



Oxford Energy

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DEPARTMENT OF
**ENGINEERING
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Bridging Sustainability and Innovation with AI in Mobility and Energy Sector

Konstantina Vogiatzaki

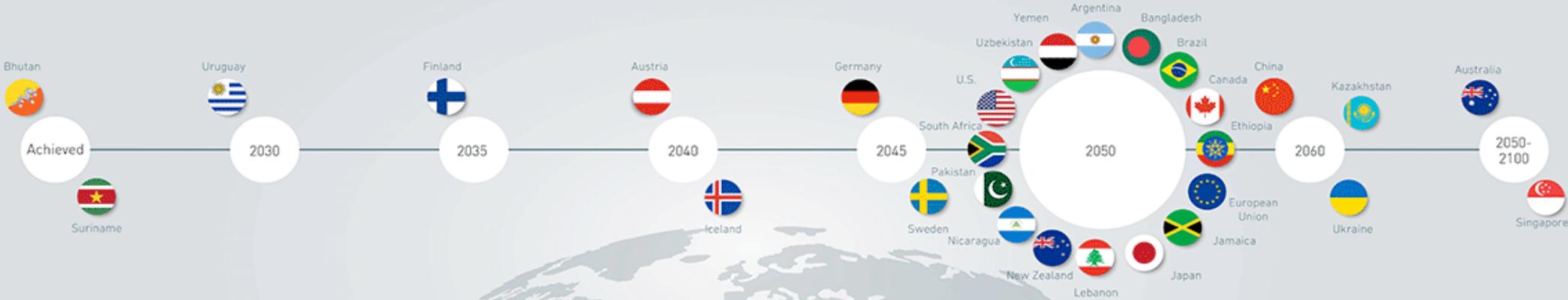
Associate Professor of Engineering Science
Fellow at Somerville College, University of Oxford

21st of January 2025

Why we need AI: Current ... Climate

WORLD COUNTRIES' CARBON NEUTRALITY TIMELINE

To limit climate change, countries of all sizes the world over have committed to achieving net zero emissions before the end of this century. While most are aiming for the Paris Agreement's 2050 target, a few are significantly ahead, and others have yet to agree on a concrete target date for reaching carbon neutrality.



Bhutan and Suriname are the only two countries that have achieved carbon neutrality and are now carbon negative, removing more CO₂ than they generate.

This is a selection of the more than 90% of the 137 countries tracked that are aiming for carbon neutrality by 2050.

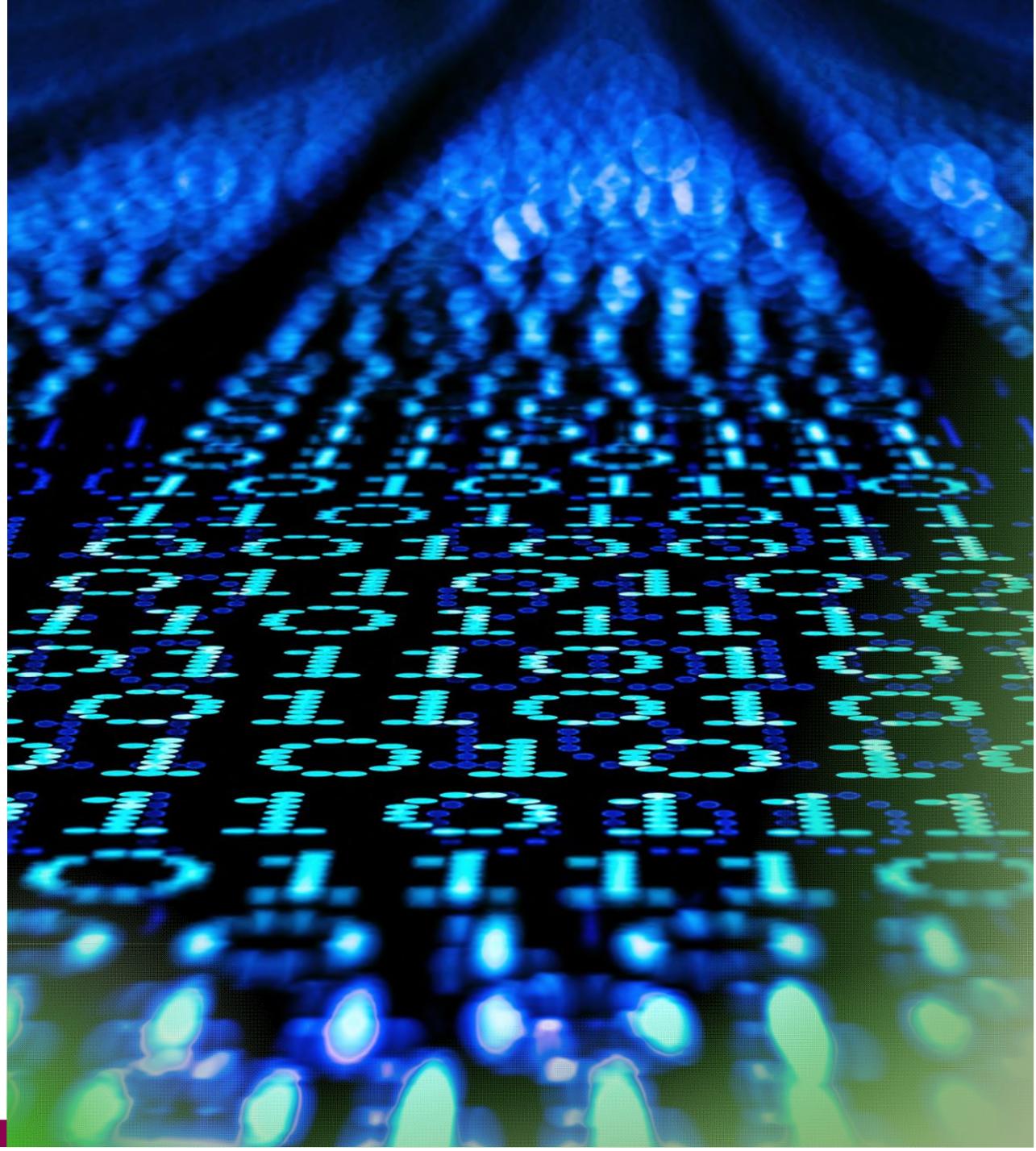
Australia and Singapore are aiming for carbon neutrality during the second half of the 21st century, but have not yet set a concrete date.

Source: Visual Capitalist

How can we speed up progress?



Digital Twins



Digital Twins: What would you do if you had a ...doppelgänger

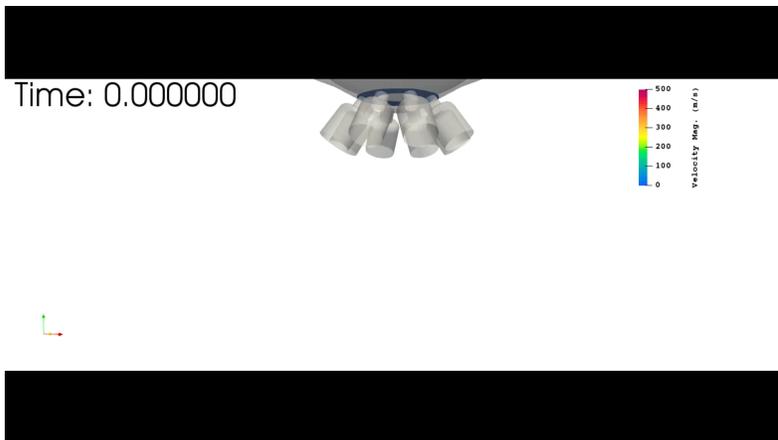
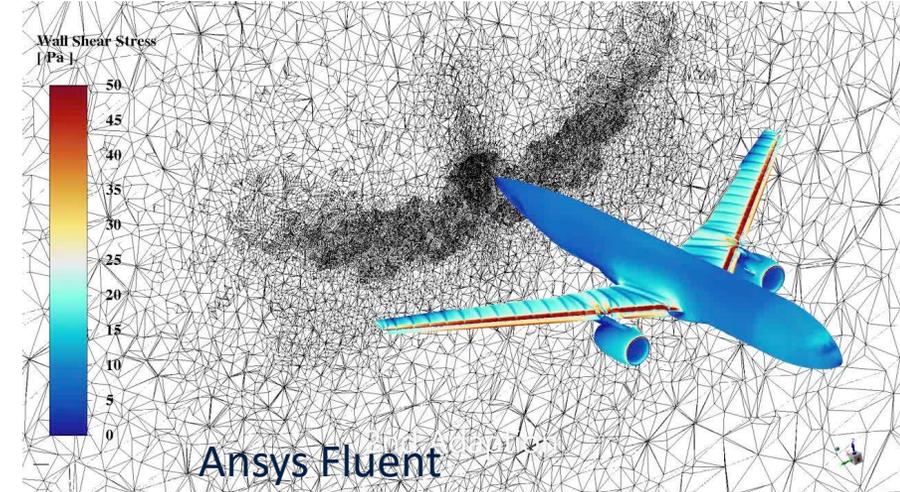


- Understand How Things Work
- Test Various Conditions (even in “dangerous operating manifolds”)
- Speed Up Manufacturing
- Active Control

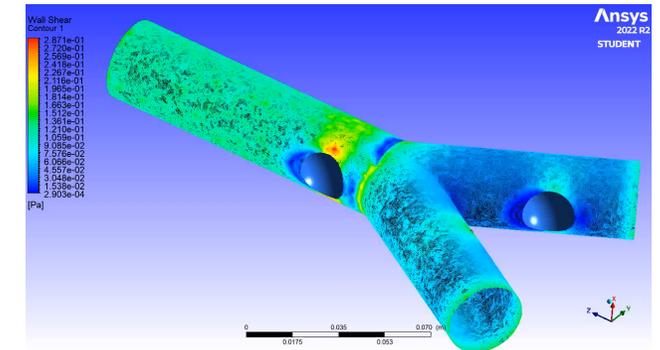
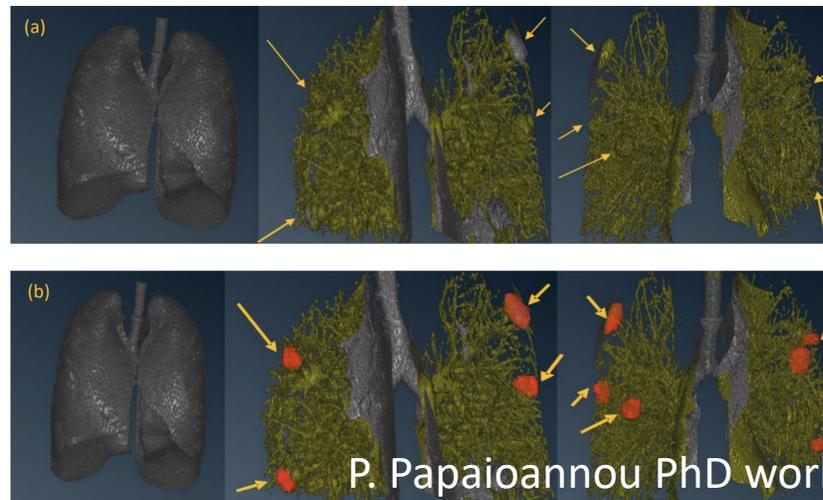
McKinsey & Company August 26, 2024

Computational Fluid Dynamics (CFD)

- A “traditional” tool of creating **Digital Twins of Fluid Systems**
- Combines applied mathematics, physics and high-performance computing
- Can be used to help understand how fluids move “around” or “inside” systems



P. McGinne, PhD work



P. Papaioannou PhD work



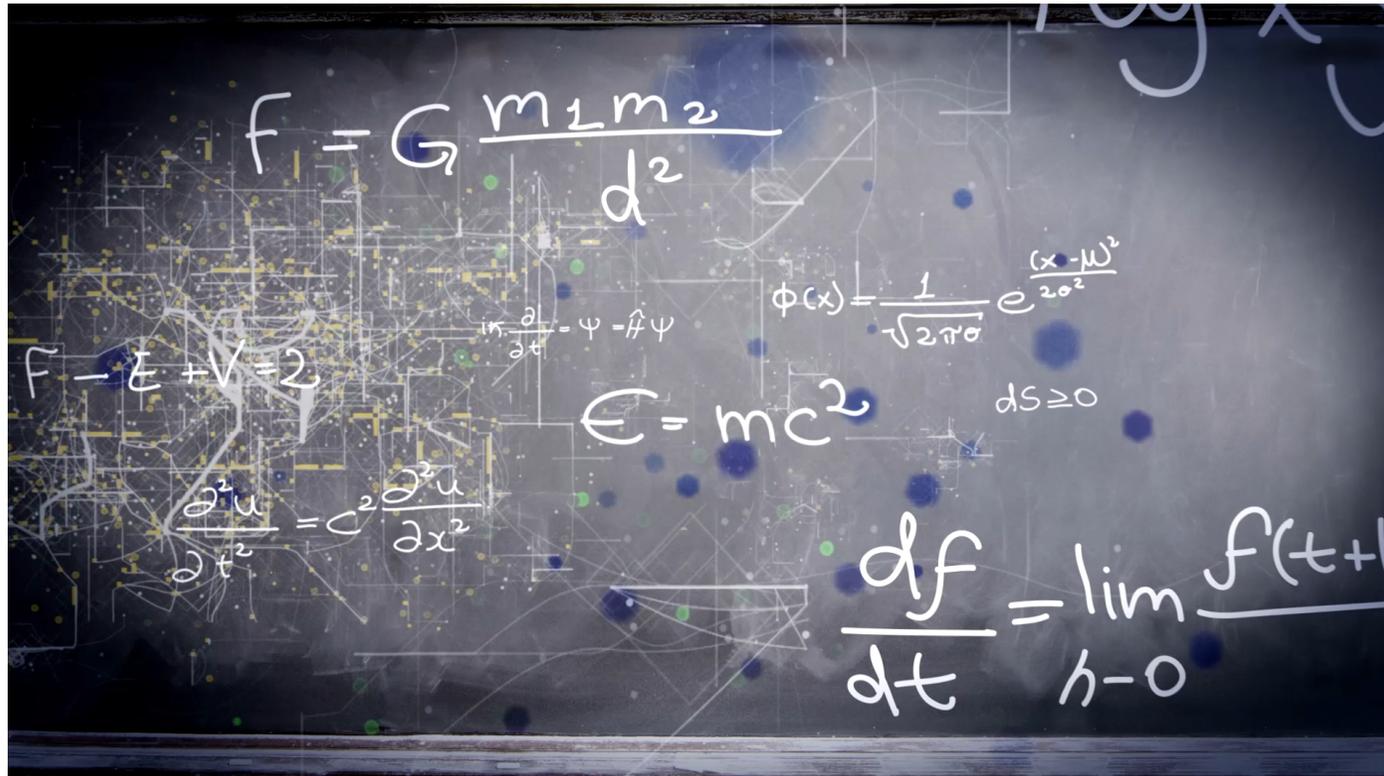
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Machine Learning

Our world is full of “correlations” of input and outputs



I.—COMPUTING MACHINERY AND INTELLIGENCE

By A. M. TURING

1. *The Imitation Game.*

I PROPOSE to consider the question, 'Can machines think?'



I have my hopes, & very distinct ones, too, of one day getting cerebral phenomena such that I can put them into mathematical equations: in short, a law or laws for the mutual actions of the molecules of the brain Ada Lovelace (c1845)



Many Opportunities

1. Speed up simulations
2. Get access to areas and operating manifolds that are hard to experiment

The No Free Lunch Theorem

David Wolpert (1996, 1997)

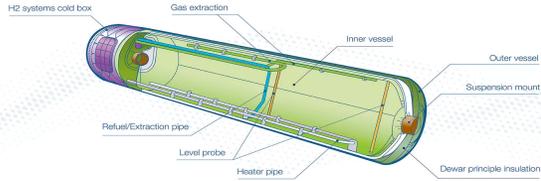
*According to the 'No Free Lunch Theorem', **no ML algorithm is universally superior**. Thus, the task of constructing such an algorithm is a **case-by-case** study. In particular, the choice of the learning algorithm is a key step in building an ML pipeline, and **many choices are available**, each suited for a particular problem and/or dataset.*

What is AI/ML vs What is not AI/ML

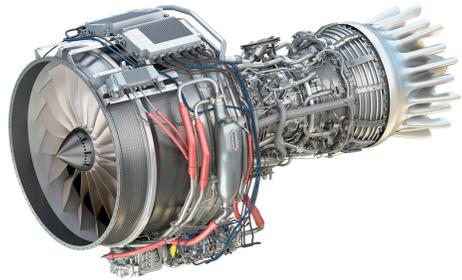


Components of H2 Integration

Liquid H₂ tank



AIRBUS



GE Passport Biz-jet engine

Cryo Storage (-253C)
Thermophysical Properties

Engine
Injection-Combustion Control

Safety
Mixing-Ignition-Detonation

SAFE-H2

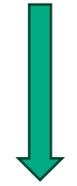


Master the power.

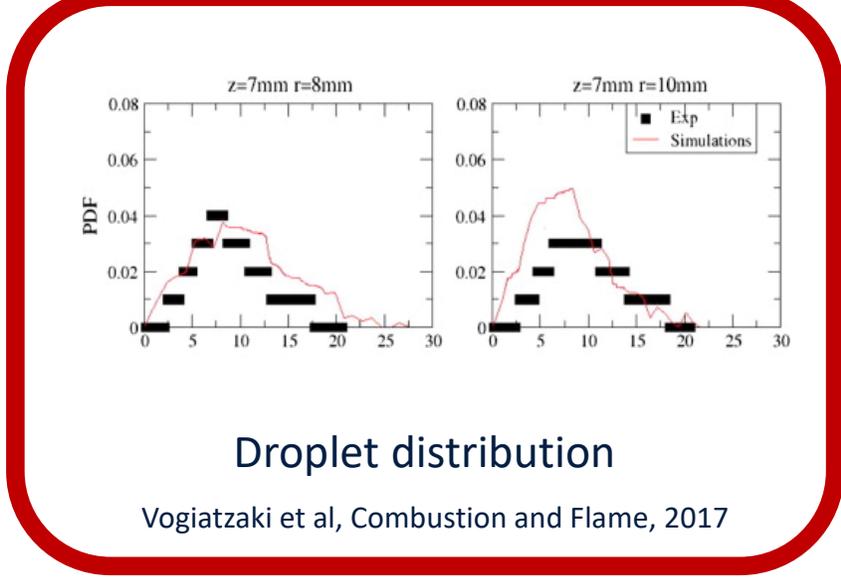
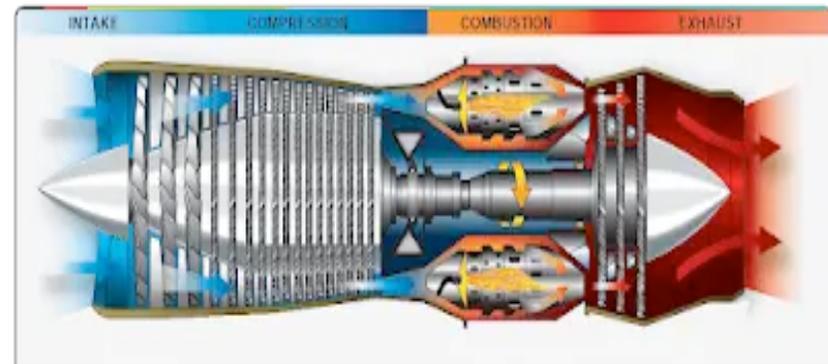




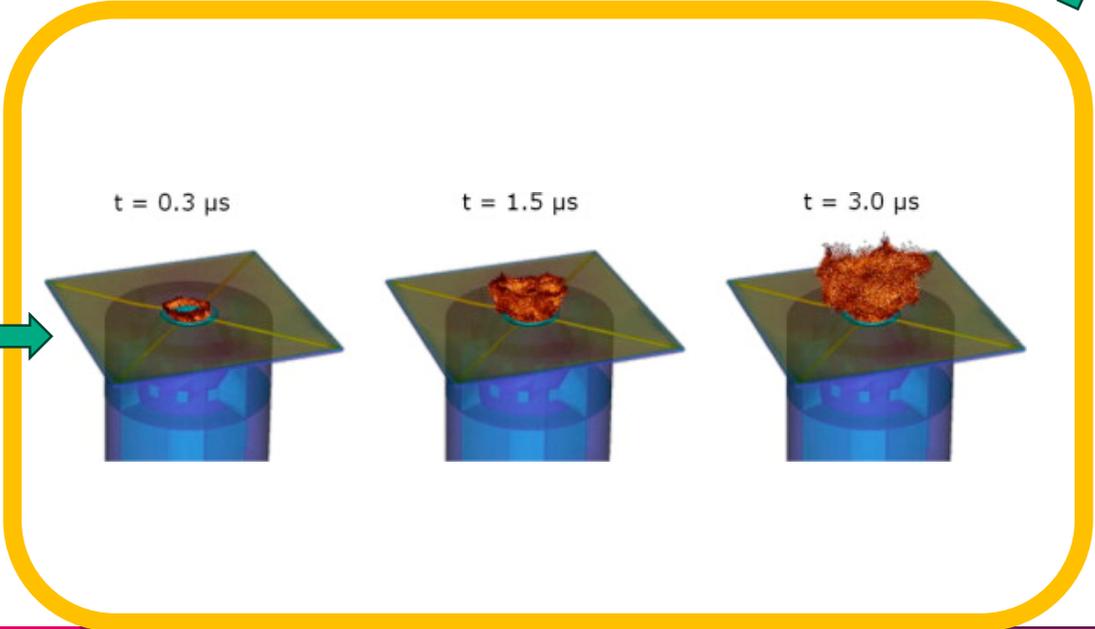
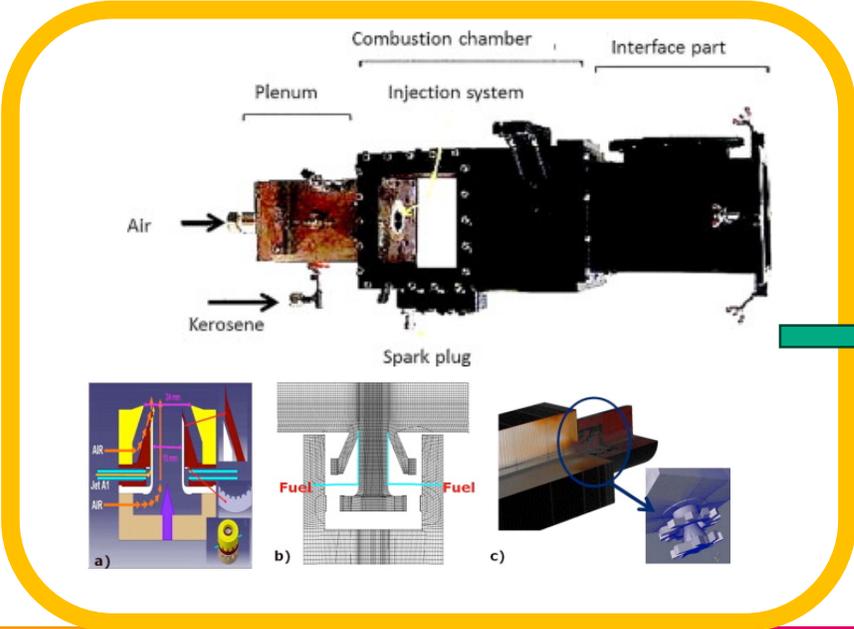
<https://www.rolls-royce.com/products-and-services/civil-aerospace.aspx>



$O(m)$

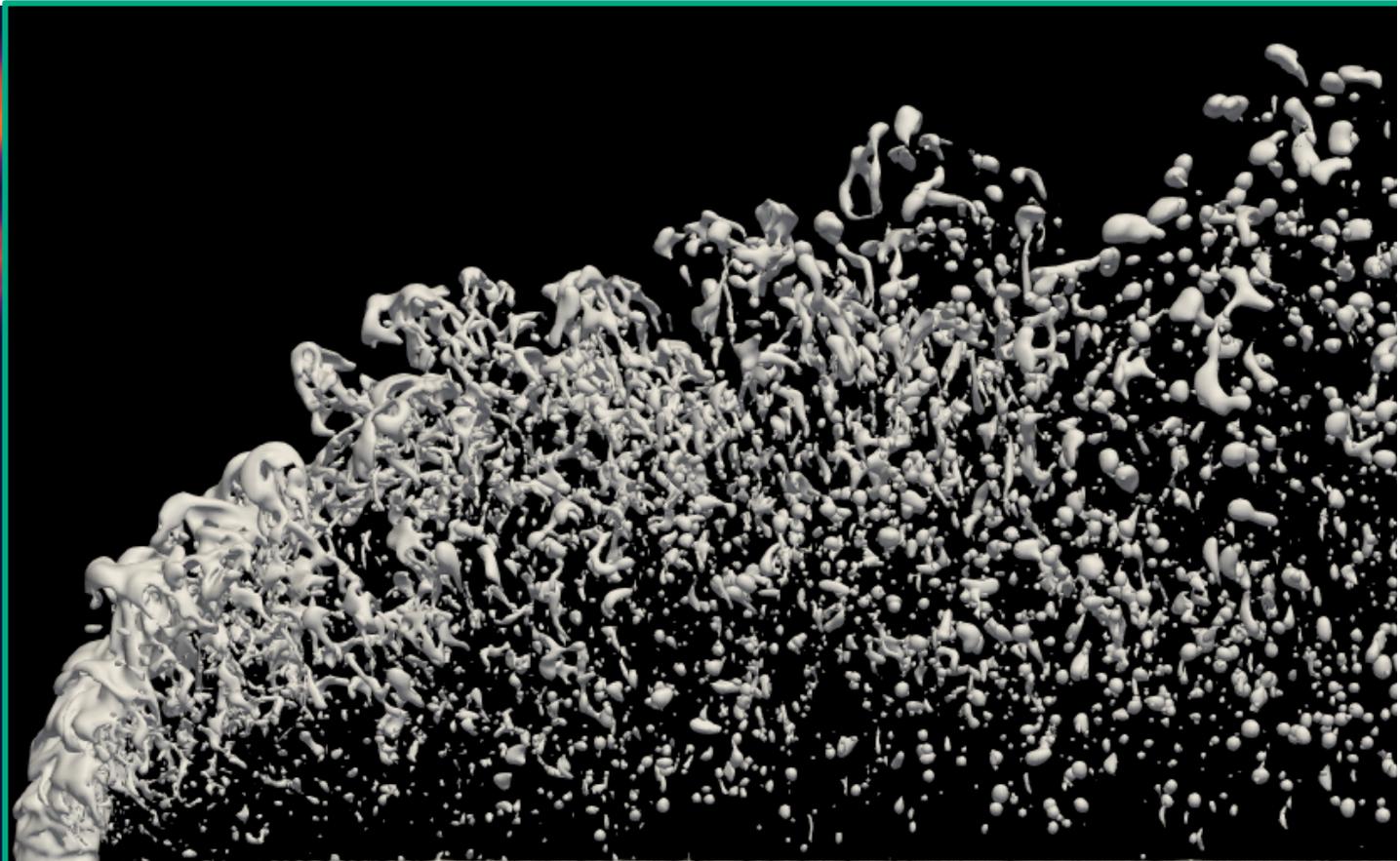
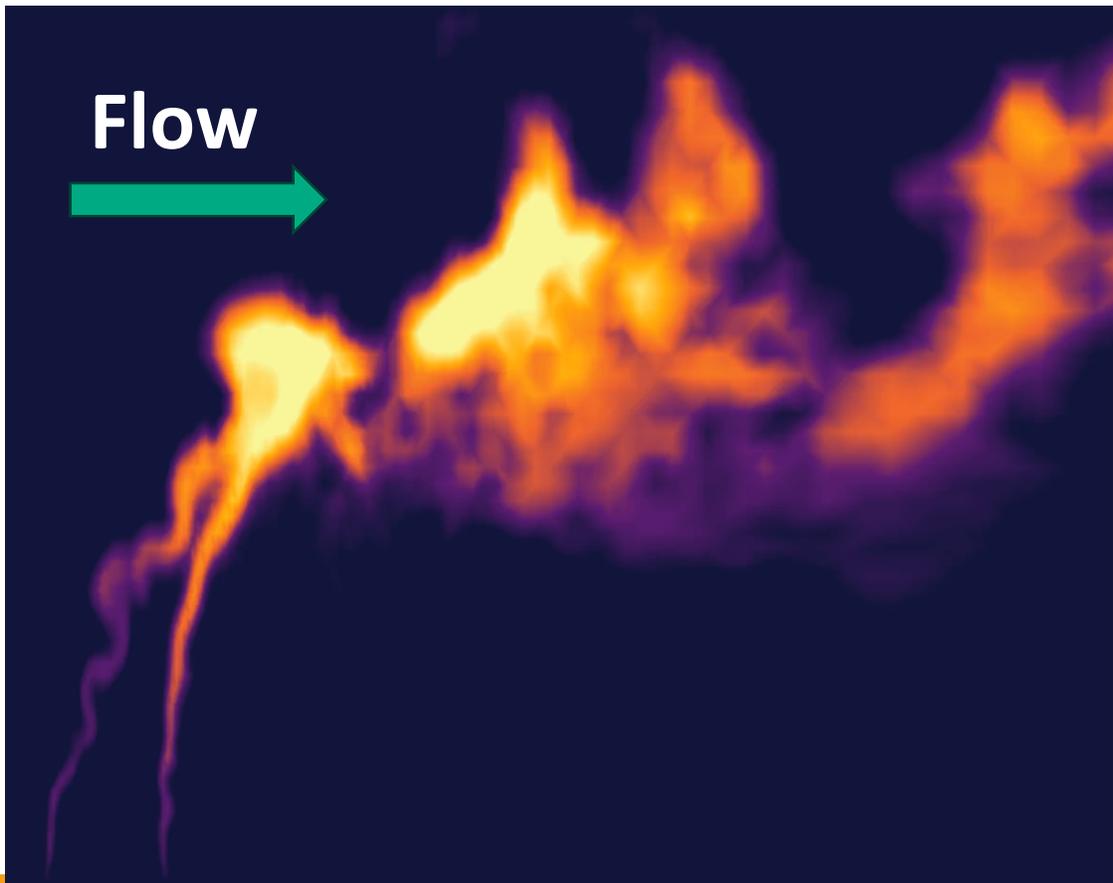


Droplet distribution
Vogiatzaki et al, Combustion and Flame, 2017



$O(\mu m)$

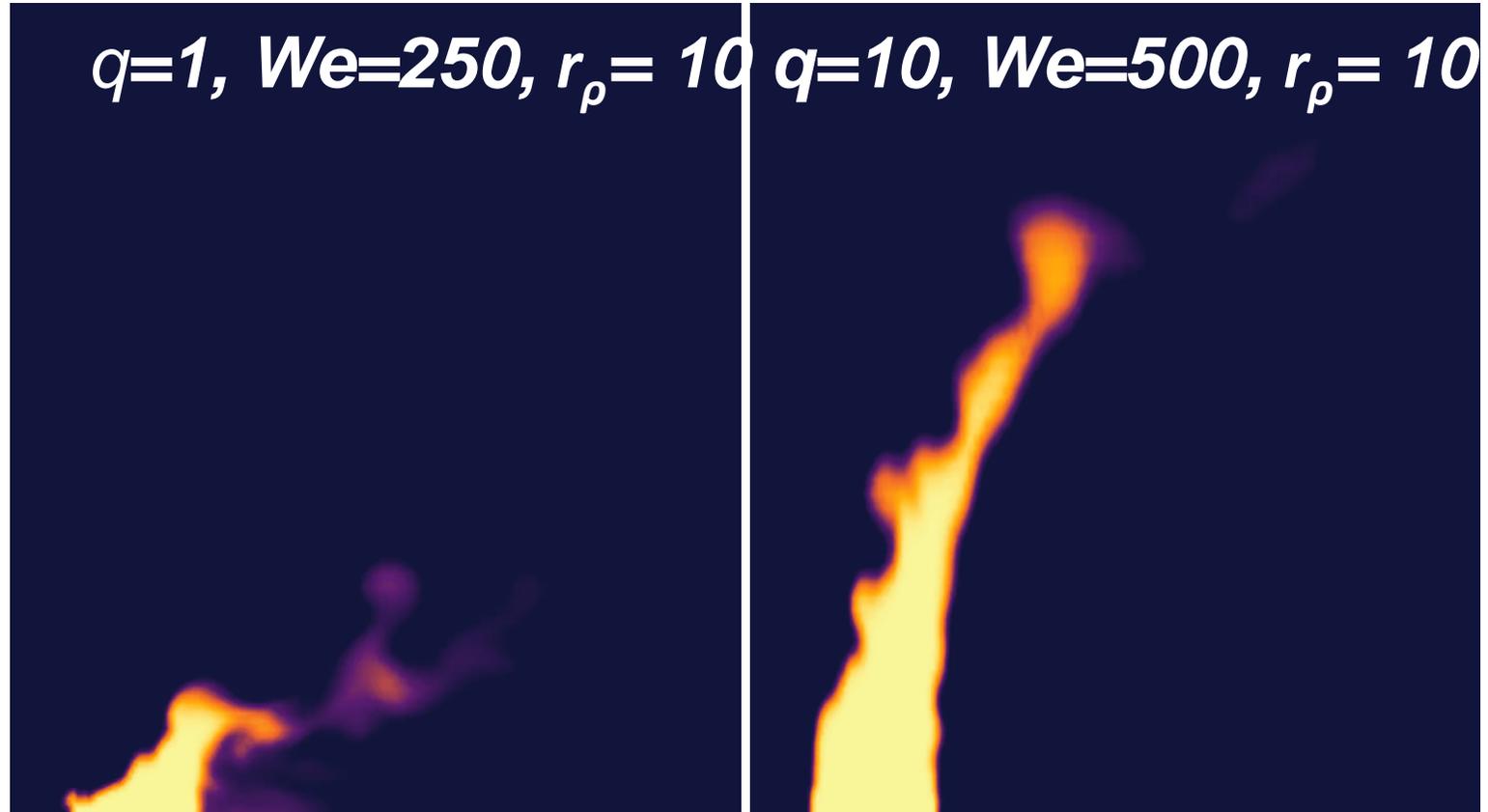
Jet in a Crossflow



Primary Breakup in JIC

Primary Break-up:

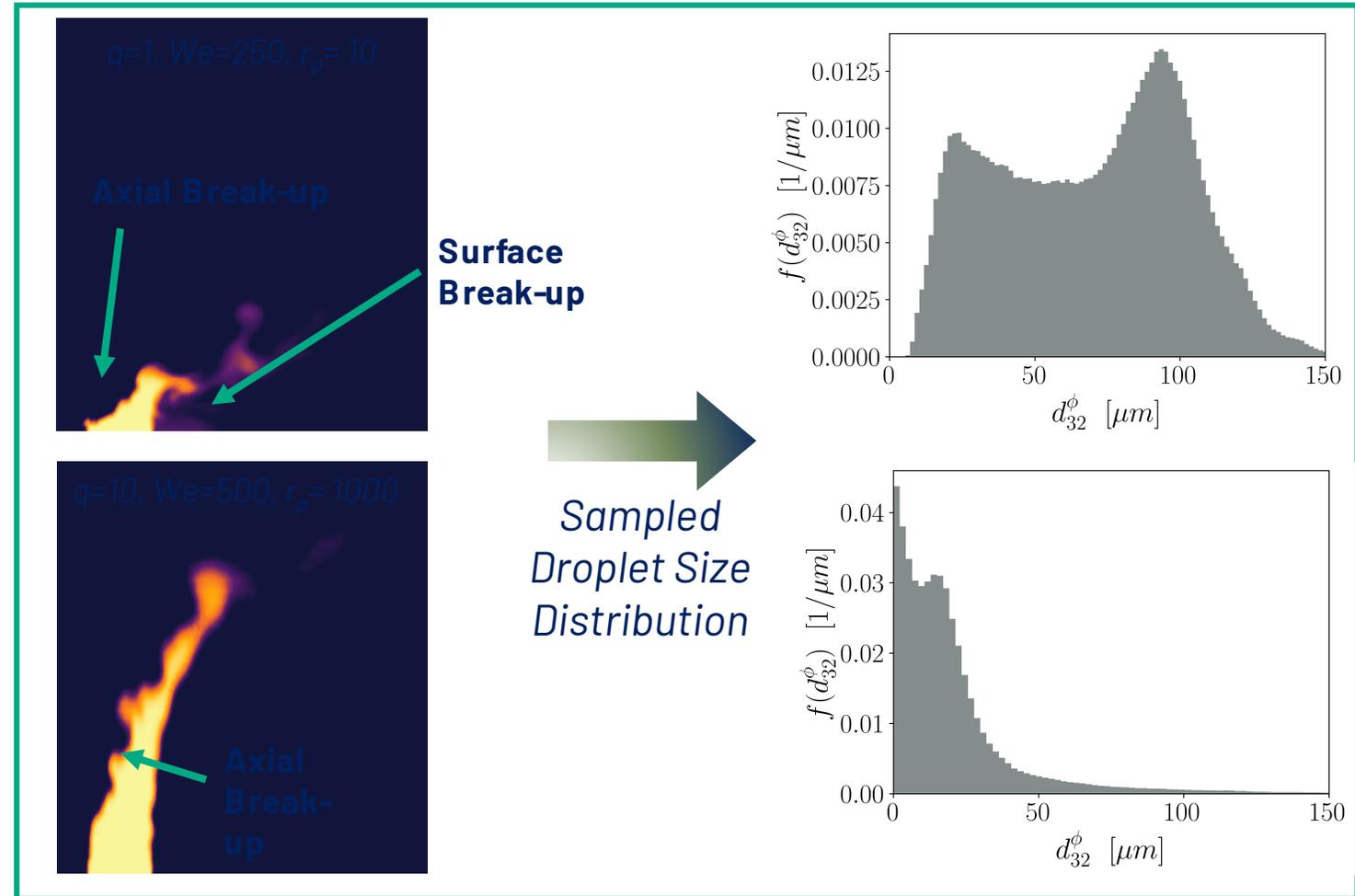
- Different liquid deformation observed
- Break-up mechanisms strongly affected by We , q , r_ρ
- Strong variation in the droplet population produced



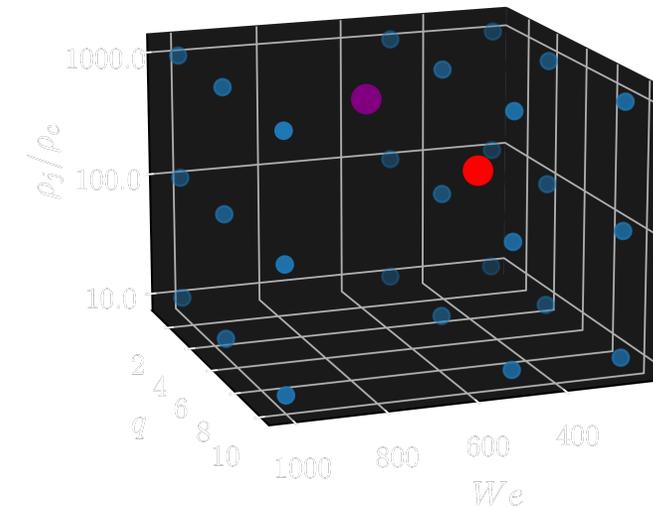
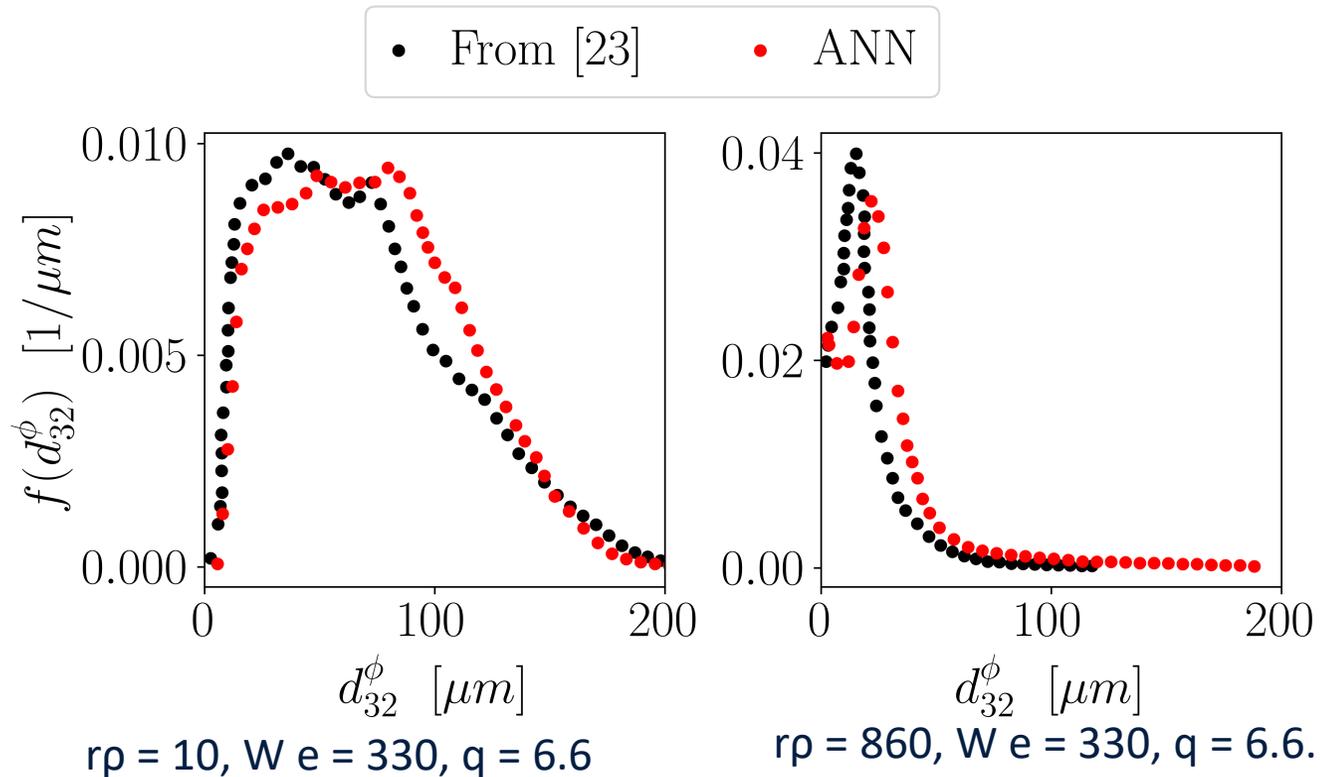
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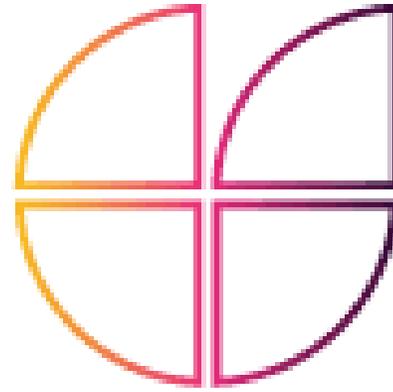
ANN Droplets



Trained DSDs obtained in less than a minute (LES: each case 144 hours on 32 CPUs)

[23]: G. Tretola, K. Vogiatzaki S. Navarro-Martinez, Effect of the density ratio variation on the dynamics of a liquid jet injected into a gaseous cross-flow, Physics of Fluids 33 (9) (2021) 092120

Thank you !



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