DNS of an Atomizing Biodiesel Jet with Basilisk

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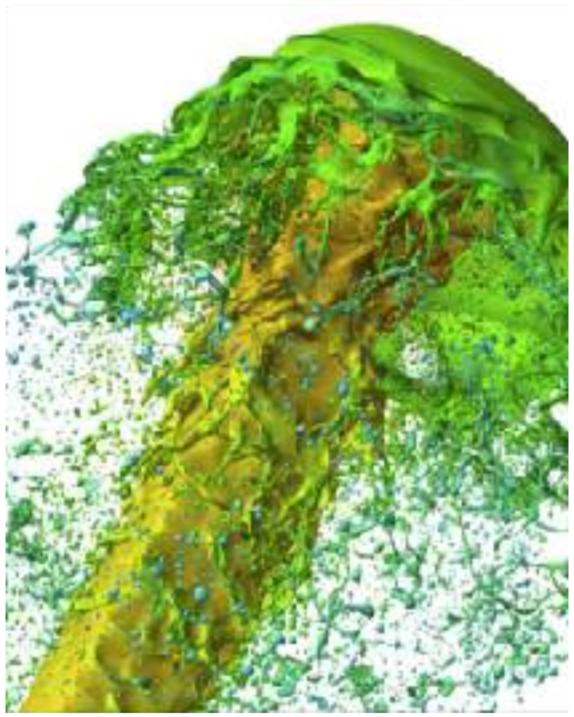
Motivations

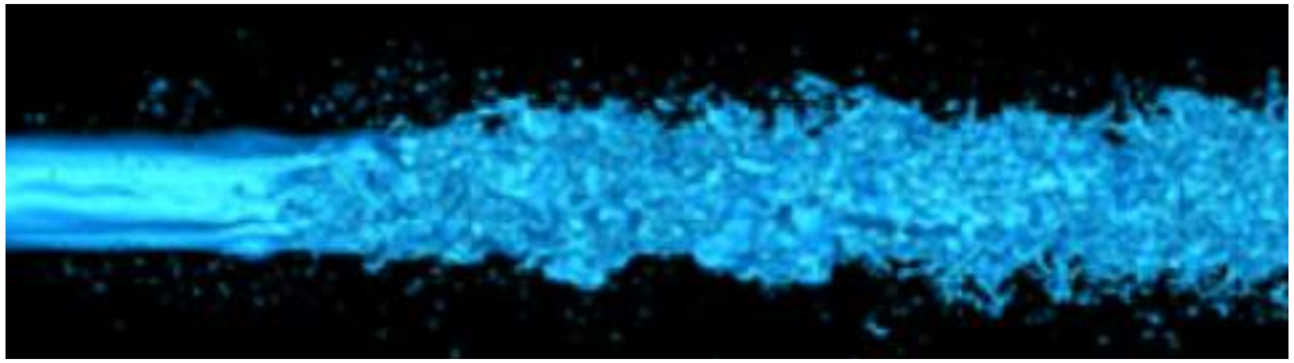
- Fuel injection and the resulting spray characteristics are critical to diesel engines
- Biodiesel fuels are increasingly popular
- Physical properties of biofuels have an impact on atomization process *(Pandey et al, 2012)*
- Direct Numerical simulations of atomization
  - Primary breakups
  - Turbulence-interface interaction
  - Droplets statistics

Detailed Numerical Simulation

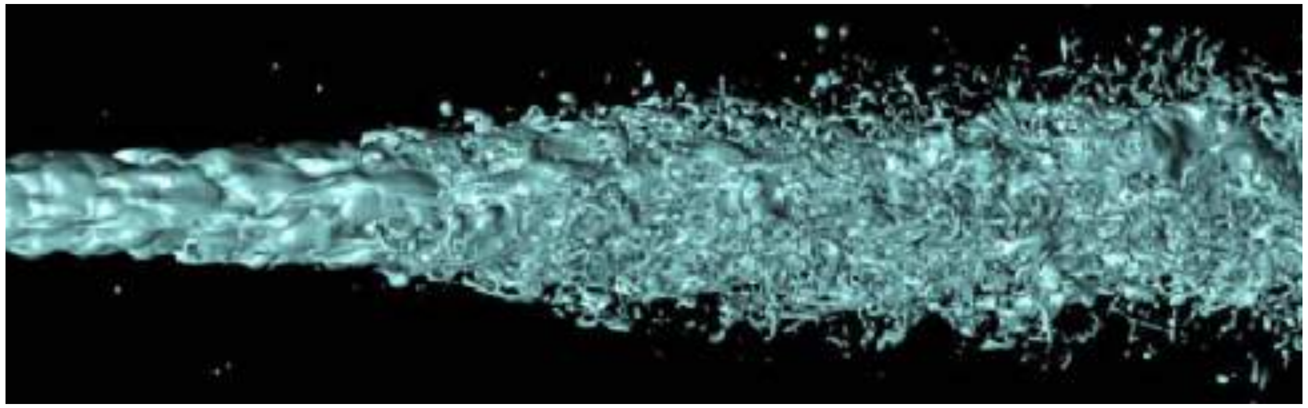


Shinjo & Umemura (2010)

Rana & Herrmann (2011)



Desjardins, Moureau & Pitsch (2008)



Lebas, Menard, Berlemont, et al. (2009)

Jarrahbashi, Sirignano, et al. (2016)

Le Chenadec & Pitsch (2013)

Equations & Solvers

- Incompressible variable-density, N-S equations with surface tension

$$\rho(\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}) = -\nabla p + \nabla \cdot (2\mu \boldsymbol{D}) + \sigma\kappa\delta_s \boldsymbol{n}$$

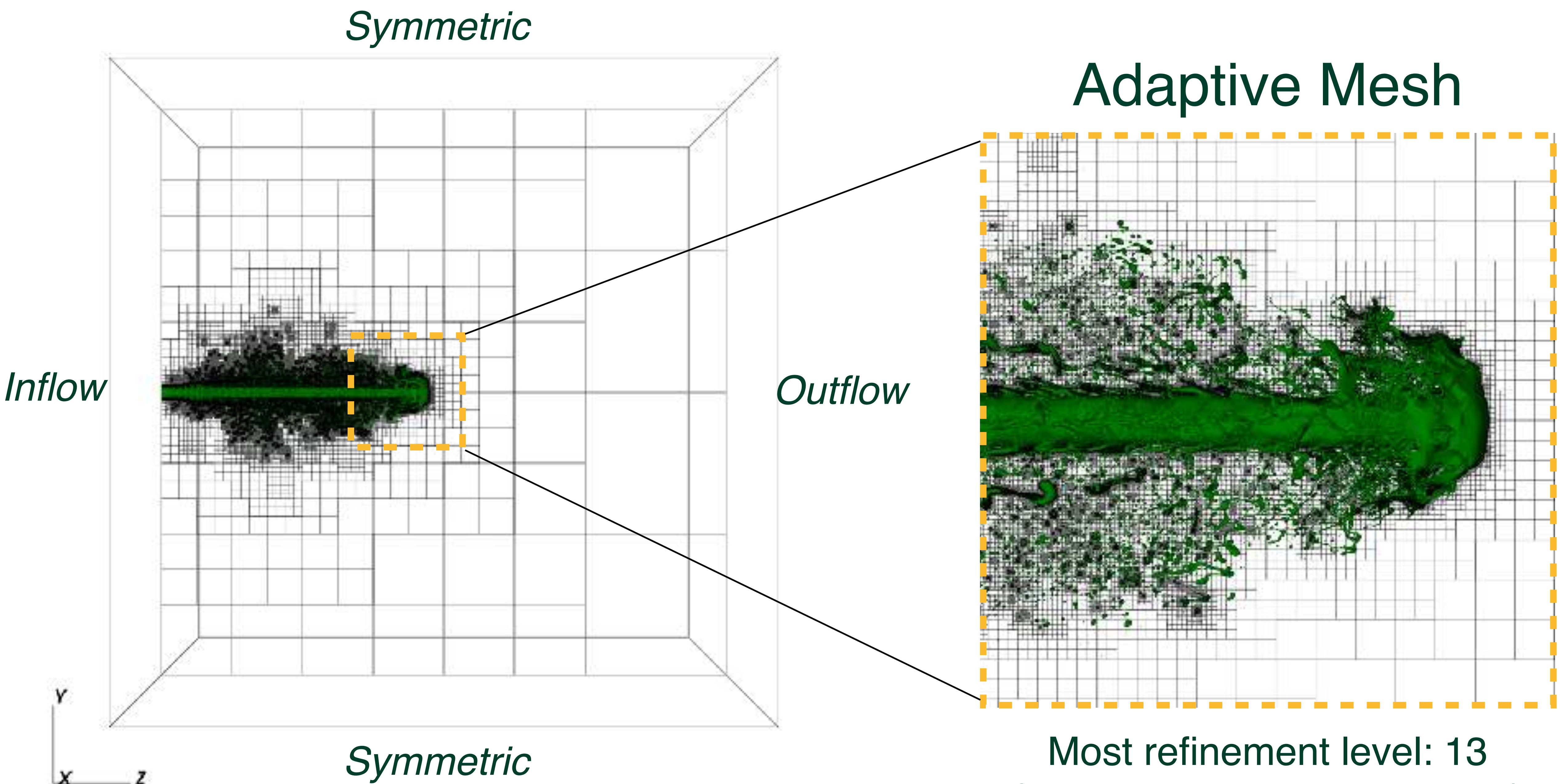
$$\nabla \cdot \boldsymbol{u} = 0$$

- Volume of fluid method (PLIC)

$$\partial_t C + \boldsymbol{u} \cdot \nabla C = 0$$

- Basilisk solver
  Finite volume approach, 2nd order in time & space,VOF, quad/octree spatial discretization, adaptive mesh refinement, height-function method for curvature, balanced-force surface tension discretization

Simulation Setup



Most refinement level: 13
(Rinj/Δmin=85, Δmin=1.5μm)

2048 CPU cores on CURIE for 5 weeks

http://basilisk.fr/src/examples/atomisation.c

Simulation Cases

Gas: compressed air (p=10 bar)

Liquid fuels: - Standard European diesel (D)

- Biodiesel of soybean Methyl Ester (B)

Fuels	ρ_g (kg/m³)	ρ_l (kg/m³)	μ_g (Pa s)	μ_l (Pa s)	σ (N/m)
Diesel	11.13	825	1.46E-05	2.10E-03	2.4E-2
Biodiesel	11.13	870	1.46E-05	3.90E-03	2.8E-2

(Battistoni & Grimaldi, 2012, Appl. Energy, 97, pp. 656–666)

Three different injection conditions

Injection Cond.	R_{inj} (μm)	U_{inj} (m/s)
1	65	70
2	40	50
3	65	50

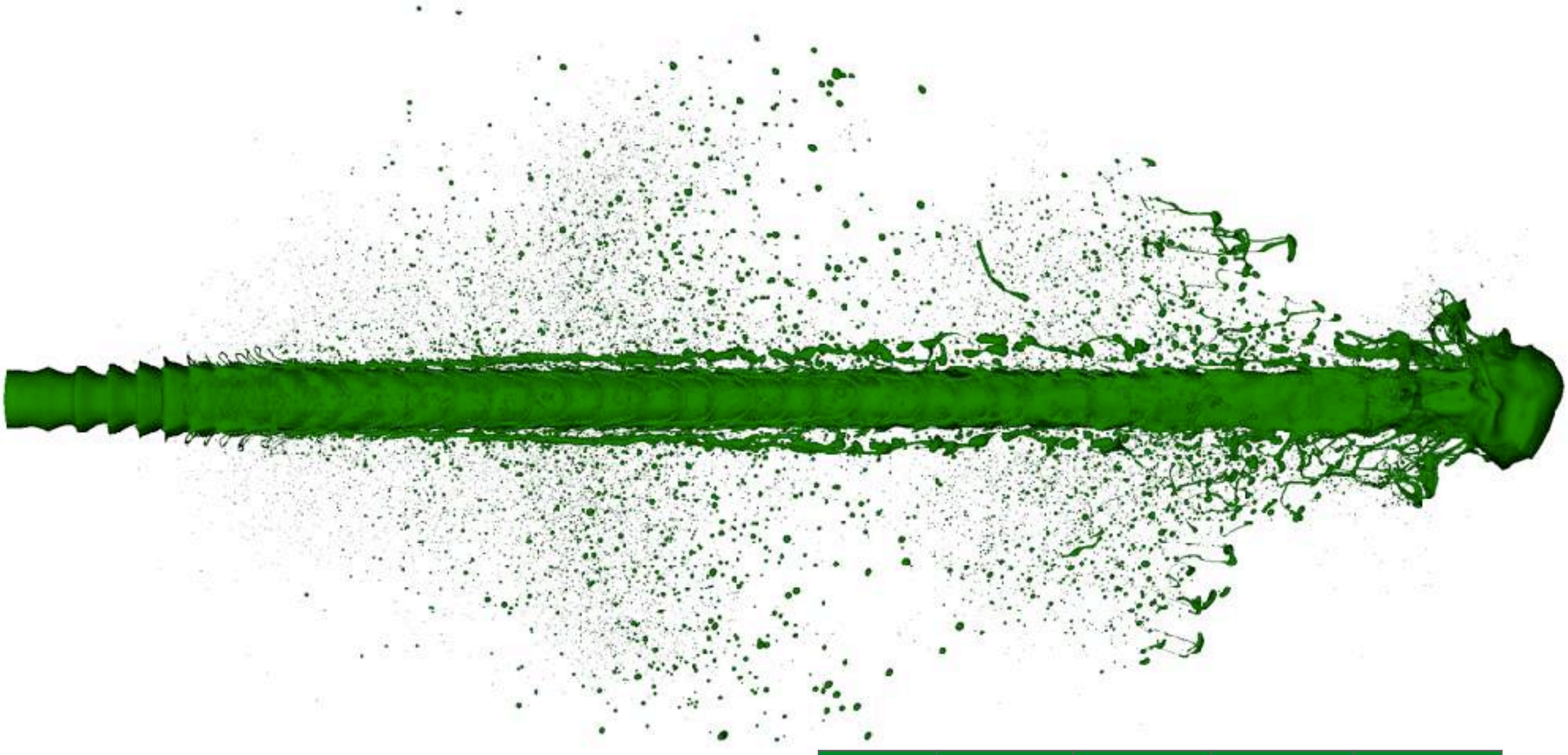
Simulation Cases

Cases	ρ_g (kg/m^3)	ρ_l (kg/m^3)	μ_g (Pa s)	μ_l (Pa s)	σ (N/m)	R_{inj} (μm)	U_{inj} (m/s)	Re_g	Re_l	We_g	We_l
D1	11.13	825	1.46E-05	2.10E-03	2.4E-2	65	70	6940	3580	295	21900
D2	11.13	825	1.46E-05	2.10E-03	2.4E-2	40	50	3050	1570	927	6880
D3	11.13	825	1.46E-05	2.10E-03	2.4E-2	65	50	4950	2550	151	11200
B1	11.13	870	1.46E-05	3.90E-03	2.8E-2	65	70	6940	2030	253	19800
B2	11.13	870	1.46E-05	3.90E-03	2.8E-2	40	50	3050	892	79.5	6210
B3	11.13	870	1.46E-05	3.90E-03	2.8E-2	65	50	4950	1450	129	10100

Gas: compressed air (p=10 bar)
Liquid fuels: - Standard European diesel (D1,D2, D3)
- Biodiesel of soybean Methyl Ester (B1, B2, B3)

1,2,3: three different injection conditions

Atomizing Liquid Jet



Case B3, R_{inj}/Δ_{min}=85
2048 Cores, about 3 weeks

Cases	Re_g	Re_l	We_g	We_l
B3	4950	1450	129	10100

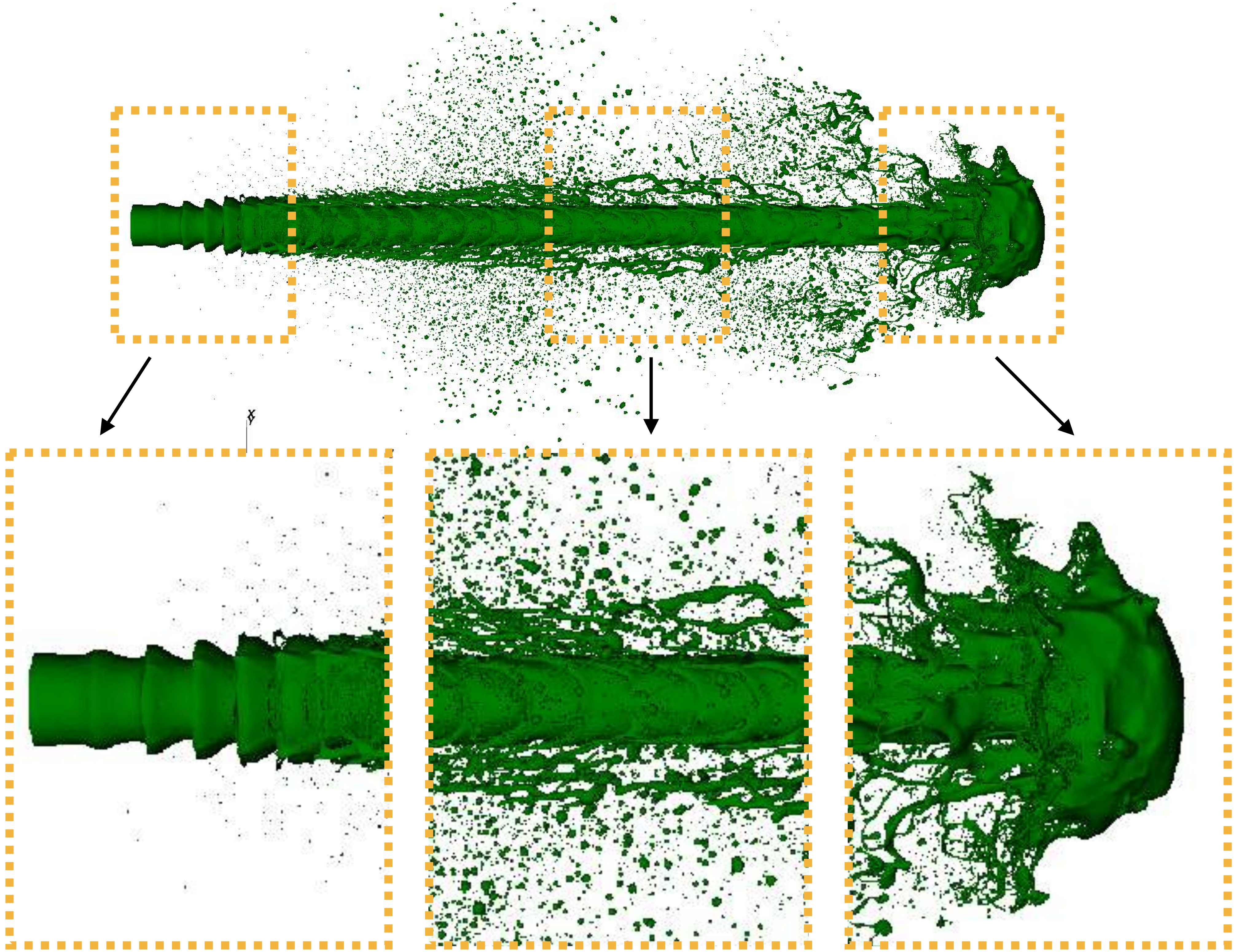
Effect of Grid Resolution (B3)

(a) Rinj/Δmin=21

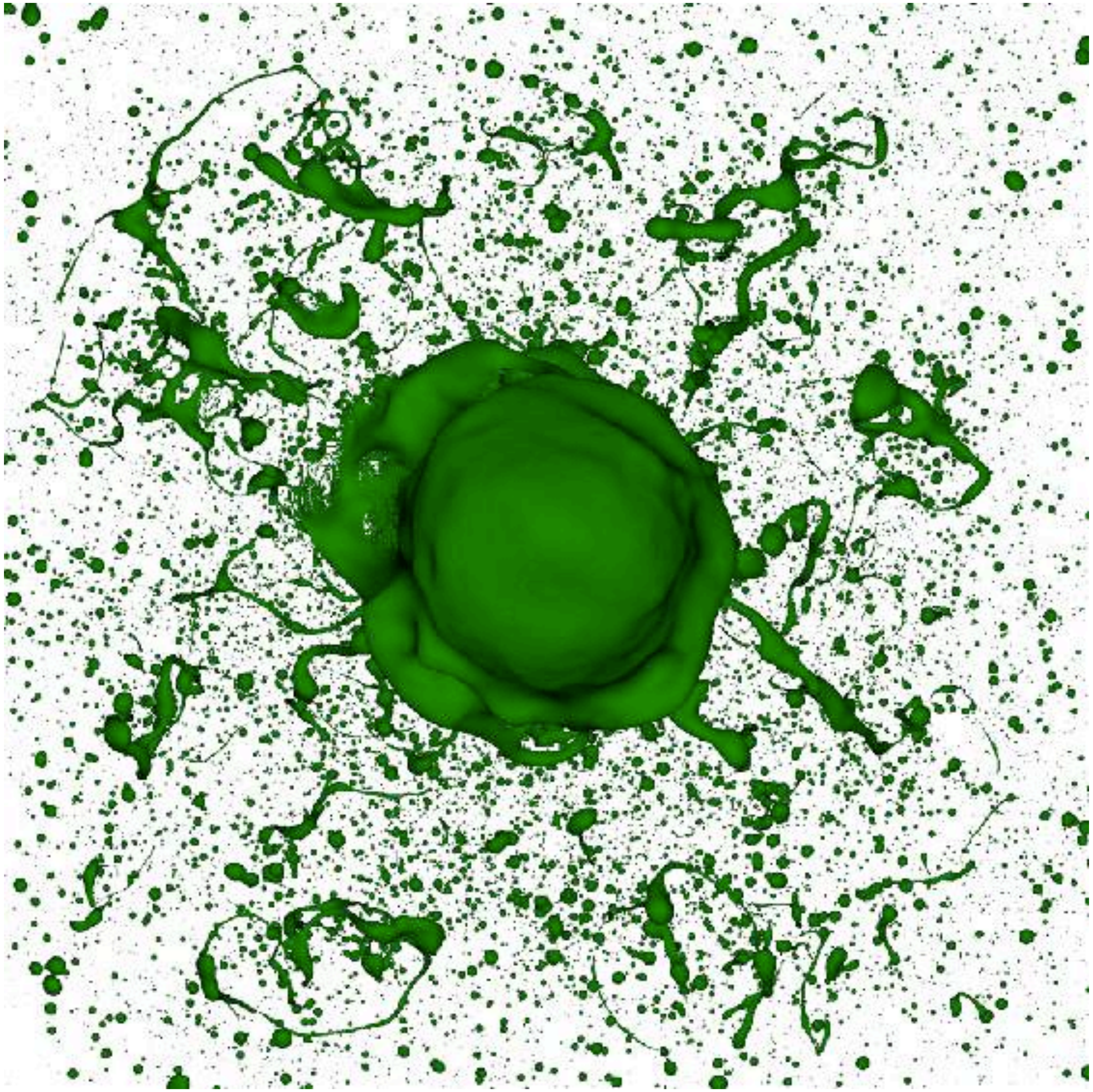
(b) Rinj/Δmin=43

(c) Rinj/Δmin=85

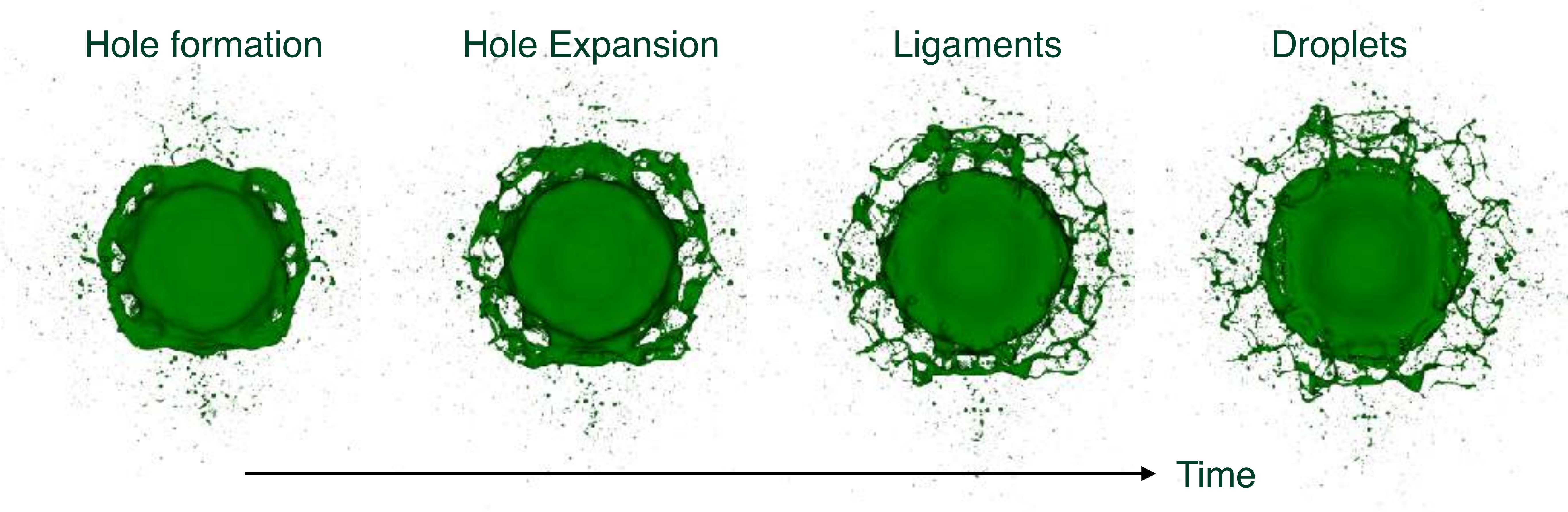
Spray Formation



Dynamics of Mushroom Head



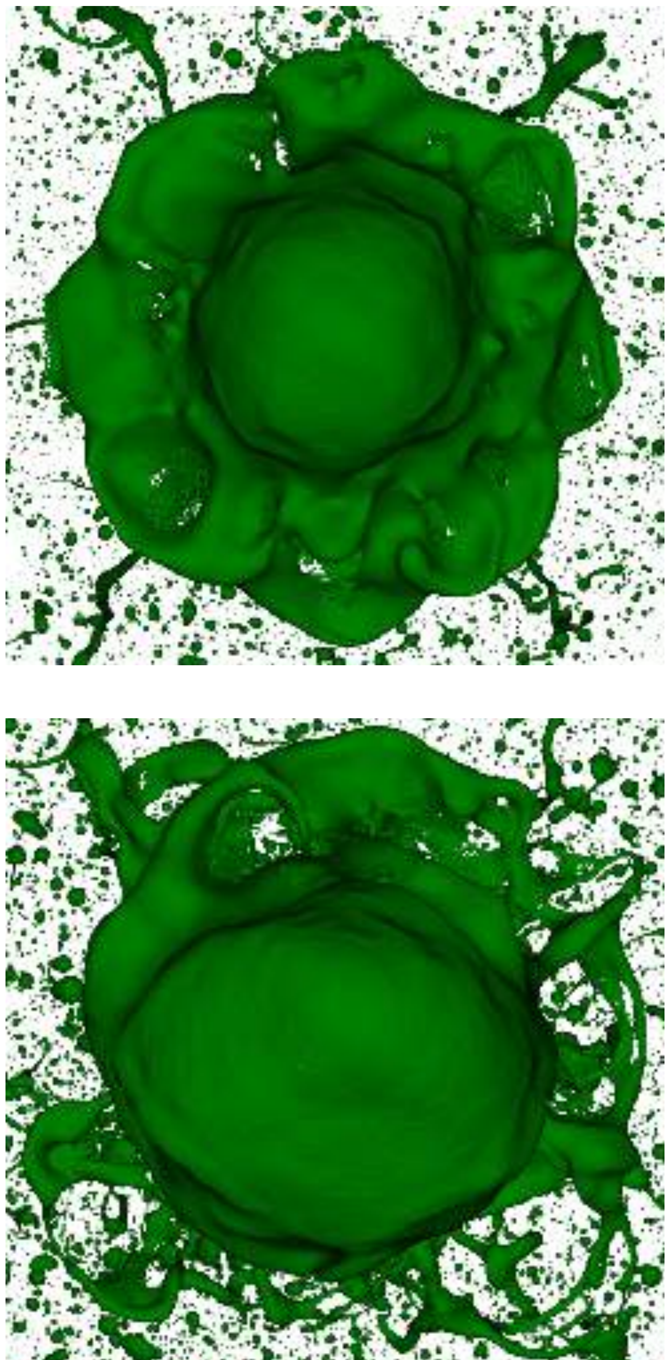
Dynamics of Mushroom Head



Instability on the Head

(Shinjo & Umemura 2010)

Time



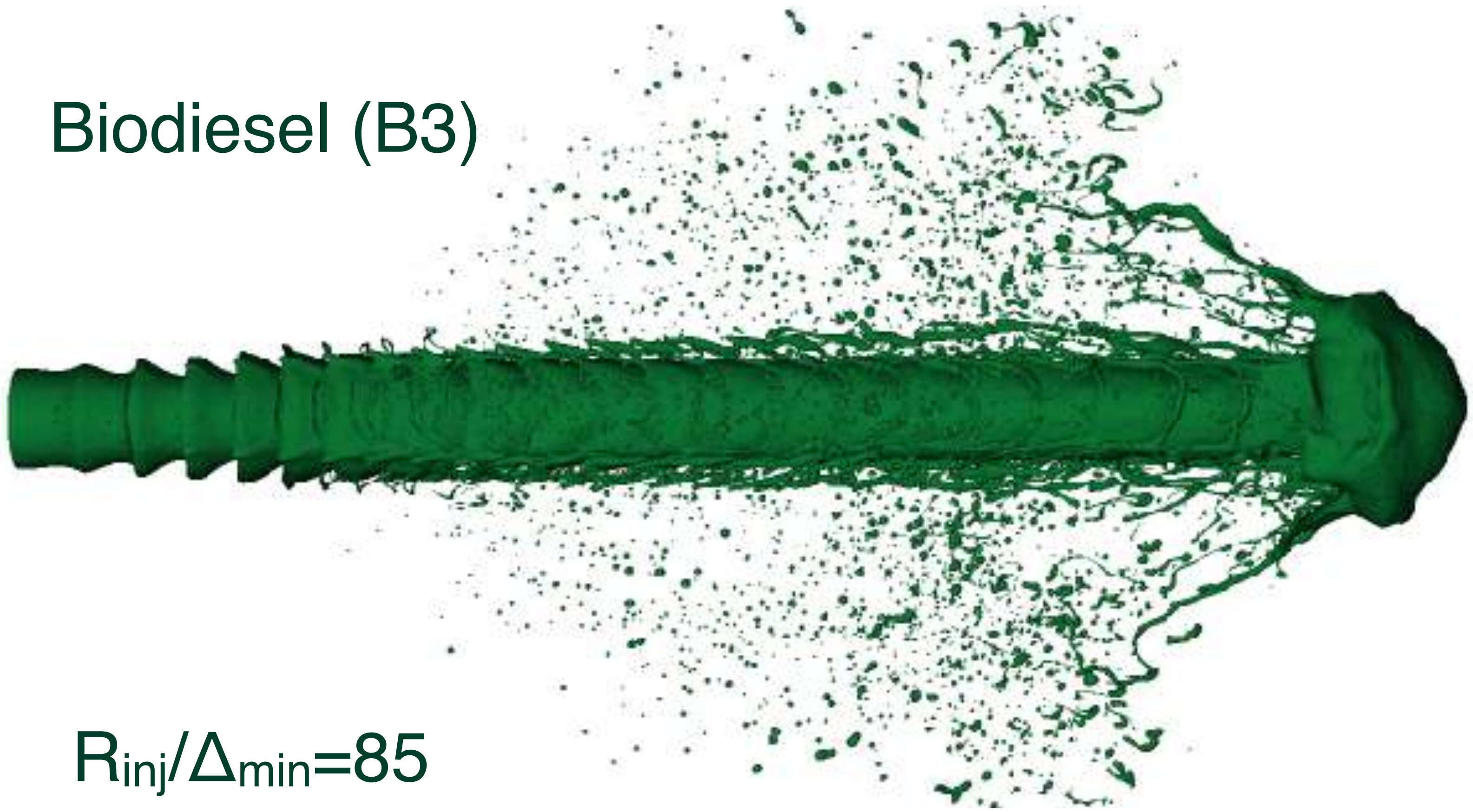
Effect of Cartesian grid fades out

Helmholtz-Kelvin Instability

Liquid sheet rolls up

Biodiesel vs Diesel

Biodiesel (B3)



- Longer filaments
- Smaller head
- Less droplets
- More large drops

$R_{inj}/\Delta_{min}=85$

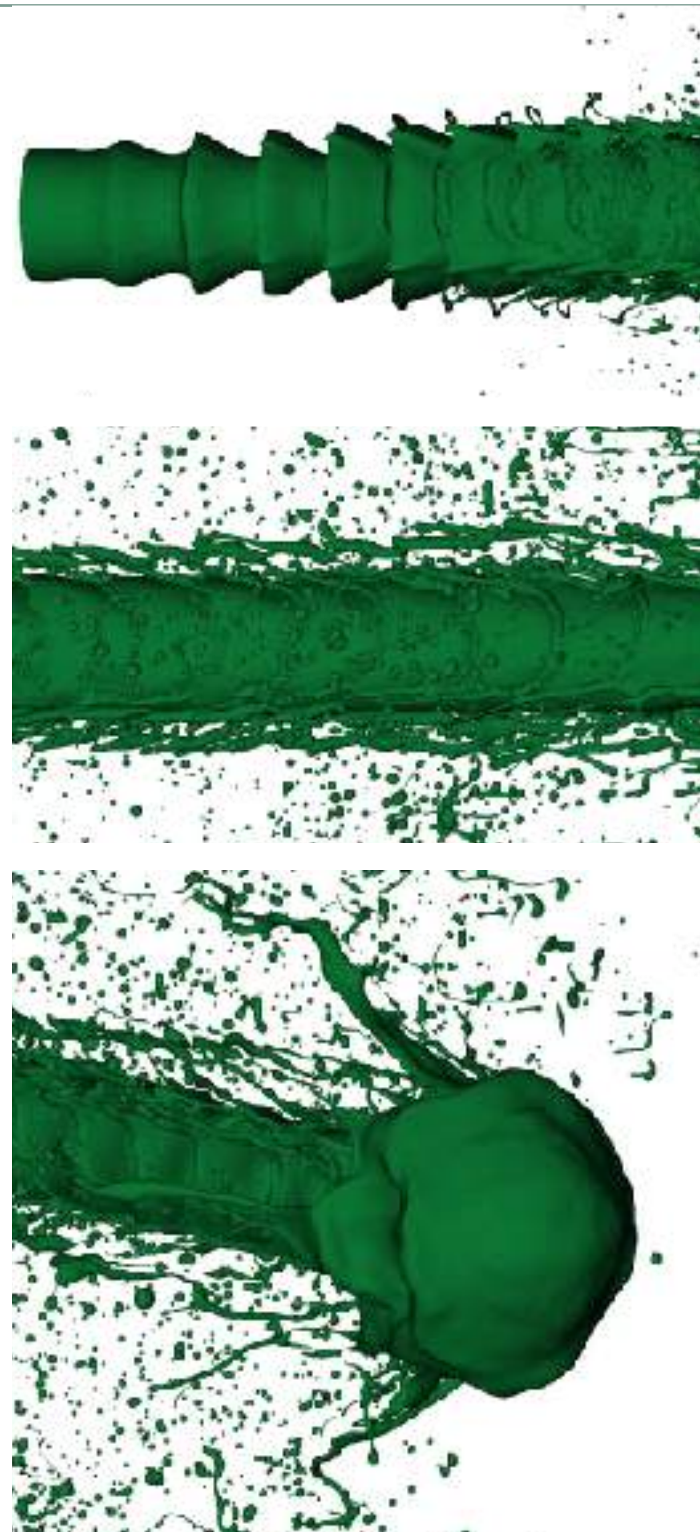
Same injection conditions:
$R_{inj}=65\mu m$, $U_{inj}=50 m/s$

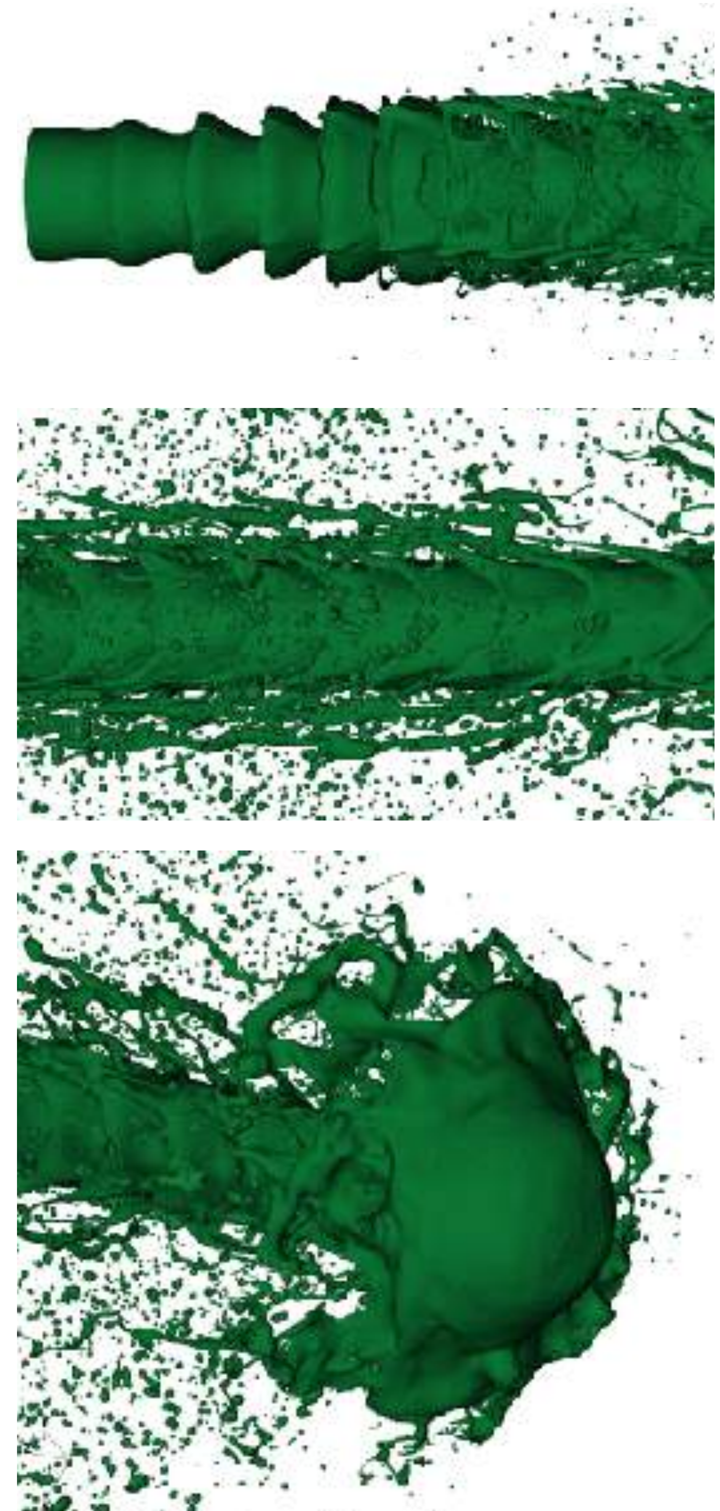
Cases	ρ_l (kg/m³)	μ_l (Pa s)	σ (N/m)
D3	825	2.10E-03	2.4E-2
B3	870	3.90E-03	2.8E-2

Diesel (D3)

Biodiesel vs Diesel: More Details

Biodiesel (B3)

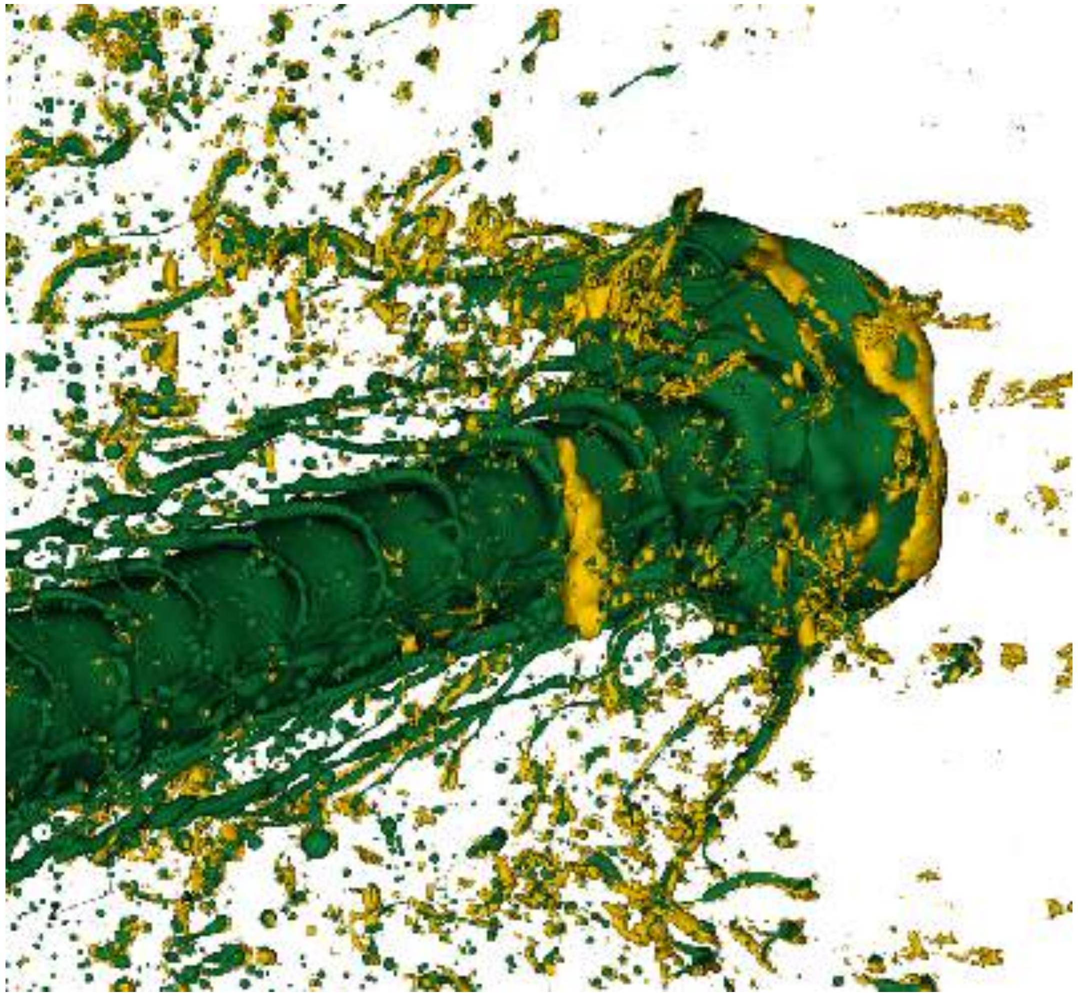




Diesel (D3)

Biodiesel vs Diesel: Vortices

λ2 iso-surface for vortical structures visualization



Biodiesel (B3)

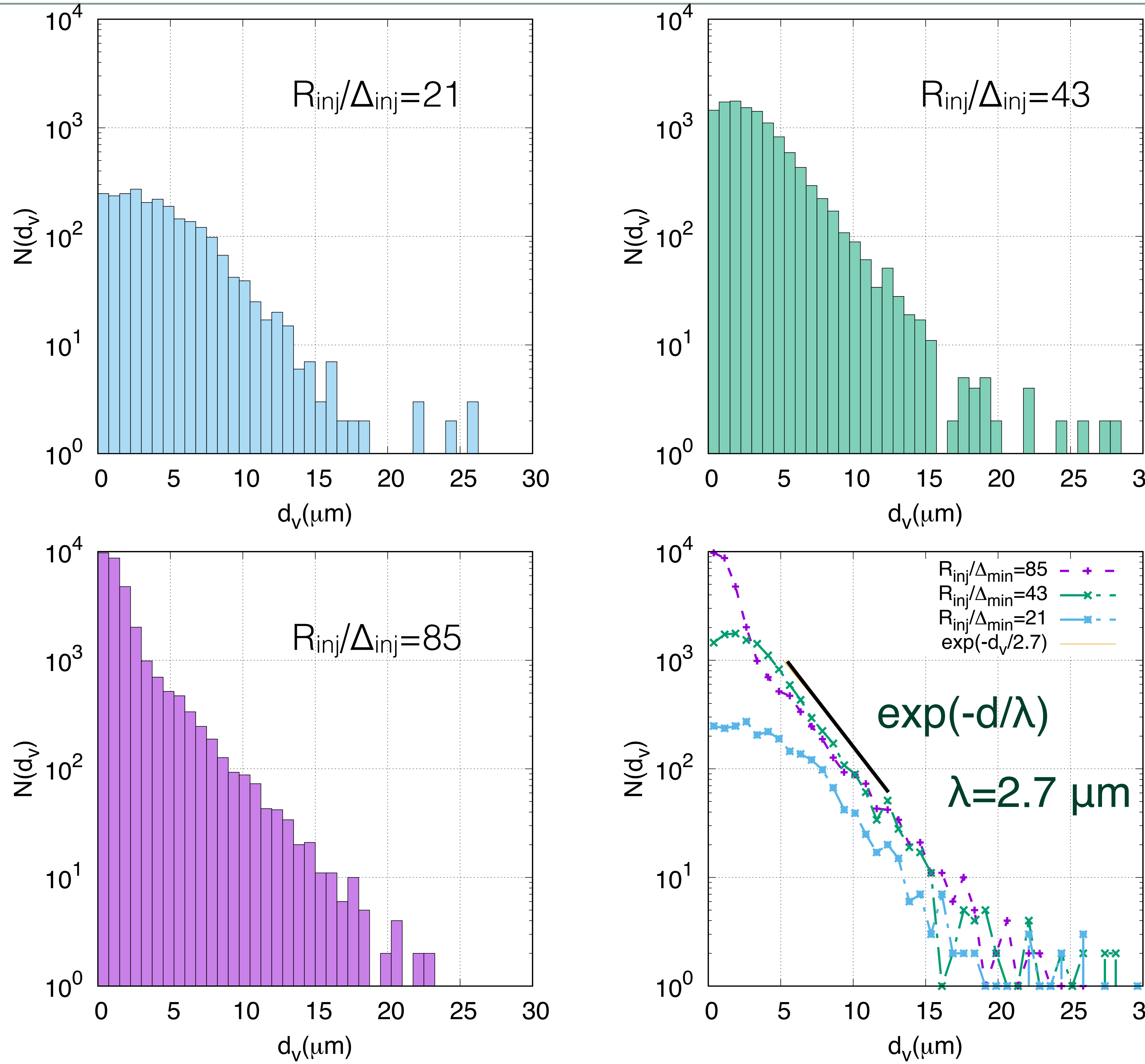
Diesel (D3)

(Vortex dynamics: Jarrahbashi, Sirignano, Popov, & Hussain 2016)

Droplet Size Distribution

Effect of grid resolution

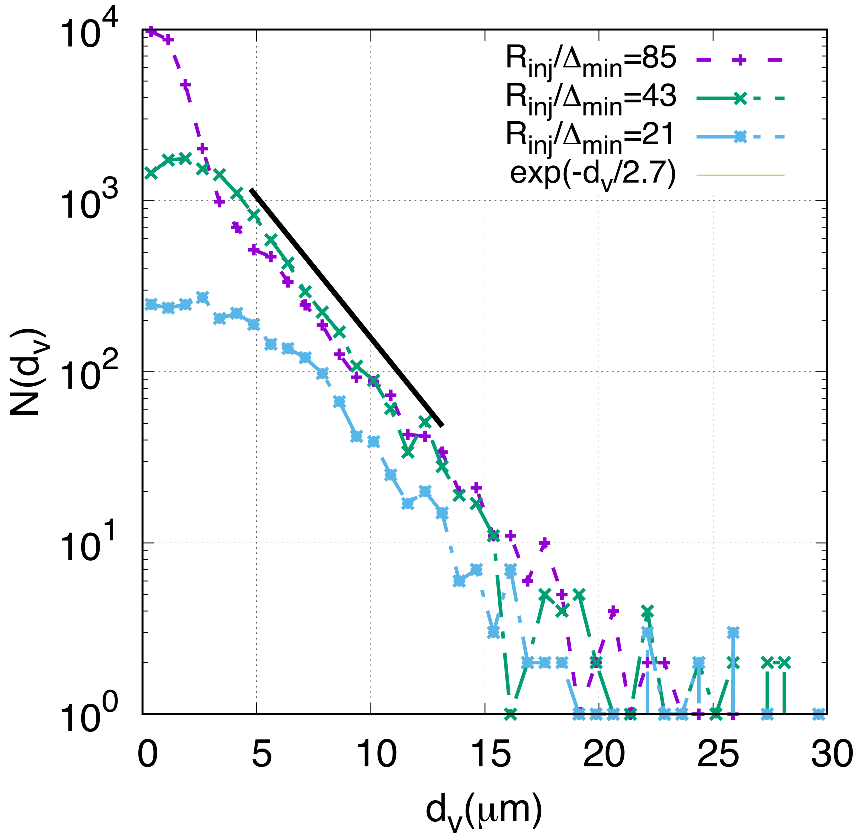
Biodiesel (B3)



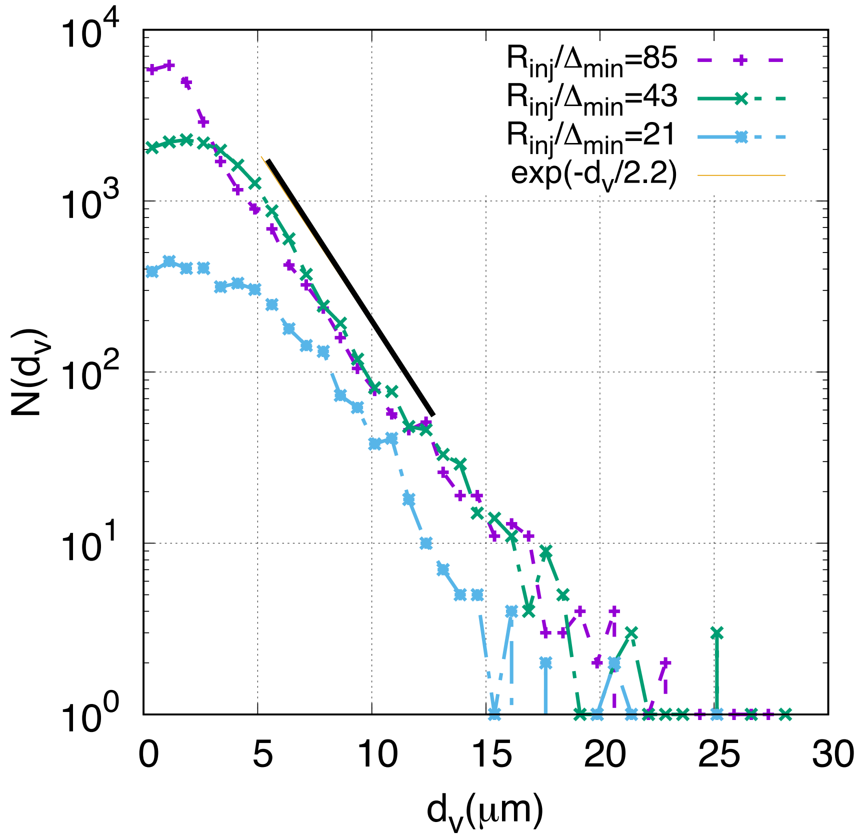
Marmottant & Villermaux 2004

Droplet Size Distribution

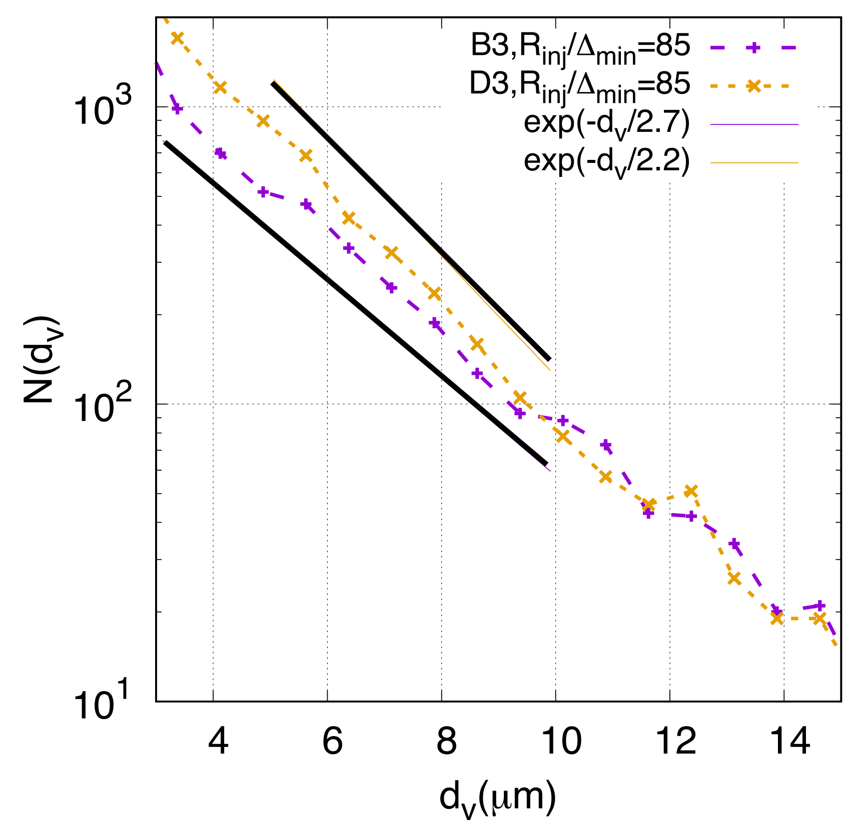
Biodiesel vs Diesel



Biodiesel (B3)



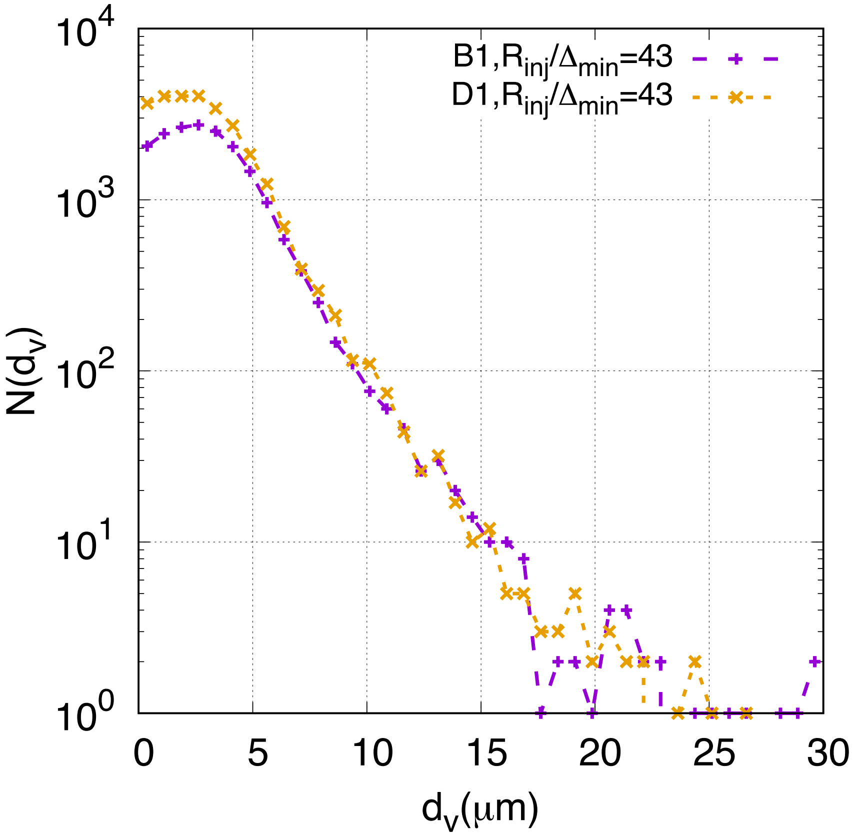
Diesel (D3)



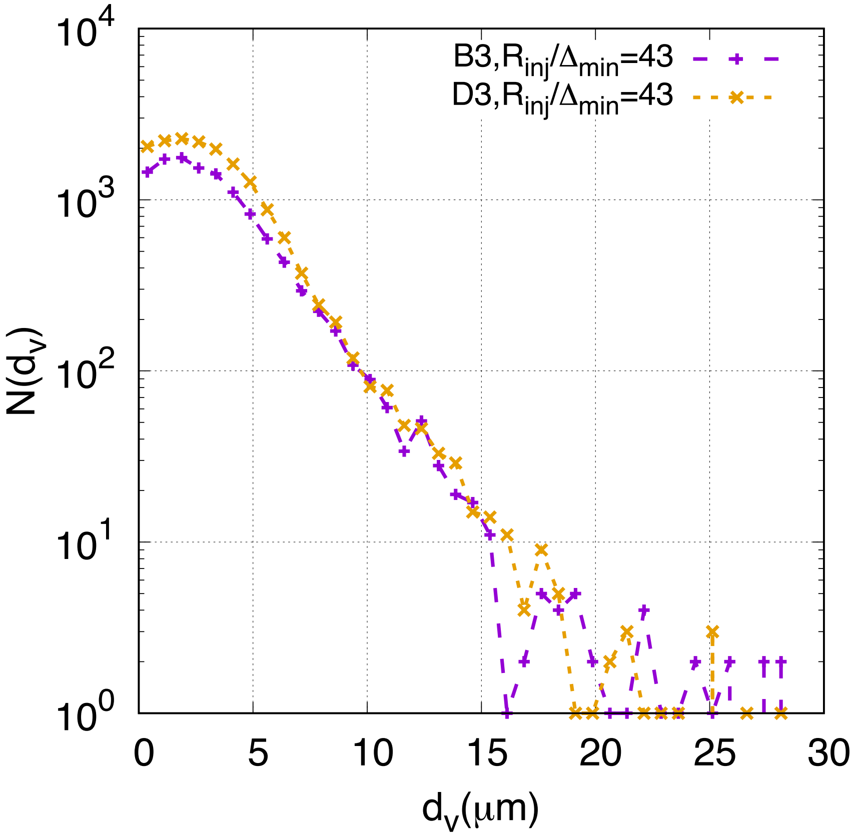
B3 vs D3

Droplet Size Distribution

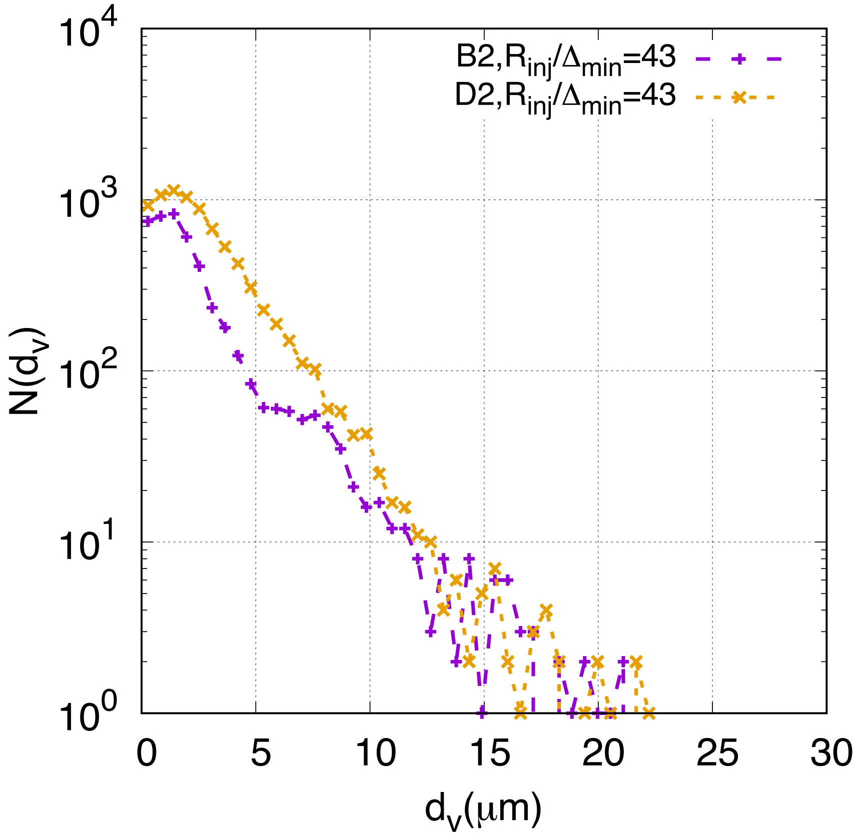
Effects of injection conditions



R_{inj}=65μm, U_{inj}=70m/s

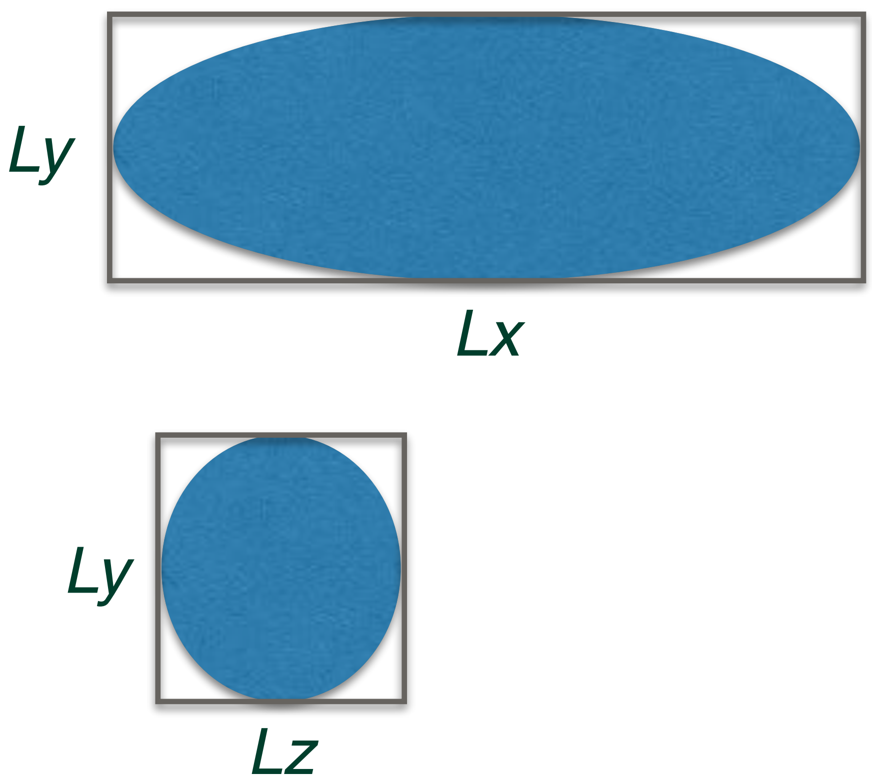


R_{inj}=65μm, U_{inj}=50m/s



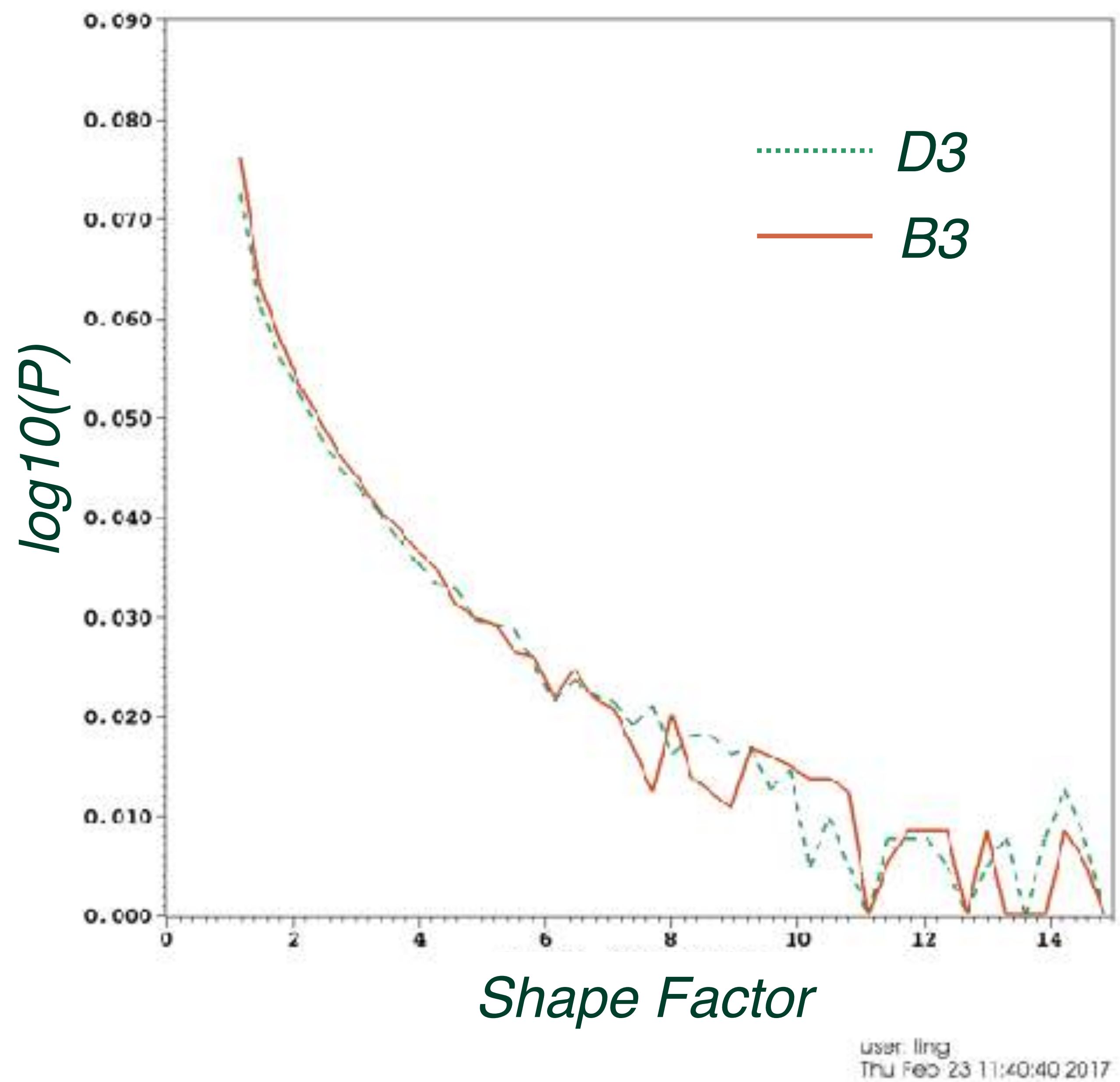
R_{inj}=40μm, U_{inj}=50m/s

Droplet Shape Characterization



Shape Factor = max(Lx,Ly,Lz)/min(Lx,Ly,Lz)

Occupancy Factor = Volume/(Lx*Ly*Lz)



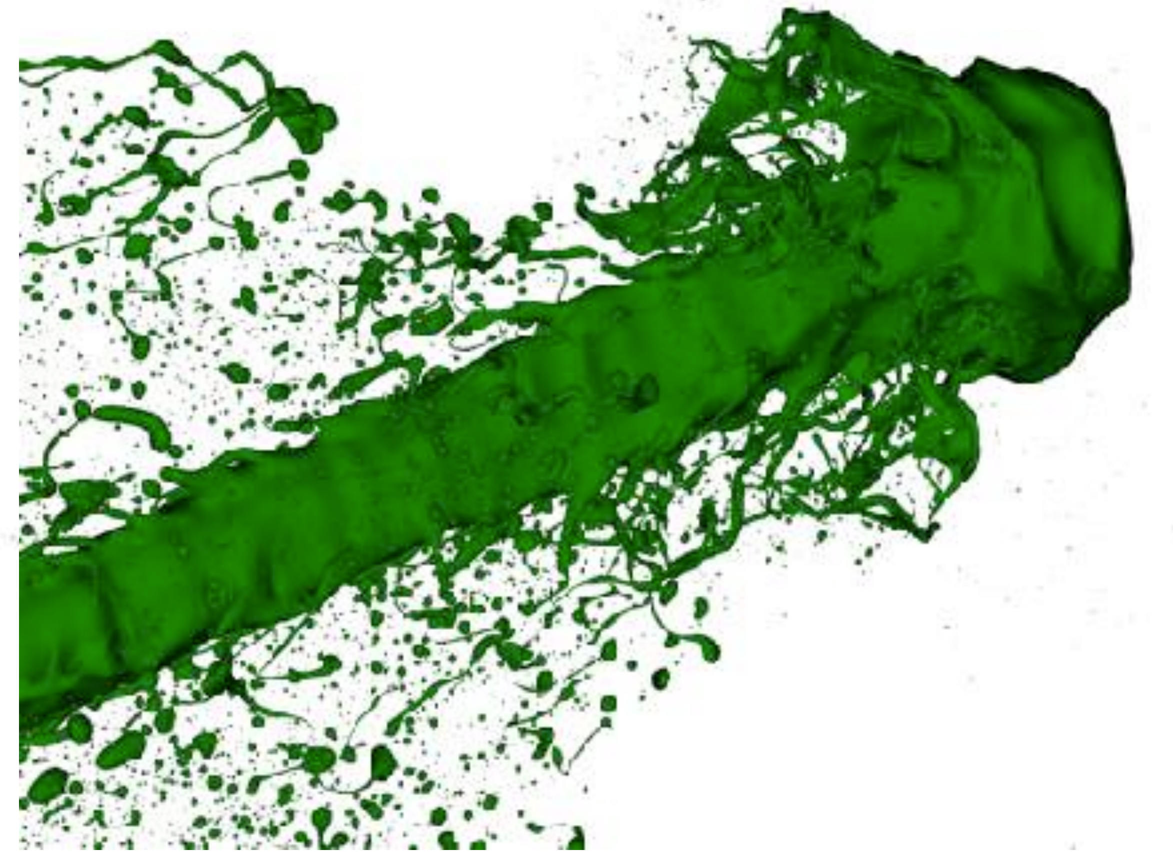
We need better methods to characterize topology!

Summary

- DNS of atomizing jets are performed for both diesel and biodiesel
- Sufficient mesh resolution is essential to capturing breakup physics and droplets statistics
- The most refined mesh yield converged PDF for droplets larger than 3 μm
- Majority of droplets are formed at mushroom head and hole dynamics play a critical role in sheet breakup
- The biodiesel jet produces less droplets but of larger size than diesel jet under the same injection conditions

Future Work

- Topology characterization & statistics
(Ligaments, holes, etc; efficient way to obtain topology & geometry information)
- More realistic injection condition
(Injection pressure > 1000 bar, U_{inj}>200m/s)
- Low fidelity averaging model
(but we need to get a statistically steady state first)
- Multi-physics
(Droplet evaporation, spray combustion, and more)



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Thank you!