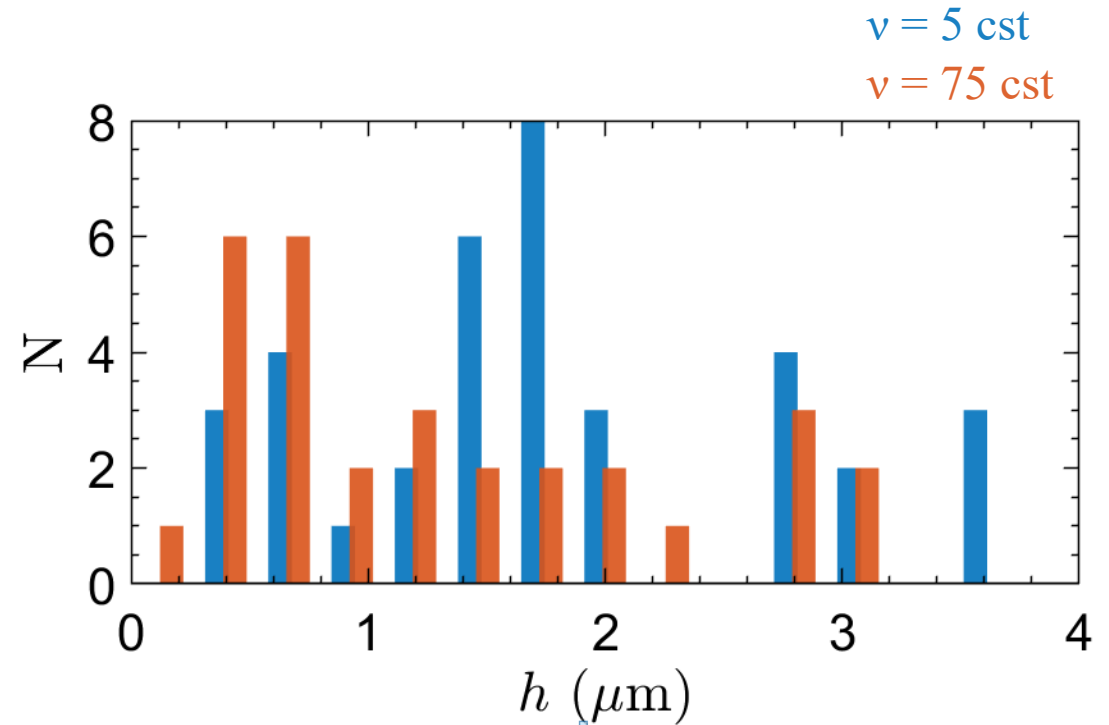
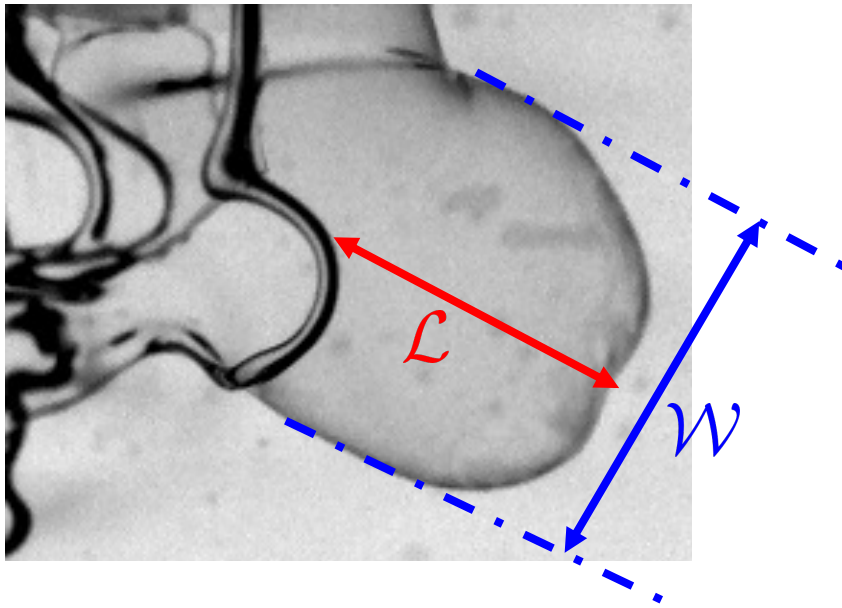
Droplet size distribution : Influence of viscosity



$\nu = 5 \text{ cst}$
 $\nu = 75 \text{ cst}$

Mathematicians
help !

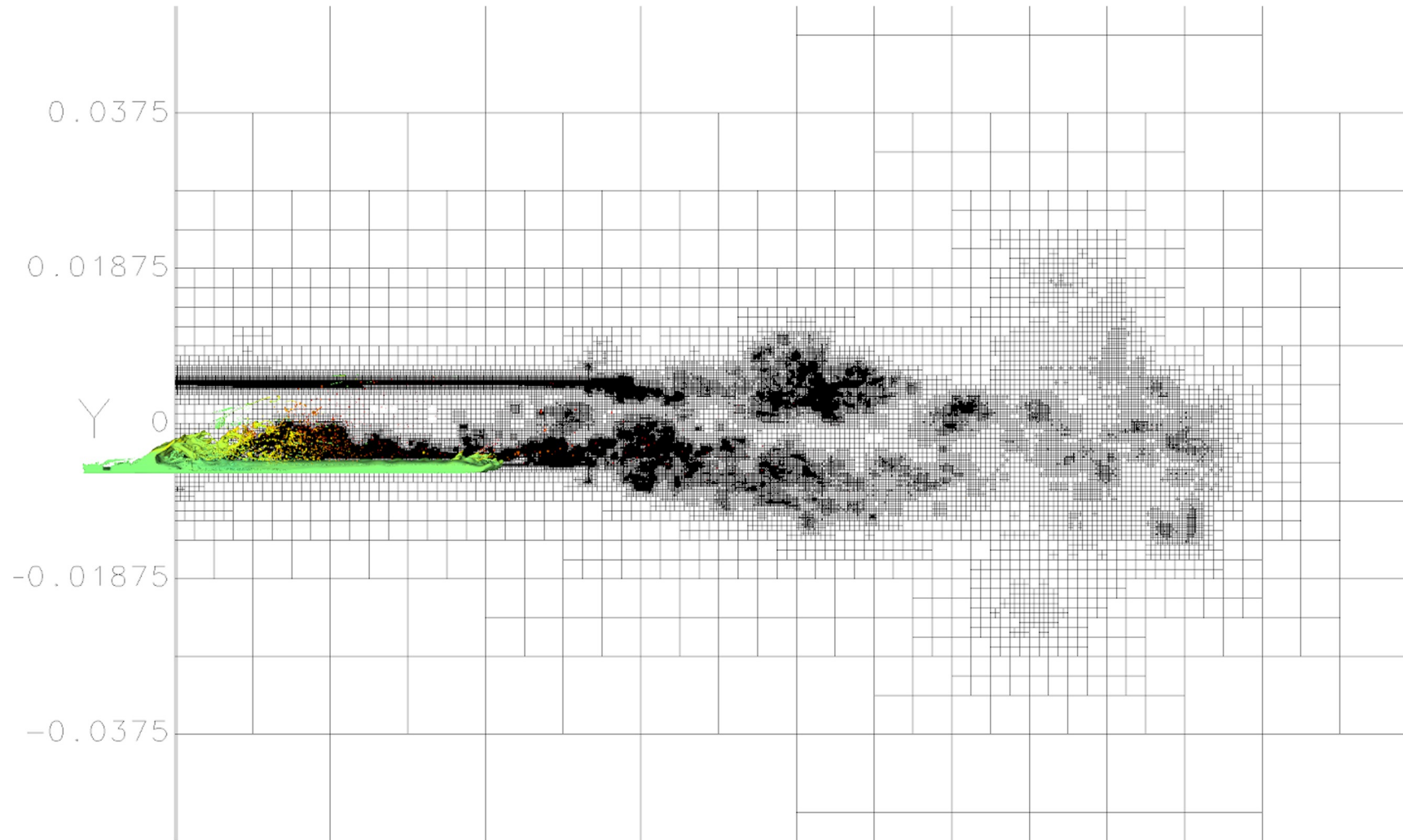
Influence of viscosity: Bag thickness



Experimental Conclusion

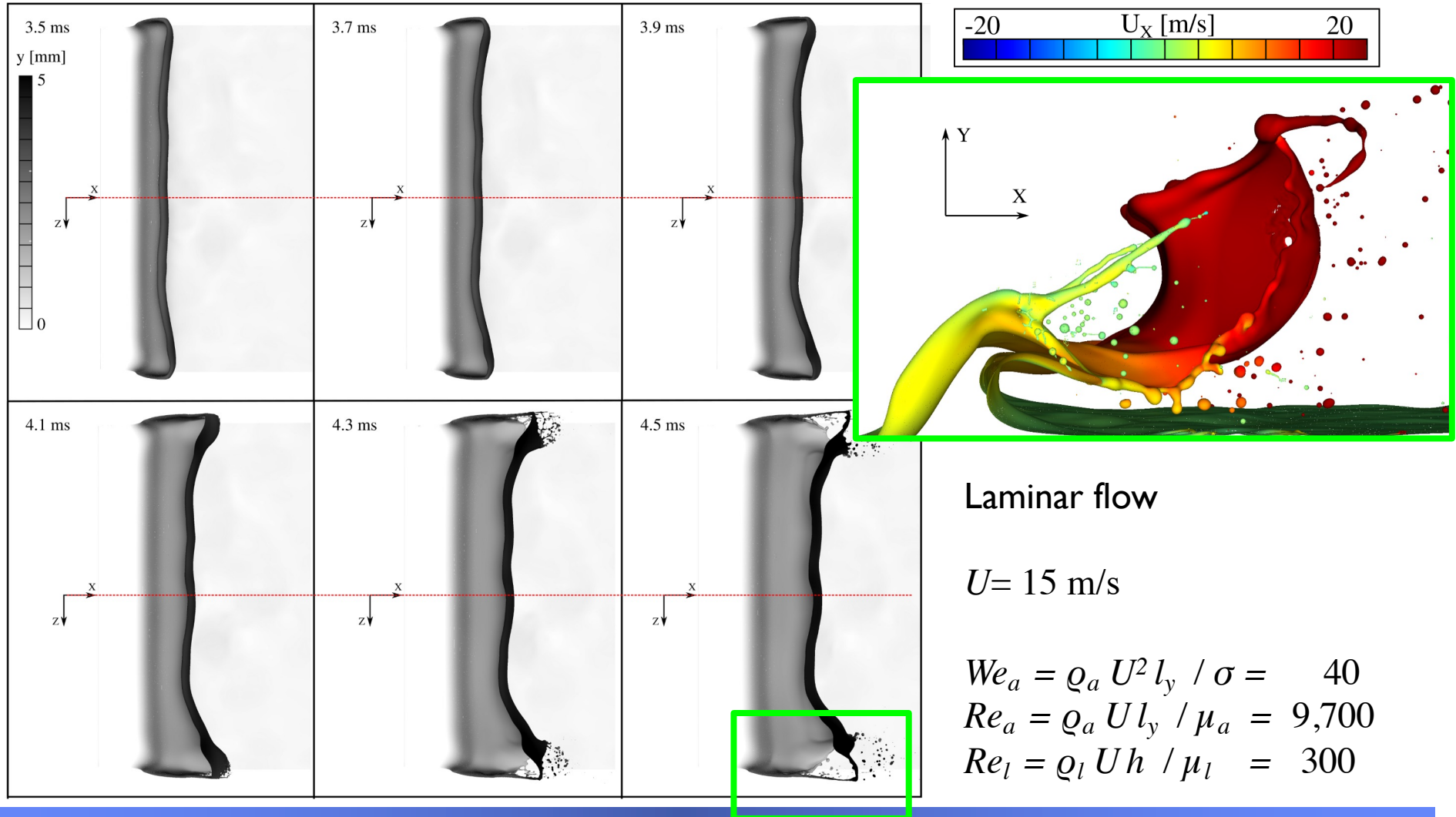
Viscosity promotes formation of deeper, wider and **thinner** bags, thus smaller droplets are generated.

Numerics of cough : octree grid (basilisk code by S. Popinet)

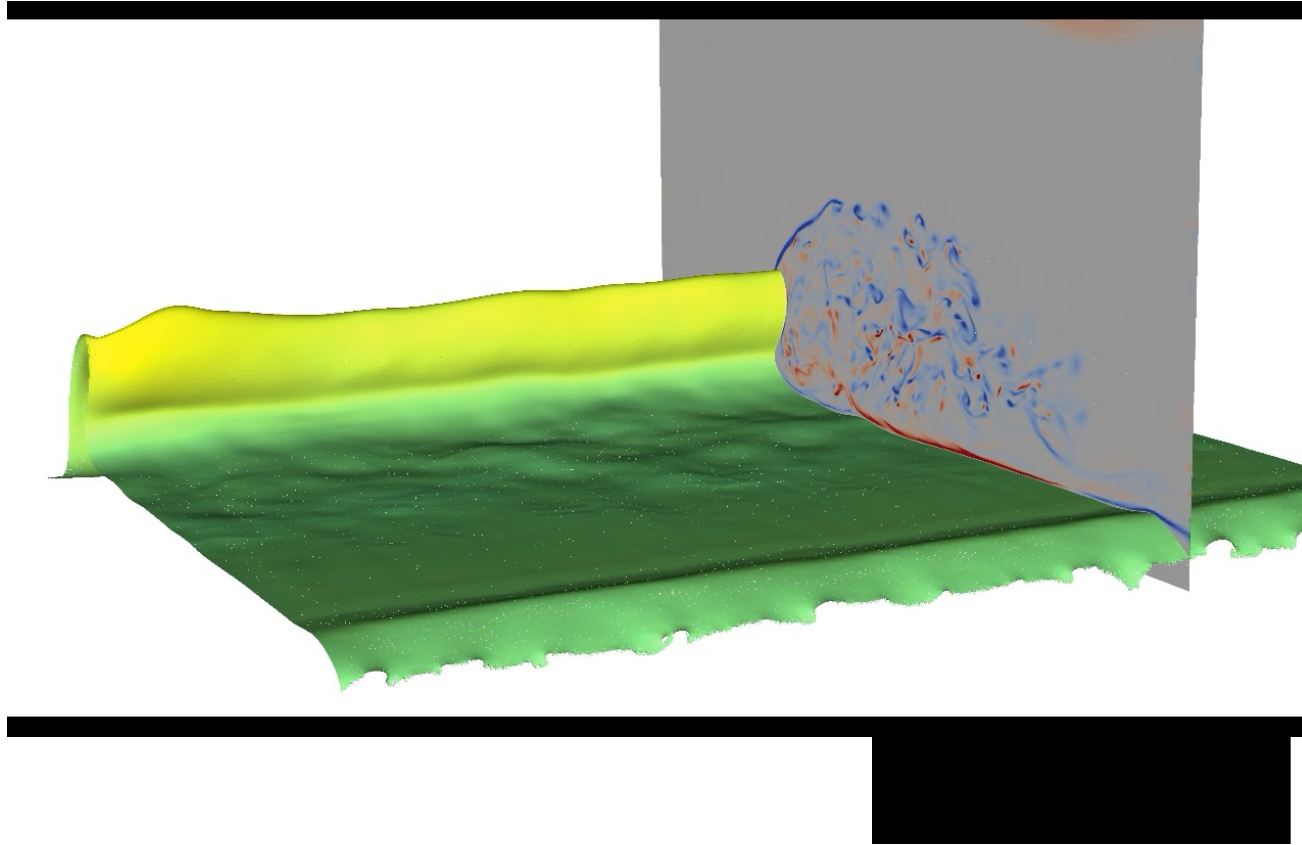


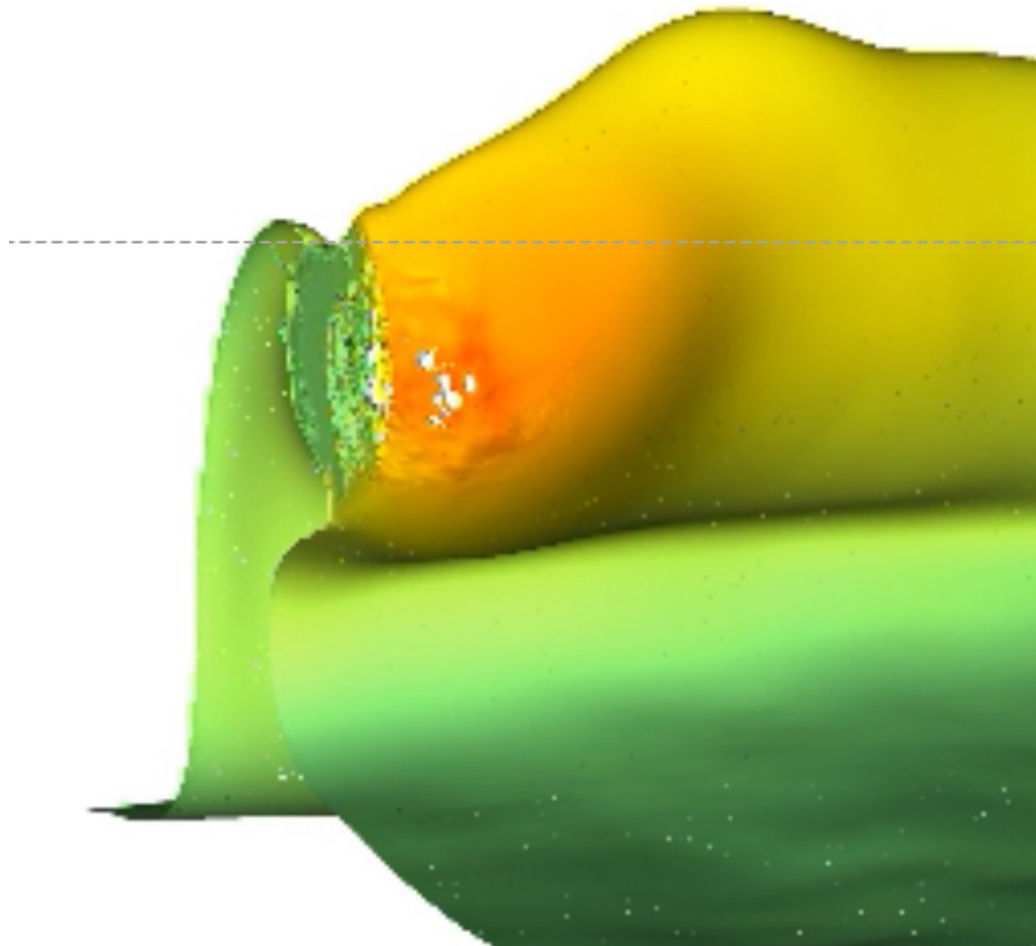
Sheet inflation and perforation regimes

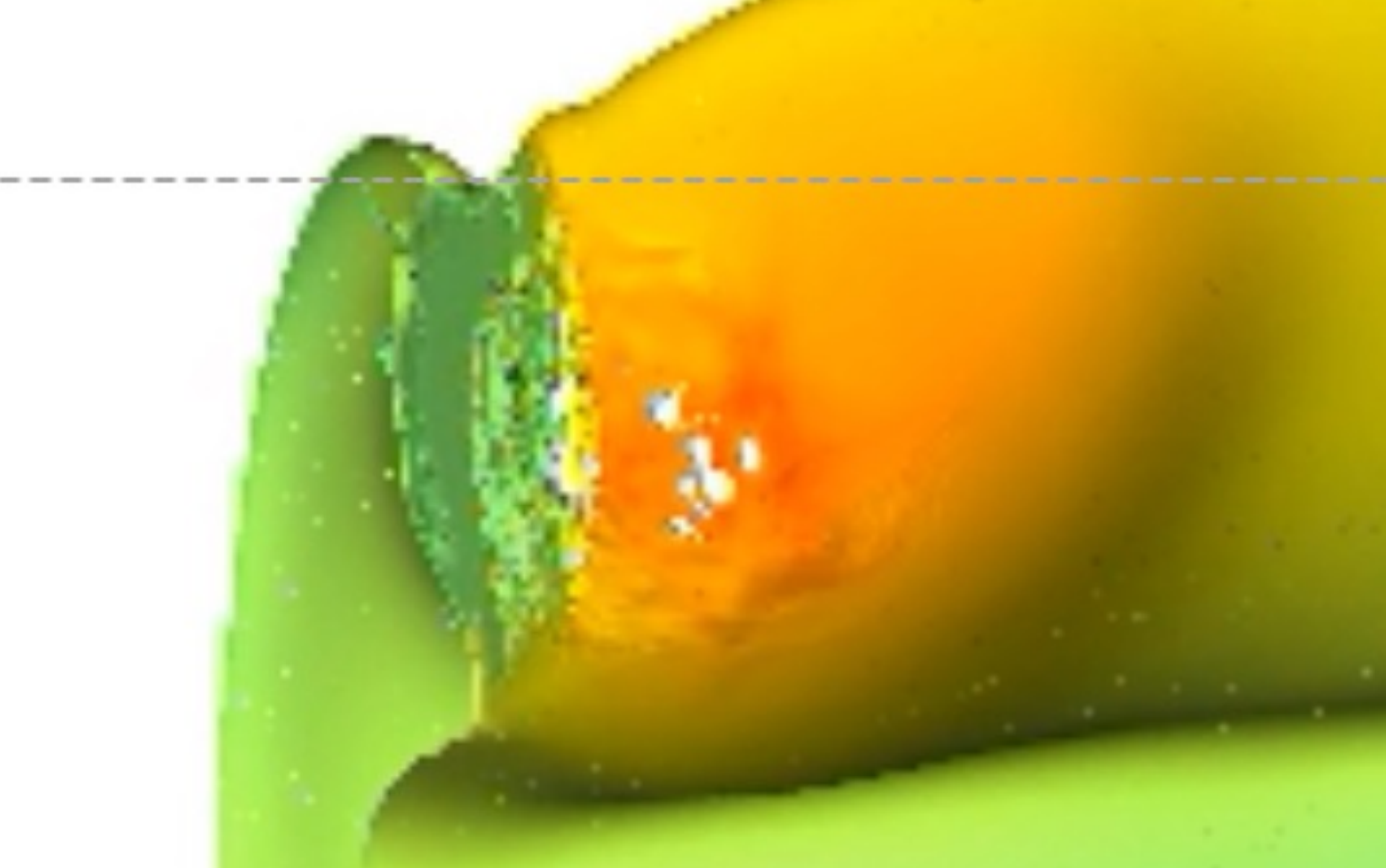
The experimental setup allows to study more viscous configurations, closer to saliva properties (silicon oil experiments). Air velocity during sneeze can also be smaller.



The liquid sheet close to the side wall deforms faster, thinning rapidly until perforation. The hole expansion forms ligaments that eventually fragment.

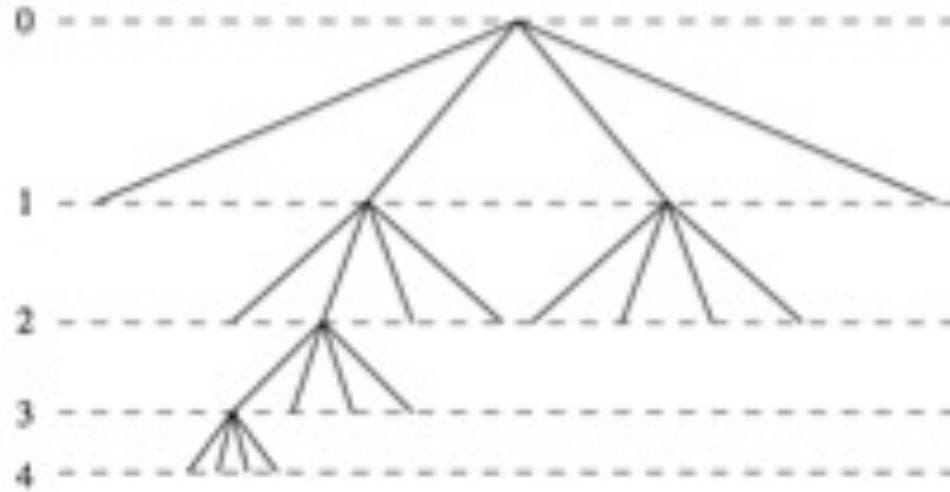
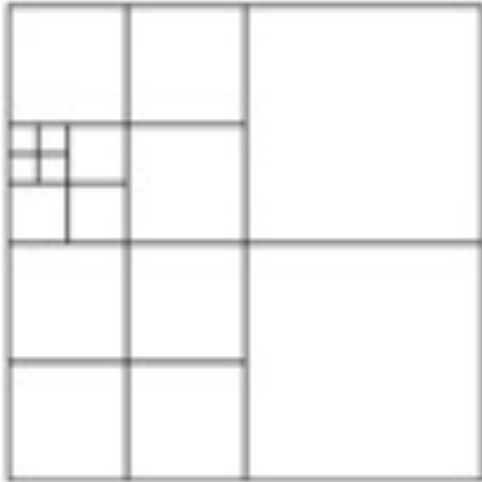






Ligament formation is similar to experiment.
We still need more computer power to determine the droplet size.

Efficient numerical methods: the octree grid.



The octree grid

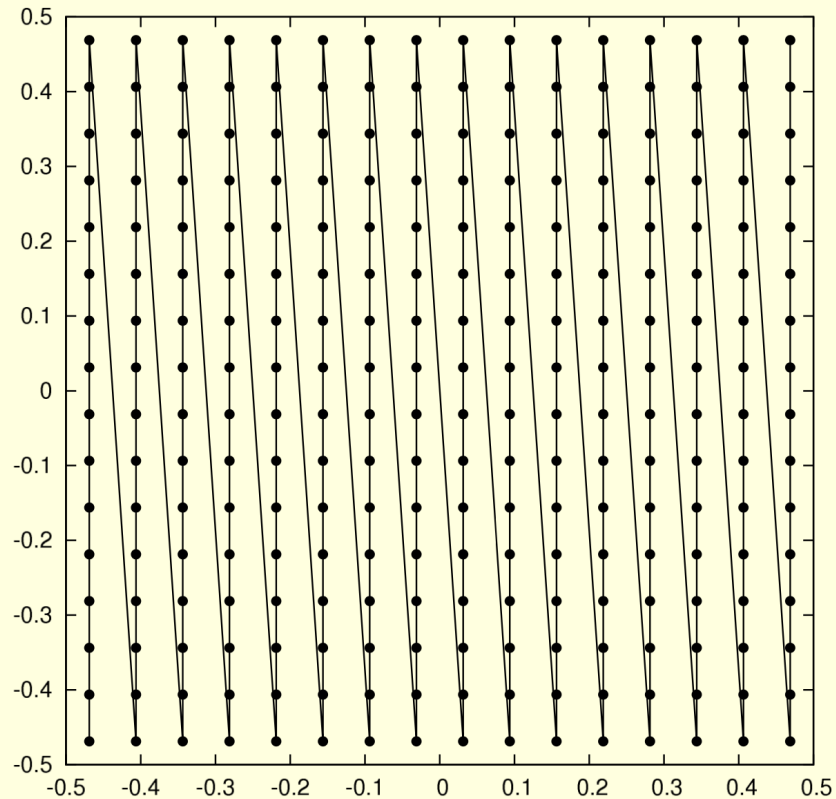
Considerable CPU time can be gained by using adaptive grids.

In 2003 S. Popinet introduces Gerris, an octree code using the “forest of trees” parallelization method.

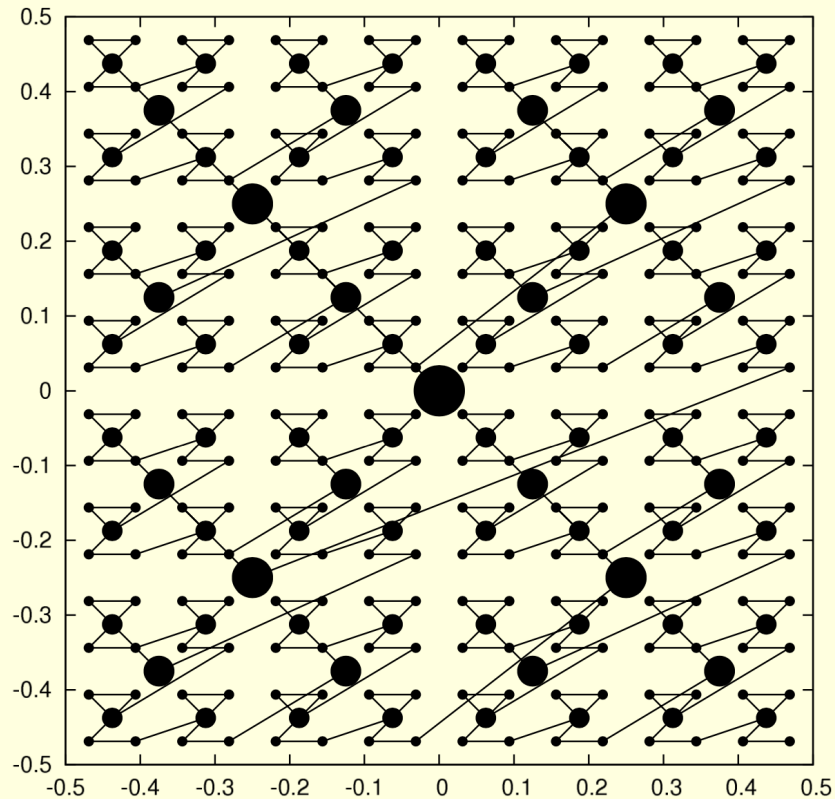
However massive parallelisation with Gerris was difficult.

Around 2016 Popinet releases a multiphase version of Basilisk, a new octree code with much better parallel performance. The forest of tree approach is replaced by space-filling curve

Memory accesses Cartesian/quadtree



Cartesian, column by column



quadtree, Z-ordering

As a result, we have a very efficient, massively parallel, adaptive method.

Add massive computers





Impossible problems



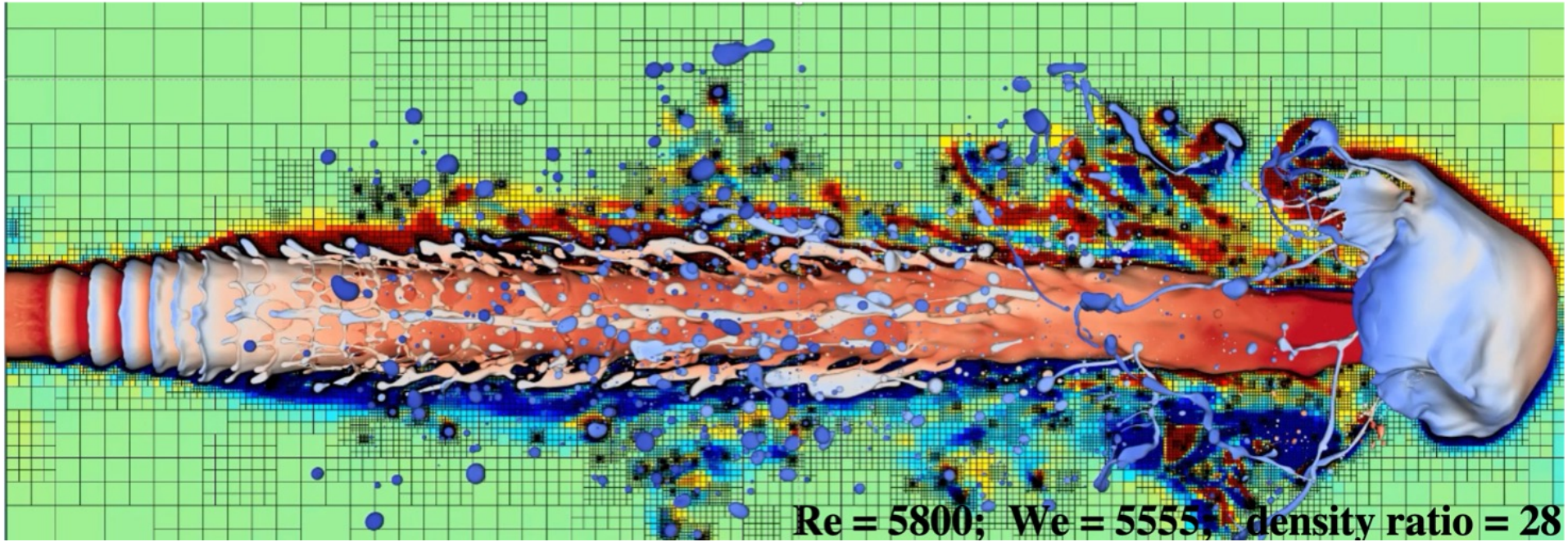
Impossible problems

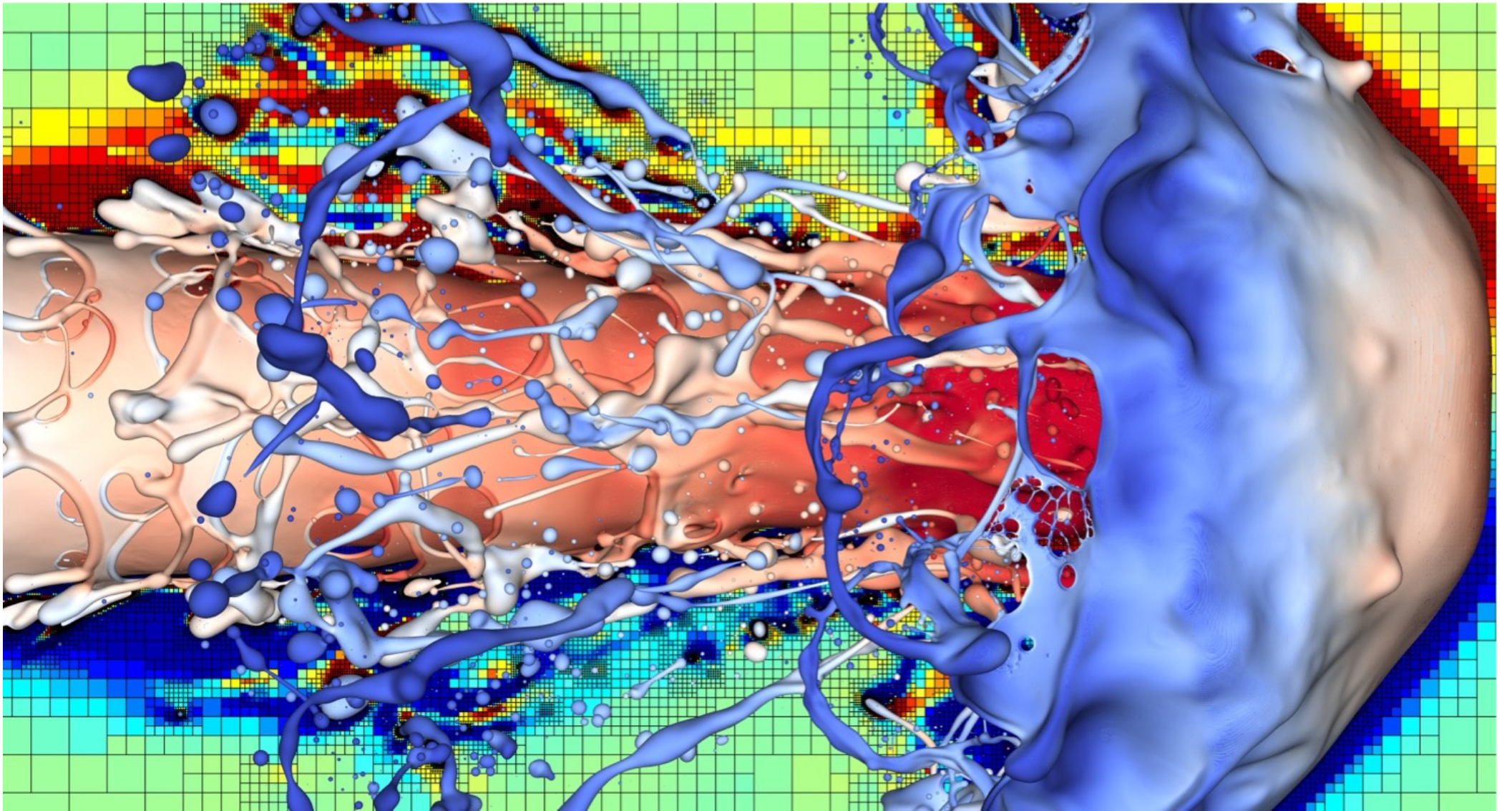
Thin liquid sheets: too thin, nanometer scale
compared to meter scale experiments or industrial processes

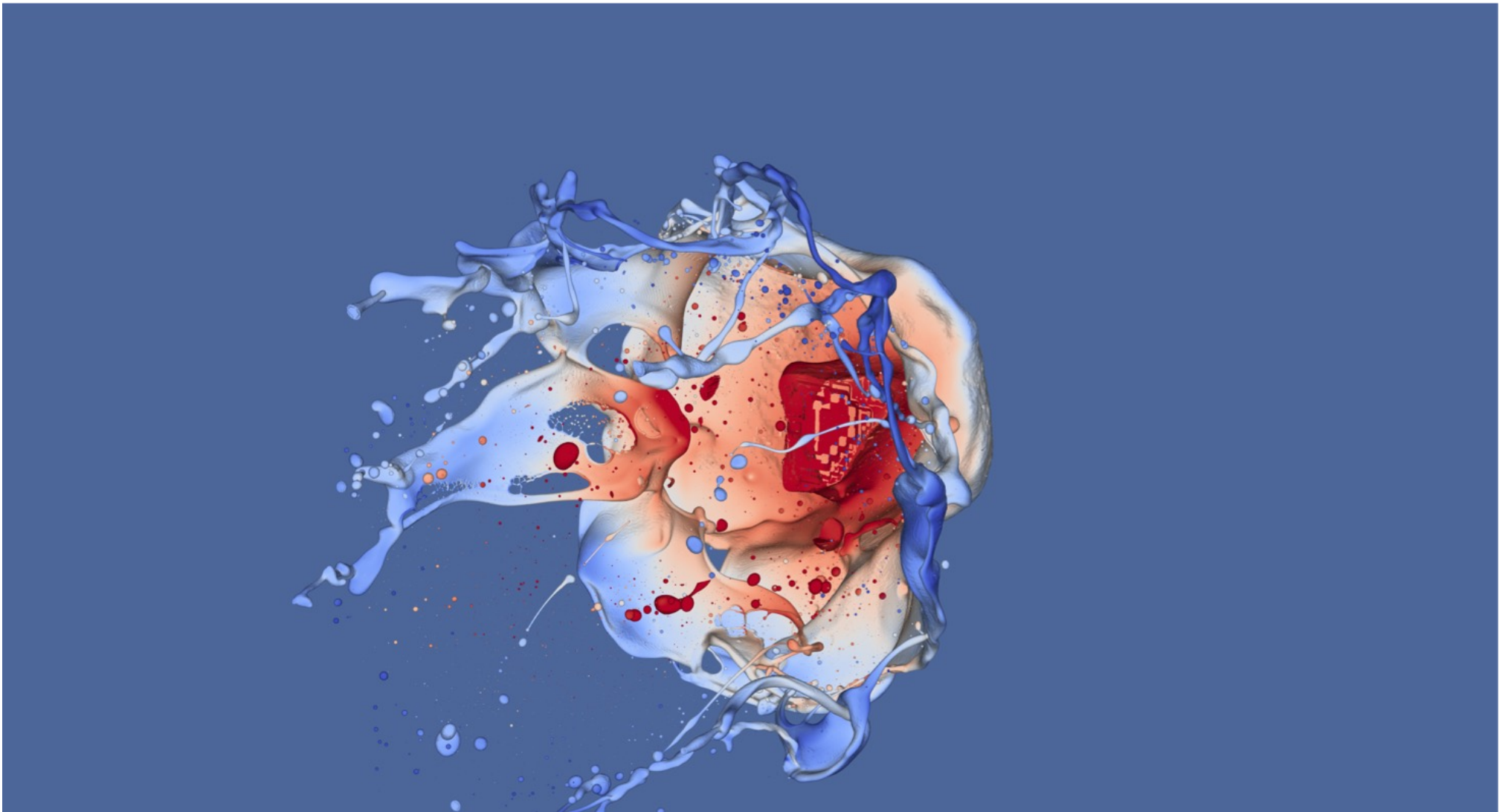
Impossible problems

Thin liquid sheets: too thin, nanometer scale
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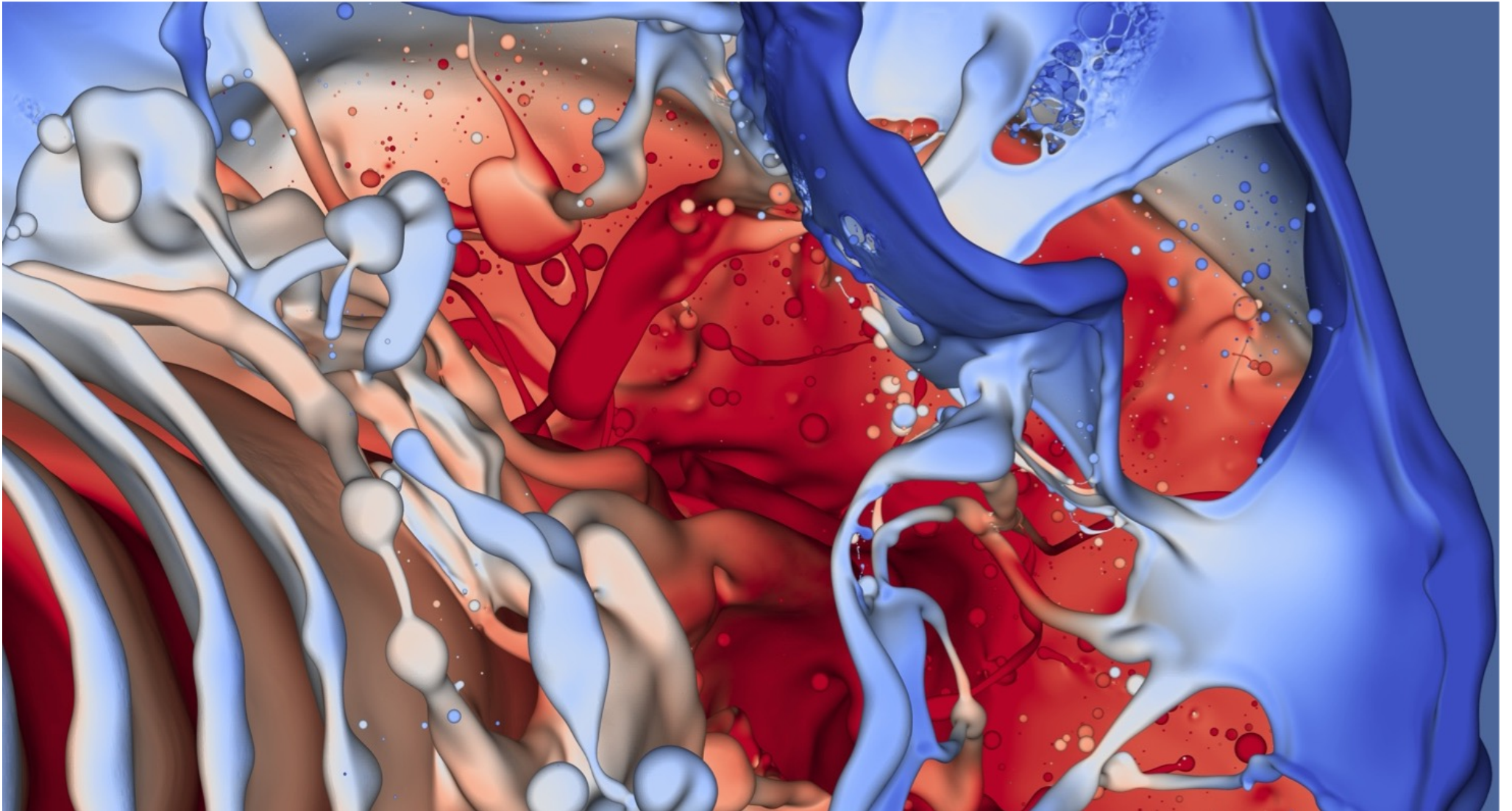
Pulsed jet case



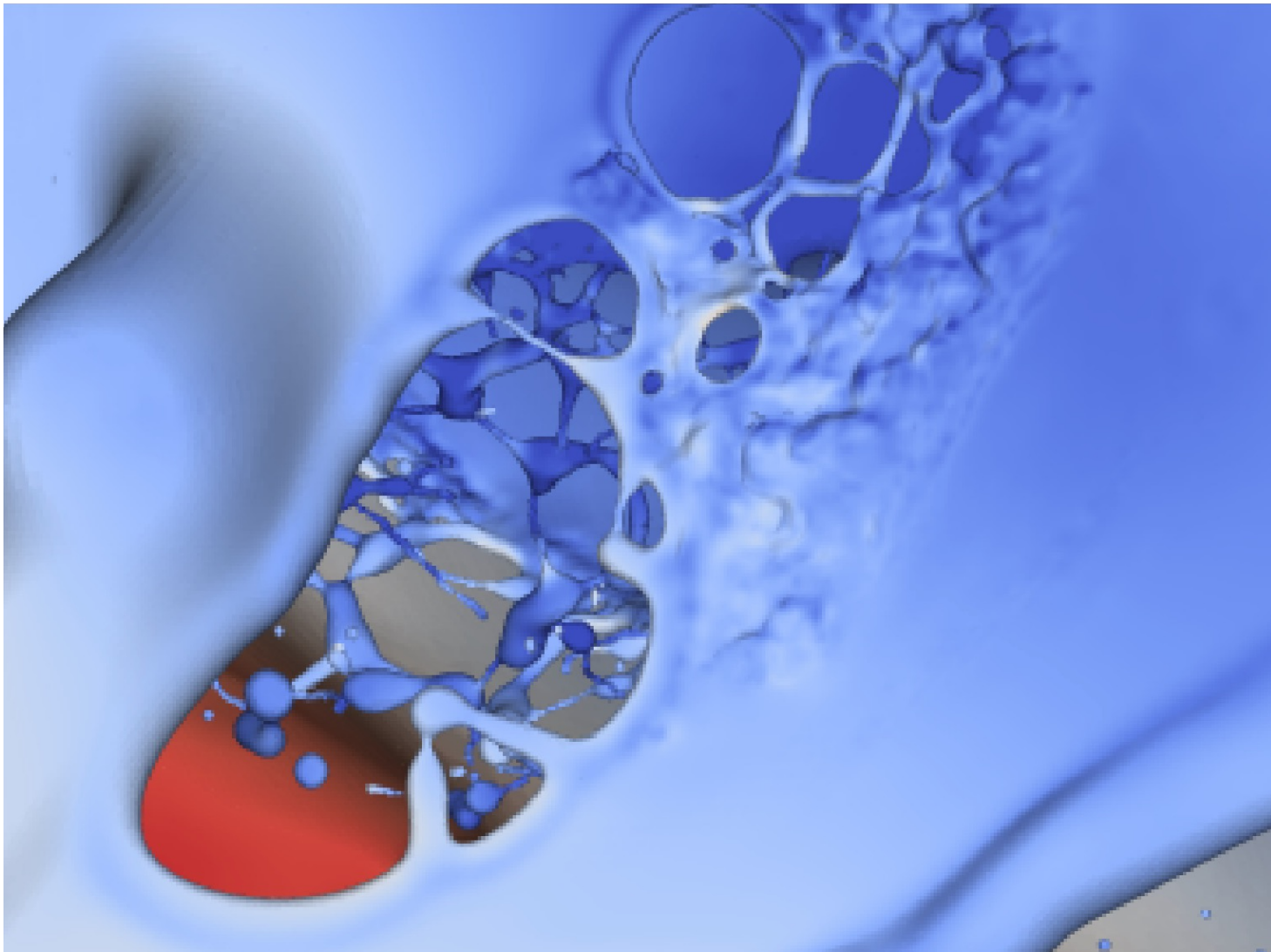




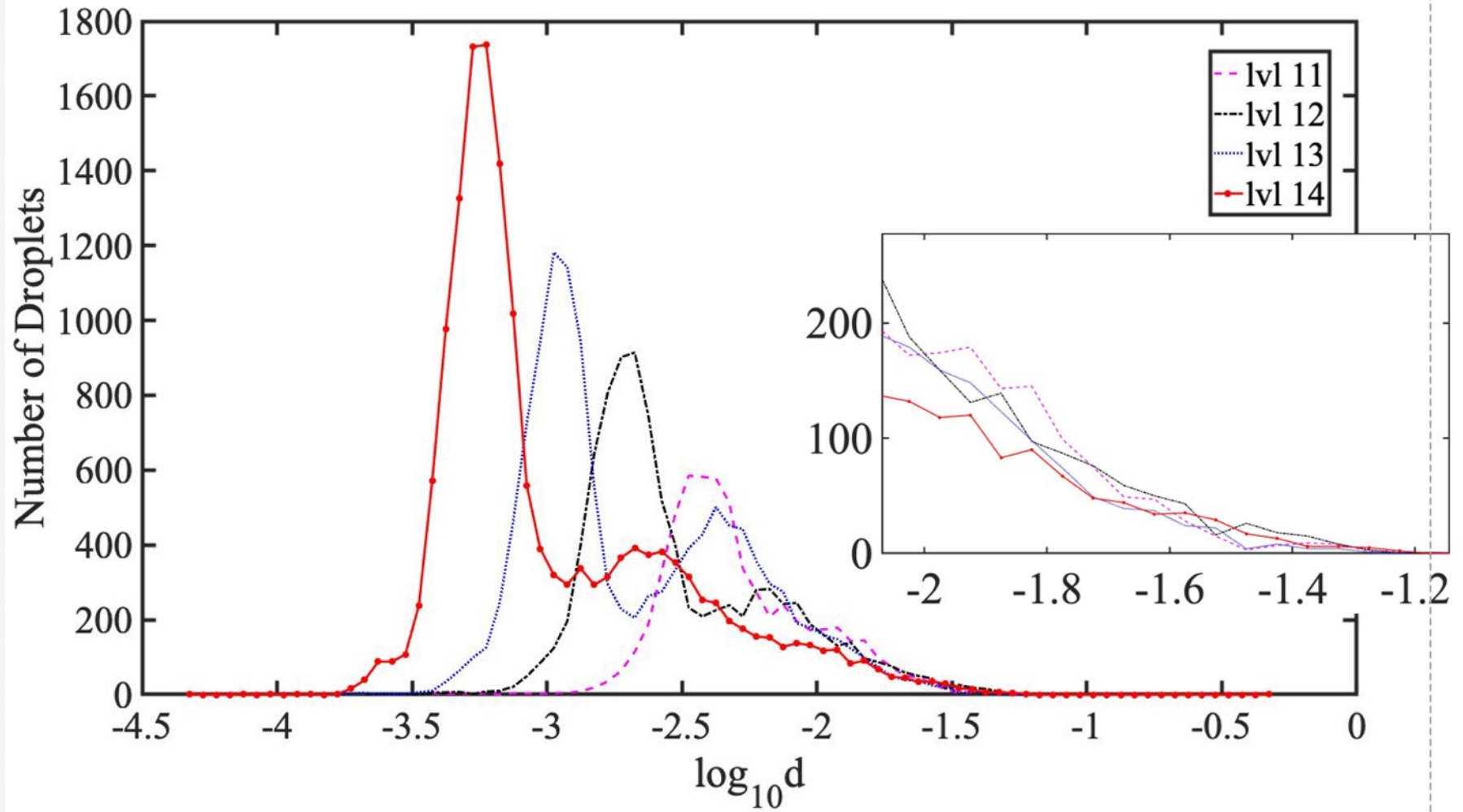
View of the mushroom head from behind



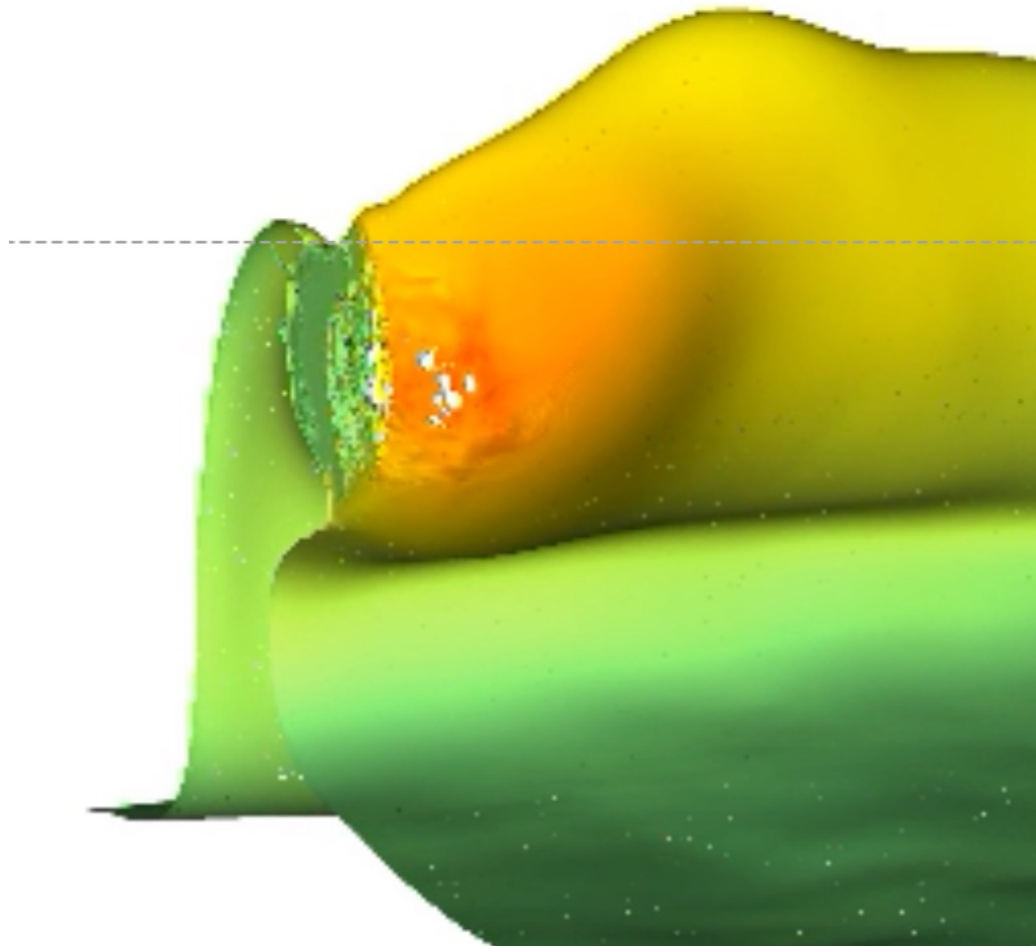
Further zoom on the mushroom head

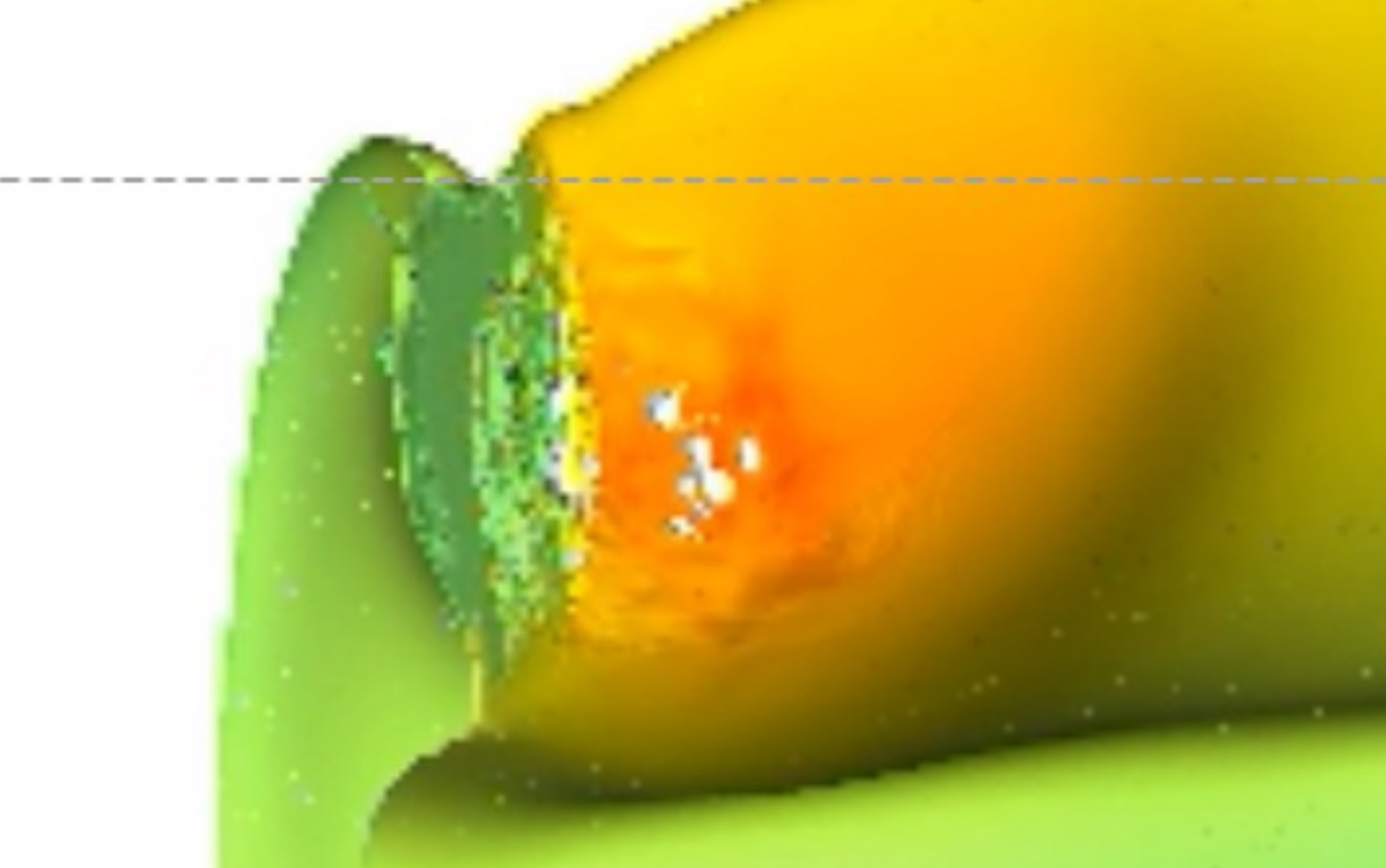


Further zoom : manifold death



sequence of droplet size PDF with increasing resolution.



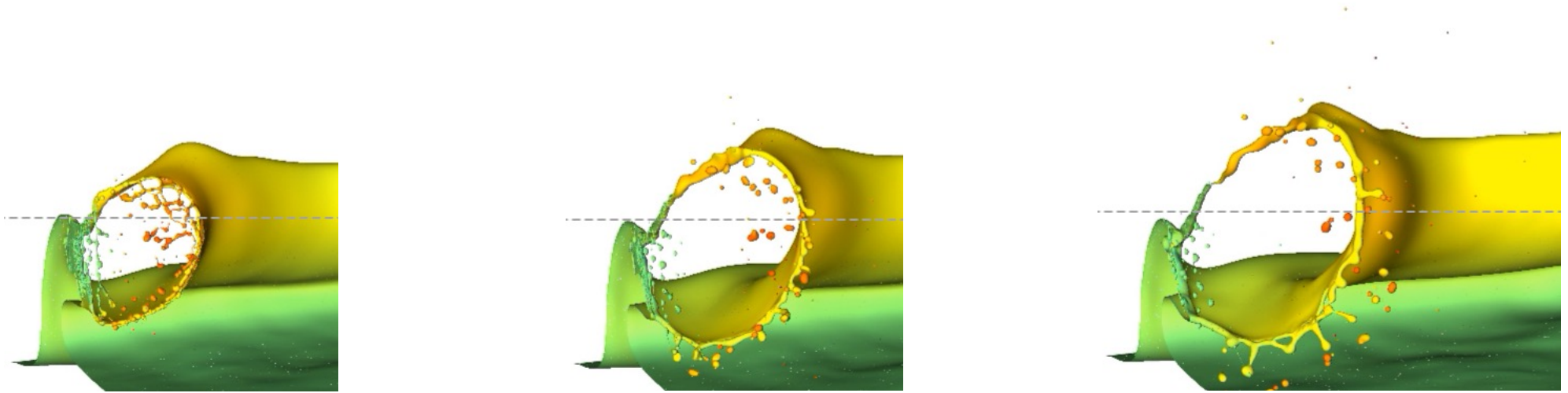




Real life is different

Mud volcano, Salse di Nirano

You can obtain something similar at high resolution



The expanding annular ring is killing the sheet (sheet = 2D manifold).
But it is imperfect: depends on grid size, and is unphysical at the initiation.

A possible solution : the “Manifold Death” procedure.

(with Leonardo Chirco)



In the last volume of Liu Cixin's trilogy, there are multiple intertwined universes which are each manifolds of dimension D , with $1 < D < 14$. War between advanced alien civilizations living in those universes results in each region after the other of any universe being destroyed by enemy aliens. The alien weapon causes a region of dimension D to be "perforated". The weapon is a small element of dimension $D-1$ inserted in it.

Thus our 3D solar system is destroyed by an attack by a small post-it-sized thin sheet (2D manifold).

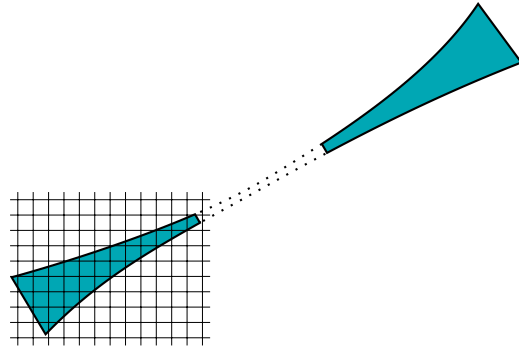
The lesson is that destruction of a D dimensional manifold is realized by a $D-1$ manifold, not a $D-2$ manifold. Thus a sheet ($D=2$) is destroyed by an expanding annular ring ($D=1$) not by a tiny point hole ($D=0$).

As a result we (Leonardo Chirco and I) call this topological transtion "Manifold Death" (MD). But the term "death" is also used for bursting bubbles.

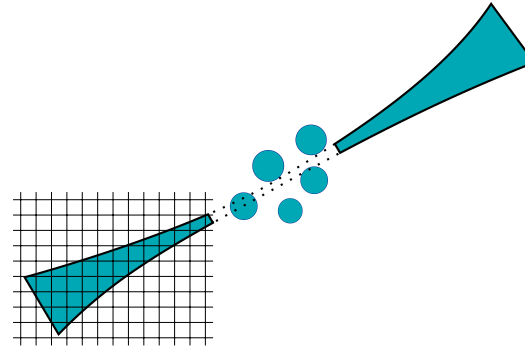
**Remembrance of Earth's Past* (Chinese: 地球往事) trilogy, the whole series is normally referred to as *The Three-Body Problem*

What happens to thin sheets in multiphase flow simulations ?

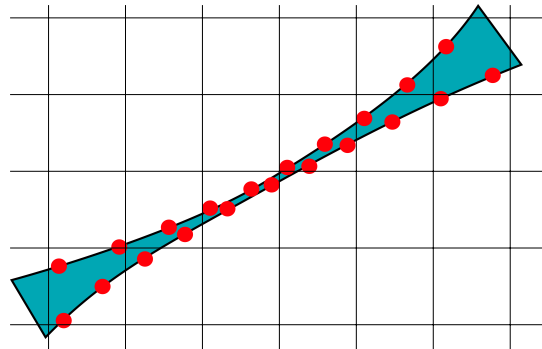
Level Set



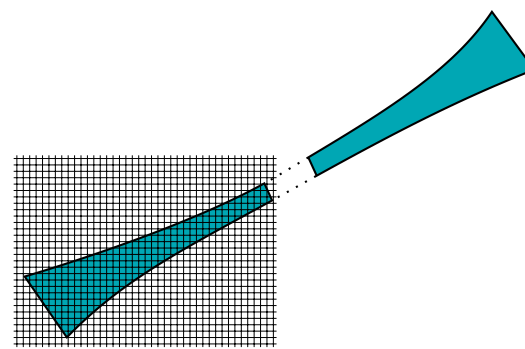
Volume of Fluid



Front Tracking



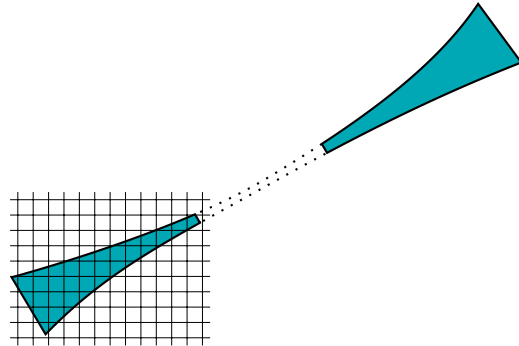
Manifold Death



What happens to thin sheets in multiphase flow simulations ?

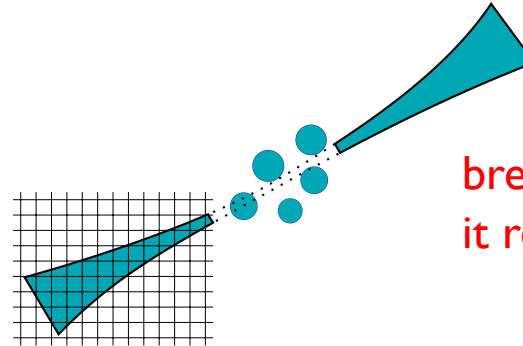
Level Set

evaporates when it reaches the grid size

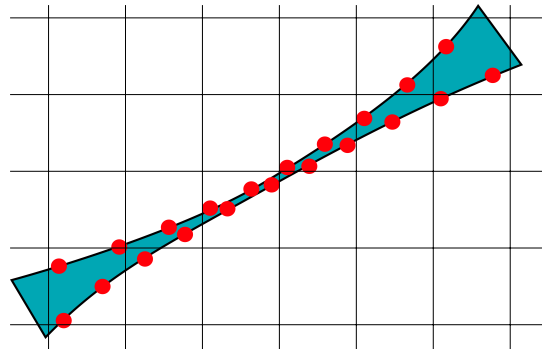


Volume of Fluid

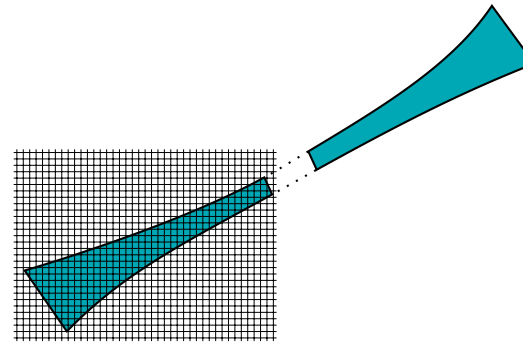
breaks into big droplets when it reaches the grid size



Front Tracking



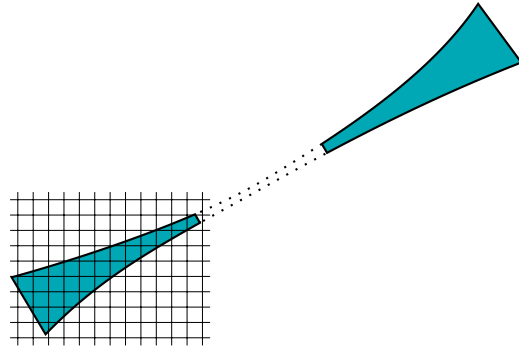
Manifold Death



What happens to thin sheets in multiphase flow simulations ?

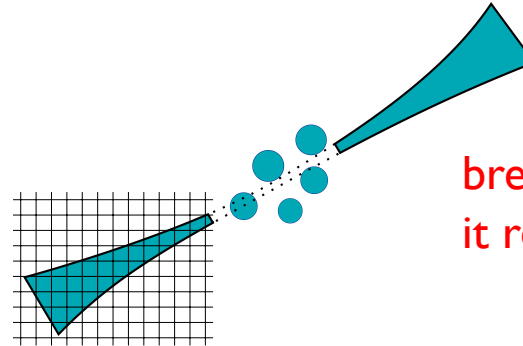
Level Set

evaporates when it reaches the grid size



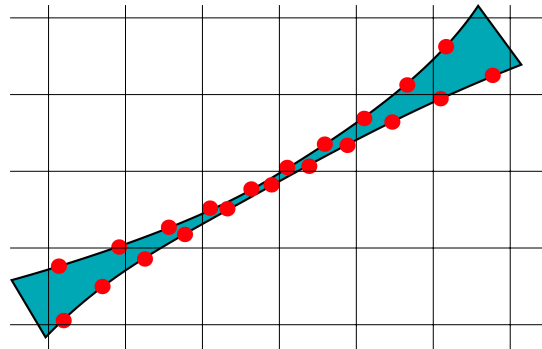
Volume of Fluid

breaks into big droplets when it reaches the grid size



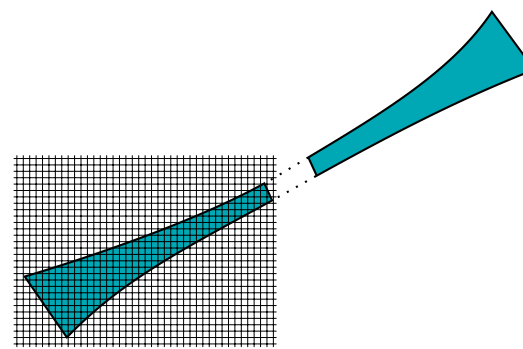
Front Tracking

never breaks



Manifold Death

breaks when we decide.



The Navier-Stokes equations must be supplemented with a law that specifies when thin sheets (manifolds) break or “die”.

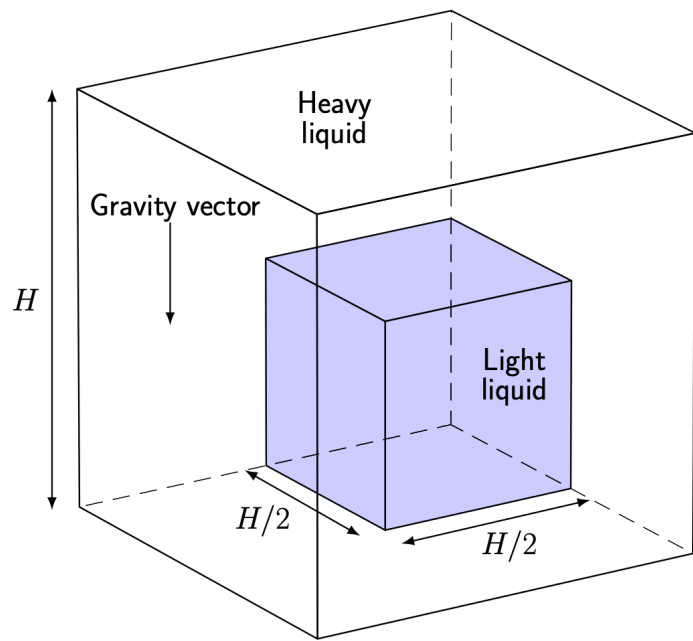
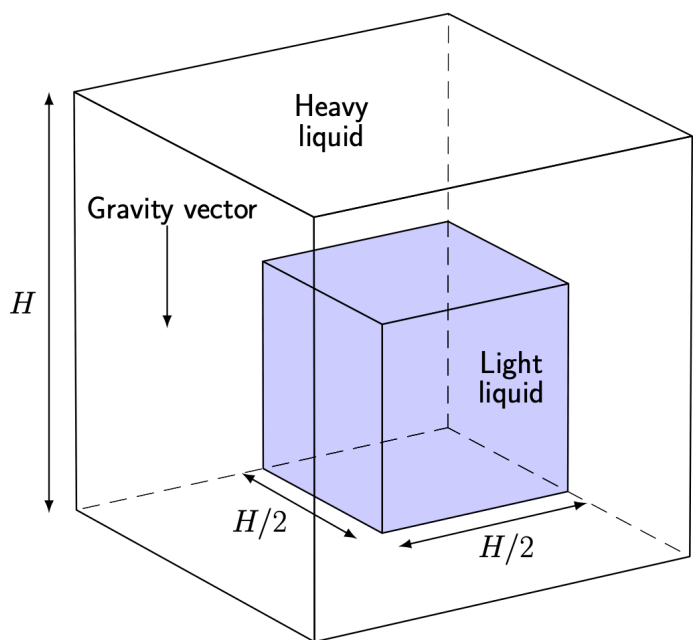


Figure 7: Configuration for the phase inversion test.



A phase inversion benchmark for multiscale multiphase flows

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J.-P. Caltagirone^f, L. Chirco^d, A. Pedrono^c, S. Popinet^d, A. Berlemont^b,
J. Magnaudet^c, T. Ménard^b, S. Vincent^g, S. Zaleski^{d,h,*}

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^h Institut Universitaire de France, Paris, France



Figure 7: Configuration for the phase inversion test.

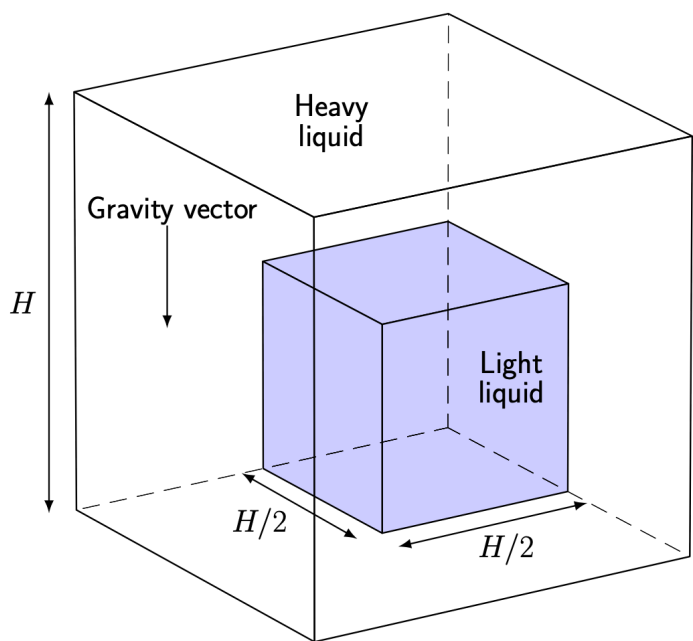


Figure 7: Configuration for the phase inversion test.

A phase inversion benchmark for multiscale multiphase flows

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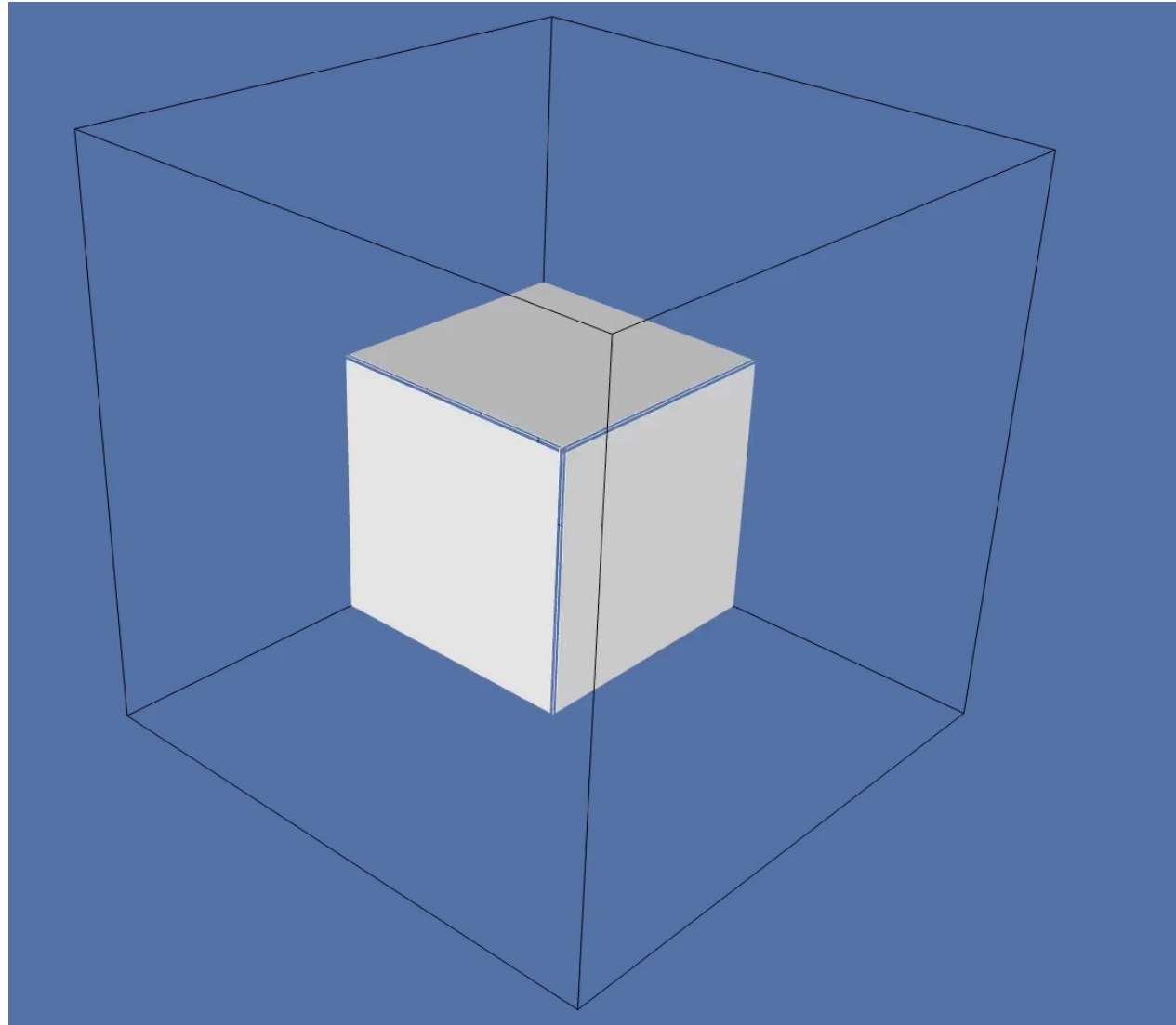
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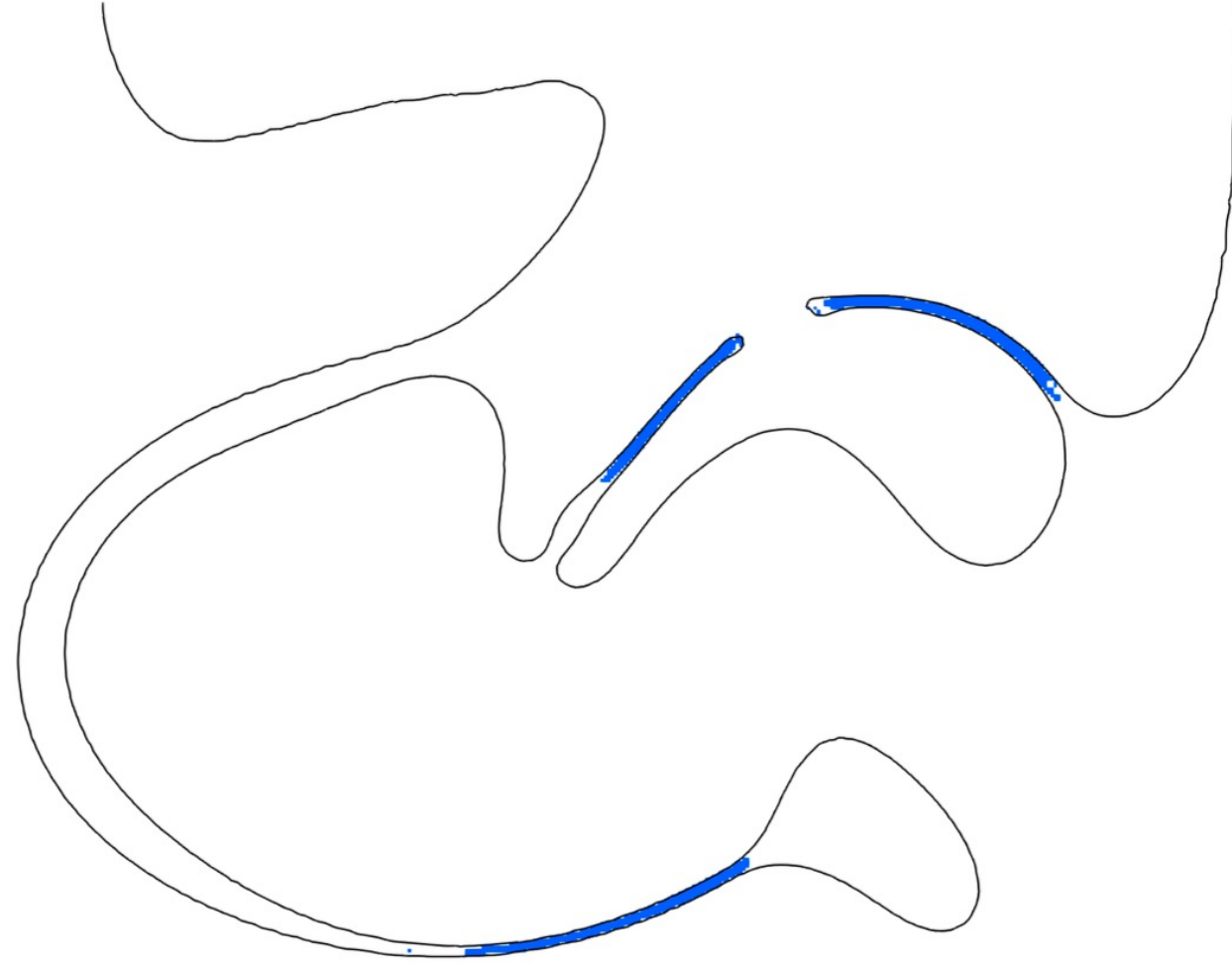


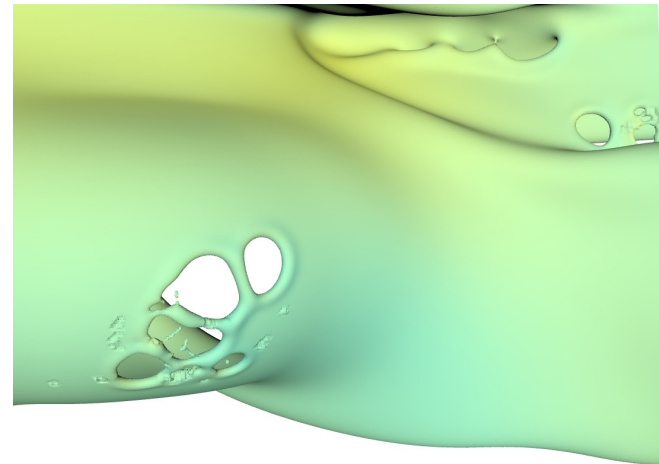
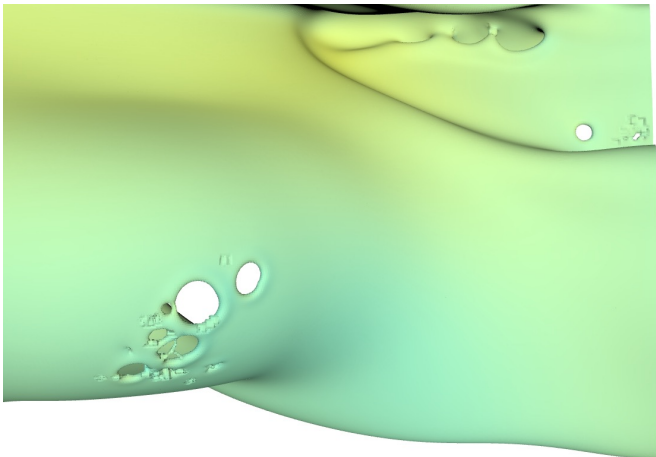
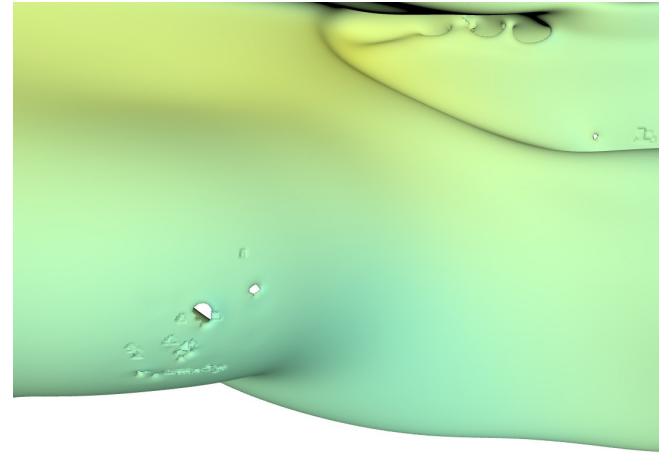
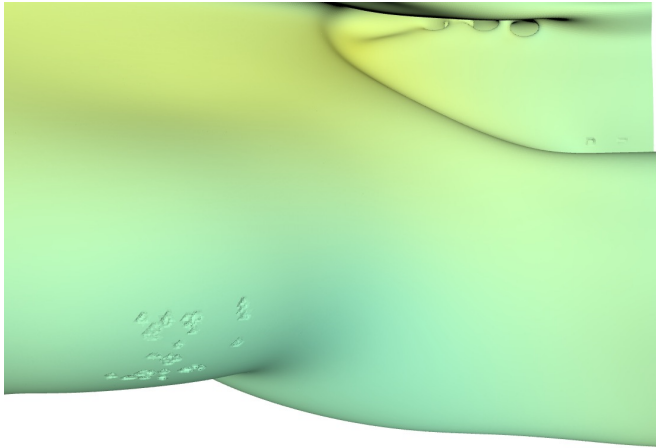
New case with smaller Reynolds numbers

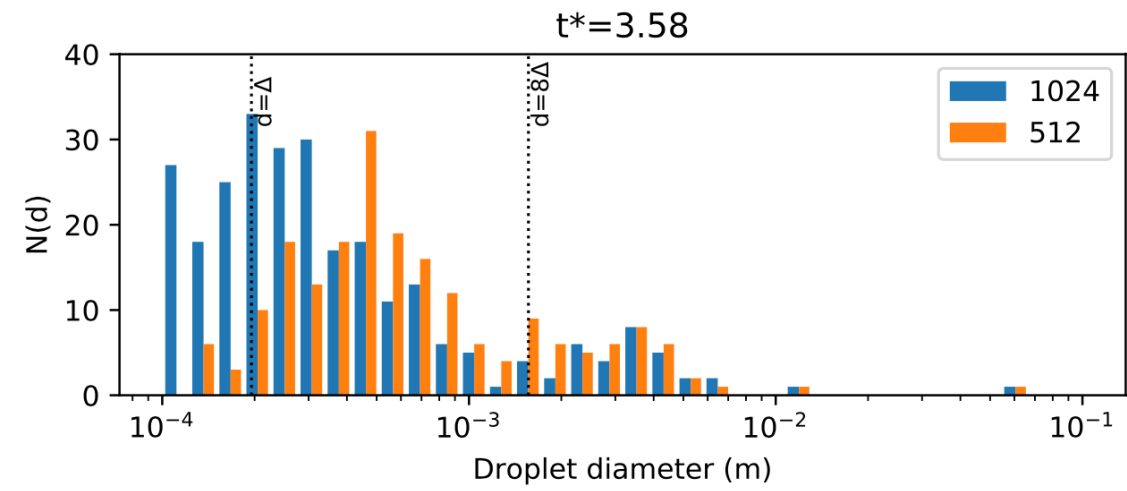
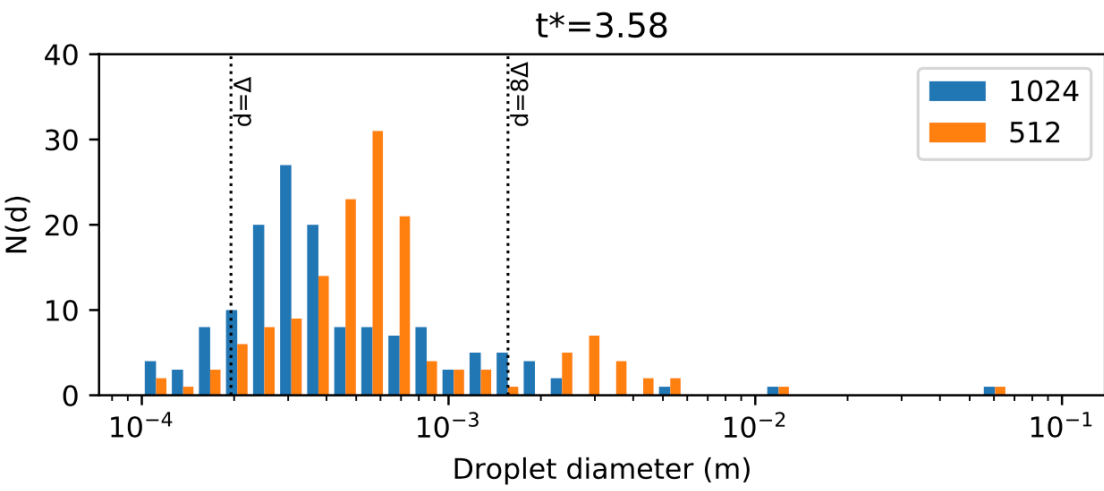
Results for case B



Sheet detection

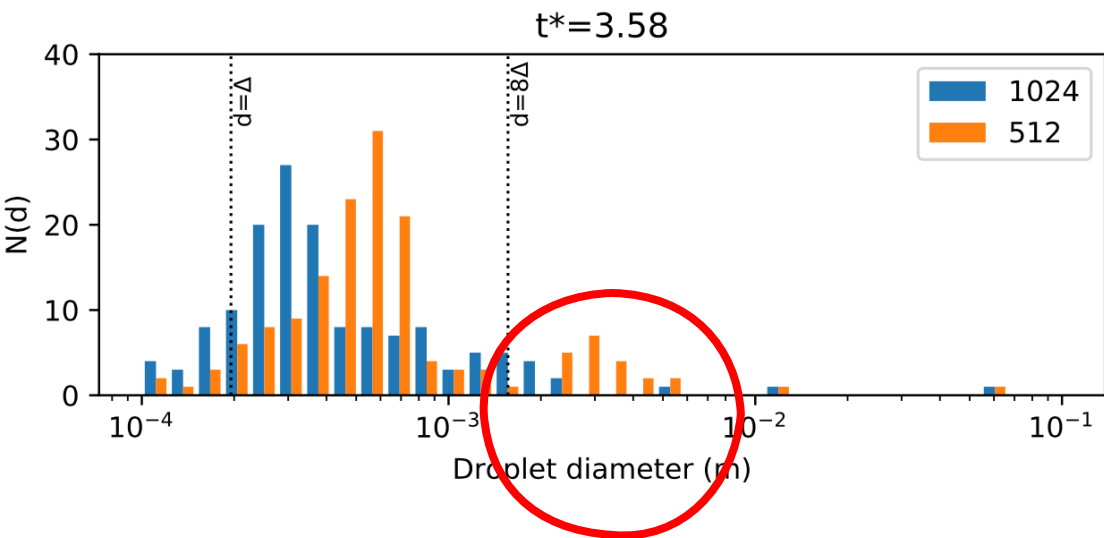




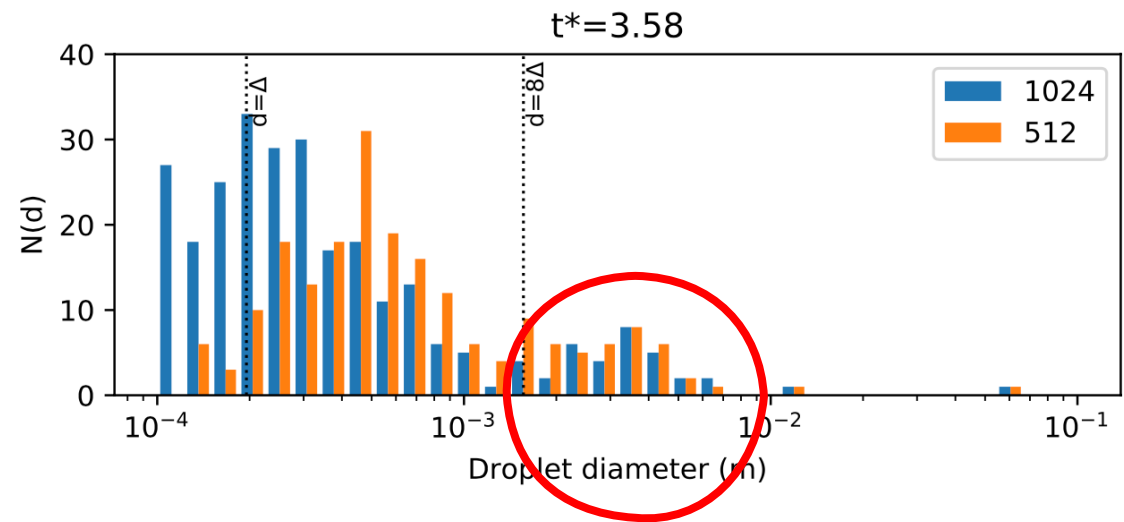


Droplet size distributions in the phase inversion test case

left: without manifold death right: with manifold death



Not converging



Converging

Droplet size distributions in the phase inversion test case

left: without manifold death right: with manifold death

Conclusion

the story of the explorations of complex multiphase solutions of the Navier Stokes equations **is only beginning.**

The End

