PROGRESS IN THE SIMULATION OF LIQUID FUEL INJECTION

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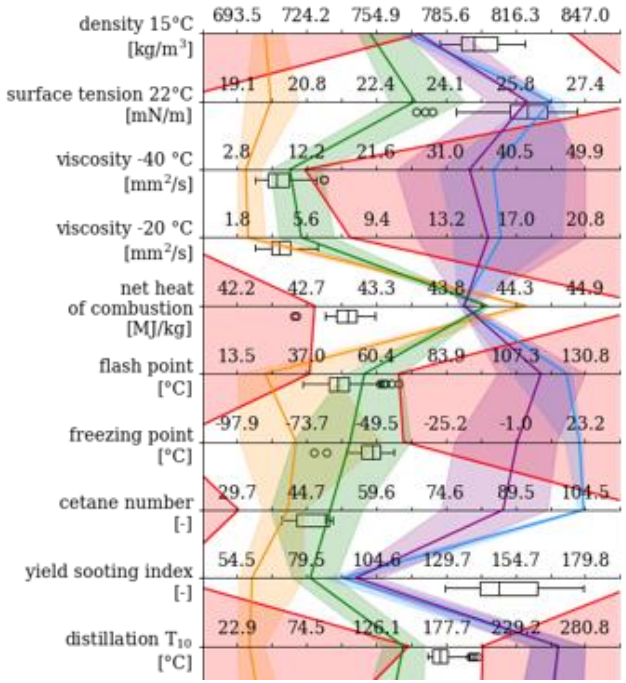
Basilisk (Gerris) User Meeting 2023

DLR

Multiphase Flow and Alternative Fuels Department

Evaluation of new sustainable fuels

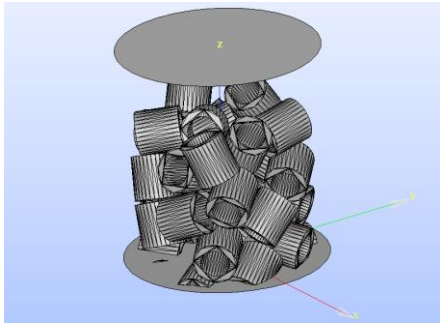
- SimFuel fuel database, physics-based and ML models to predict properties and behavior in combustion chambers.
- Prescreening, sustainable aviation fuels, blending, non-CO2 effects.

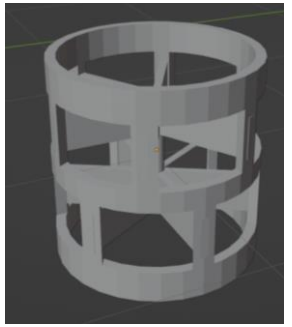


CFD of reacting multi-phase flows

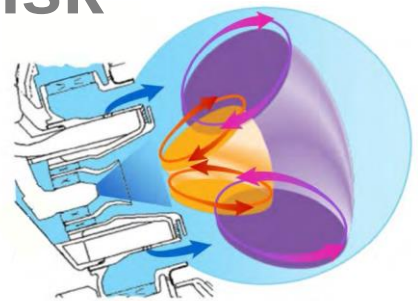
- Liquid phase: Lagrange solver SPRAYSIM, quasi-steady forces, multi-component discrete or distributions, equivalent species, evaporation, turbulent dispersion.
- Two-way coupling with weakly compressible gas phase code THETA, physico-chemical models for combustion, turbulence models, grid adaptation.
- **BASILISK for spray boundary conditions, „virtual injector“**

- Direct Air Capture





Atomisation of a liquid jet in crossflow with basilisk



DNS simulations with basilisk

Air flow $\boldsymbol{u_x = 100\ m/s}$, boundary layer of width $\delta = 2{,}5.10^{-3}\mathrm{m}$

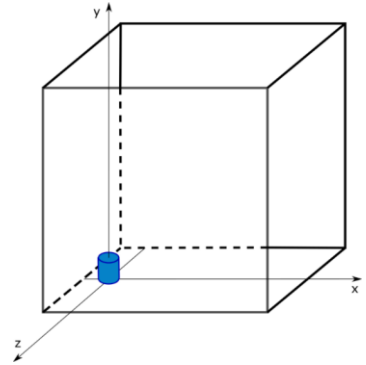
Liquid jet mean velocity $\boldsymbol{u_y = 22,99\ m/s}$, parabolic profile

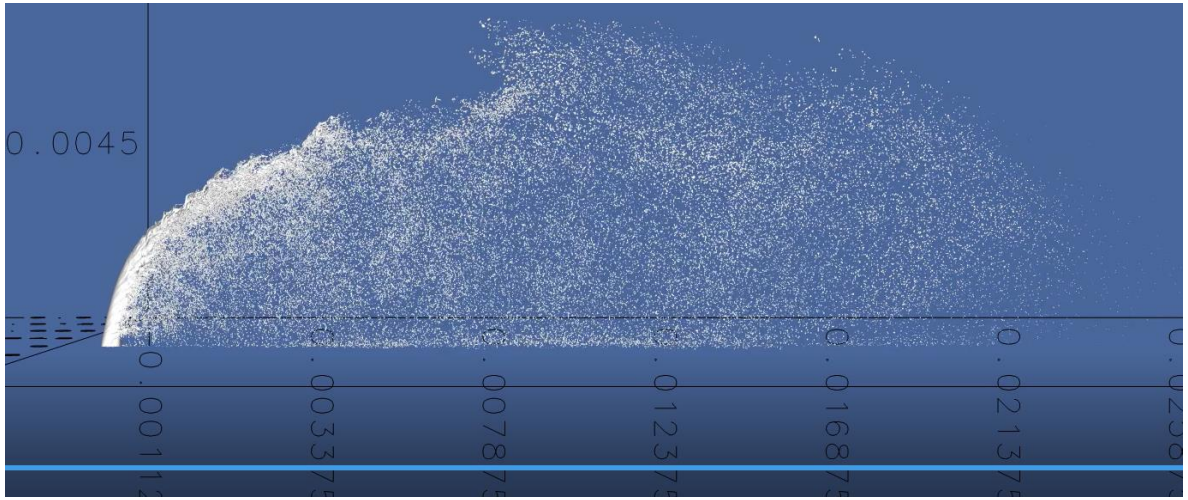
Ambient conditions $\boldsymbol{p_{air} = 5,8\ bar \quad T_{air} = 280\ K}$

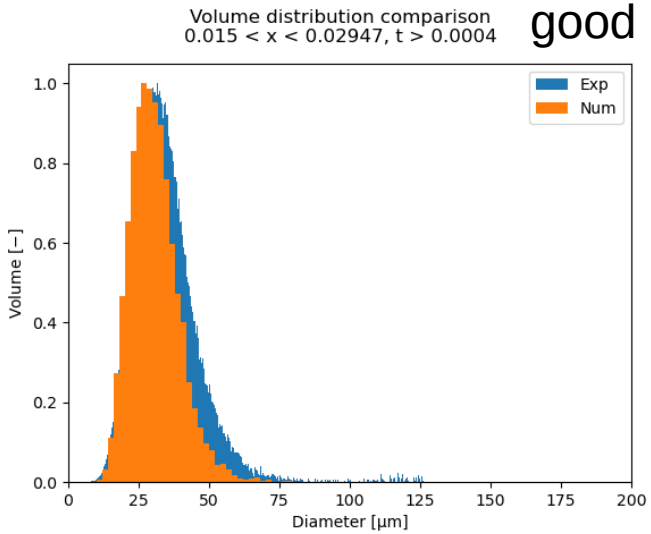
Orifice diameter $0{,}45mm$ = size of the initialized jet

Cubic domain size $0.036\ m$

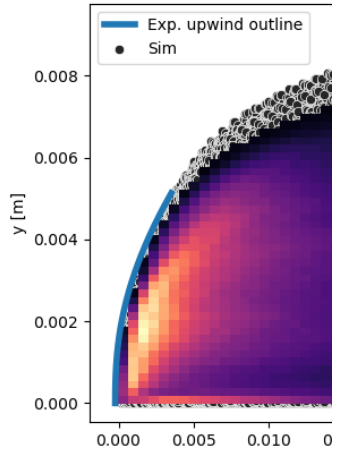
For 12 levels of refinement, the smallest cell size is $\boldsymbol{8,789\ \mu m}$







good match with experiments



Origine of the elements of the Lagrangian method

- X. Li, M. Arienti, M. C. Soteriou, M. M. Sussman, „Towards an efficient, high-fidelity methodology for liquid jet atomization computations“, AIAA 2010, coupled Level Set and VOF, AMR
  Criteria: sphericity, local concentration of resolved liquid phase

- G. Tomar, D. Fuster, S. Zaleski, S. Popinet, „Multiscale simulations of primary atomization“, Computers & Fluids 2010, **Gerris**
  Detailed consideration and validation of the forces acting on Lagrange droplets
  Momentum source term in the Navier-Stokes equation

- Y. Ling, S. Saleski, „Multi-scale simulation of primary breakup in gas-assisted atomization“, AIAA 2015, **Paris Simulator**
  Criteria: size, aspect ratio, proximity to VOF interface
  Estimation of the undisturbed flow velocity

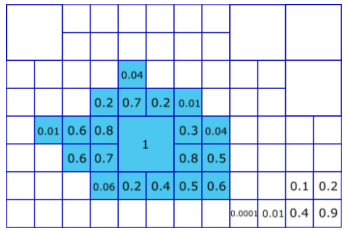
- **Antoon van Hooft‘s particle framework**: **create/add/remove particles, update particle list for MPI, dump/restore, iterators …**

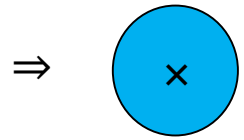
- **Spraysim: Lagrange particle solver at our institute, Lagrange time step, Cd(Re)**

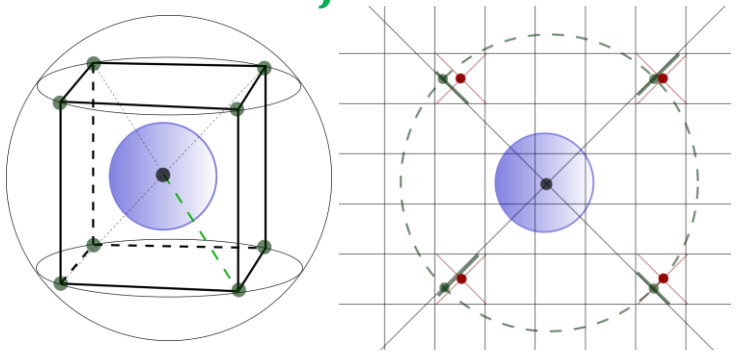
Simulation of a liquid jet in crossflow with basilisk

Basilisk DNS coupled with Lagrange solver

Identify liquid structures with tag function, transfer to spherical point-droplets in Lagrange solver, parameters $\boldsymbol{x_p}$, $\boldsymbol{u_p}$, d_p, undisturbed gas velocity $\boldsymbol{u_f}$ around the droplet







- Criteria:
  - aspect ratio < 2.5
  - diameter > 2 * smallest cell size
  - We < 12 so that transferred droplets do not break-up anymore
- Remove structure from DNS, reset gas velocity in region around particle position.
- Lagrange particle back to DNS? Yes, if **too near to interface**, in **recirculation area -> basilisk functions refine and fraction (not for We>12)**

Simulation of a liquid jet in crossflow with basilisk

Basilisk DNS coupled with Lagrange solver

- **Equation of motion**: only quasi steady force for spherical particles – different intervals for $\boldsymbol{c_d}(Re_p)$ correlations, relaxation time τ, velocity of gas phase $\boldsymbol{u_f}$ (interpolated at particle position)

$$\frac{d\boldsymbol{x_p}}{dt} = \boldsymbol{u_p} \qquad \frac{d\boldsymbol{u_p}}{dt} = \frac{\boldsymbol{u_f}-\boldsymbol{u_p}}{\tau} + \left(1 - \frac{\rho_g}{\rho_l}\right)\boldsymbol{g}$$

$$\tau = \frac{4 d_p \rho_l}{3\rho_g \boldsymbol{c_d}(Re_p)\|\boldsymbol{u_f}-\boldsymbol{u_p}\|} \qquad Re_p = \frac{d_p \rho_g \|\boldsymbol{u_f}-\boldsymbol{u_p}\|}{\mu_g}$$

⇒ Time discretisation: explicit or iterative calculation of relaxation time with mean particle velocity.

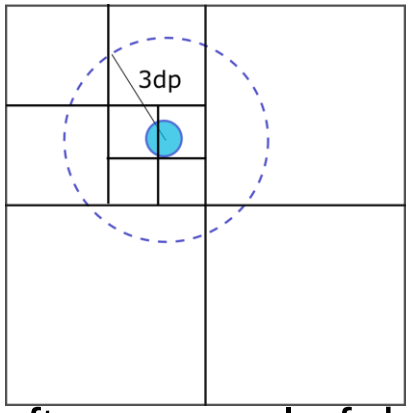
- **Lagrange time step: $\boldsymbol{5.10^{-6}s}$,** so no time discretisation issues

Simulation of a liquid jet in crossflow with basilisk

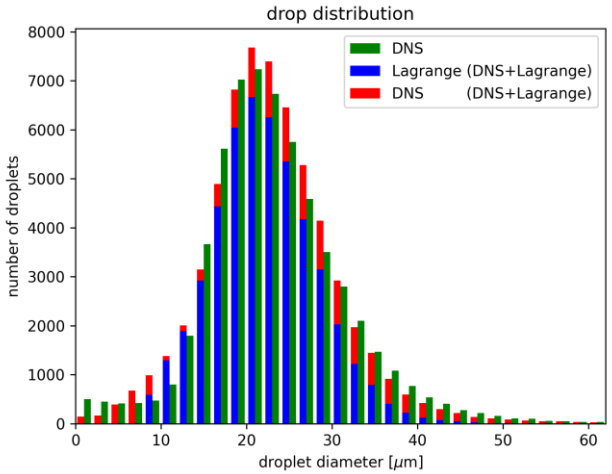
Basilisk DNS coupled with Lagrange solver

- Parallelisation issues:
  determine big region around droplet where MPI exchange is needed

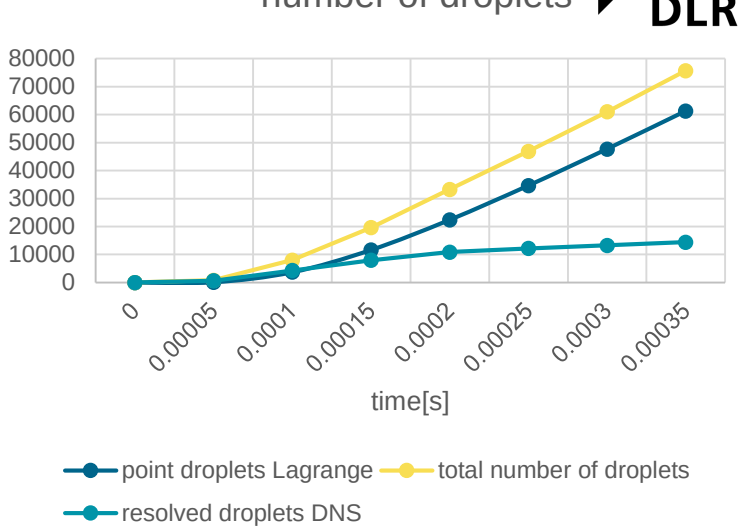
  (see Tomar, Gerris)

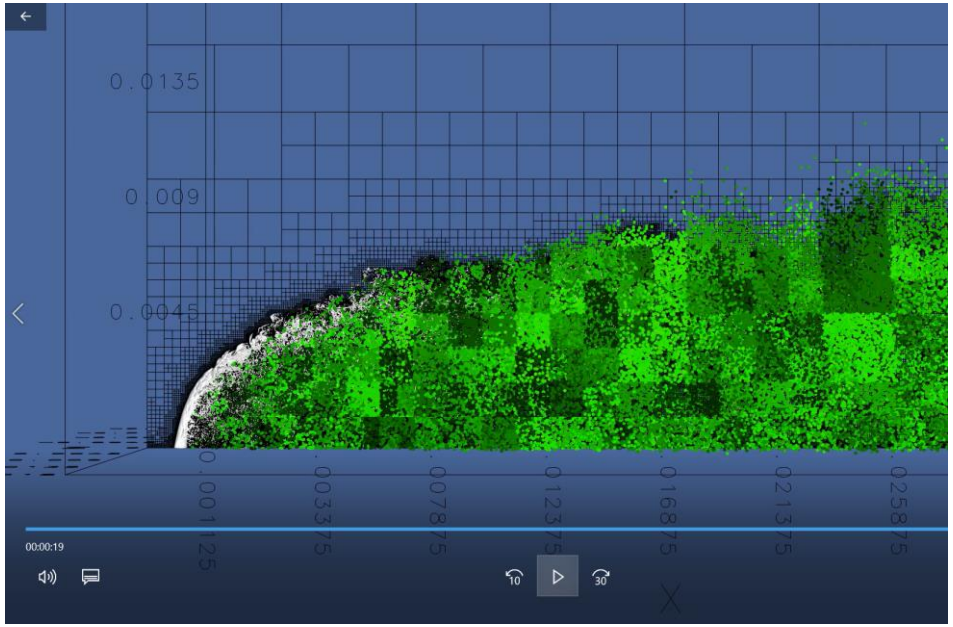


- Used to:
  reset gas velocity after removal of droplet
  add **momentum source** to acceleration in DNS
  (distribution evaluated up to distance $3d_p$)
  evaluate **proximity to interface** with volume fraction in the „big region“
- Maximum level of refinement for velocities: 10



Droplet distributions for $t = 0{,}0003\ s$

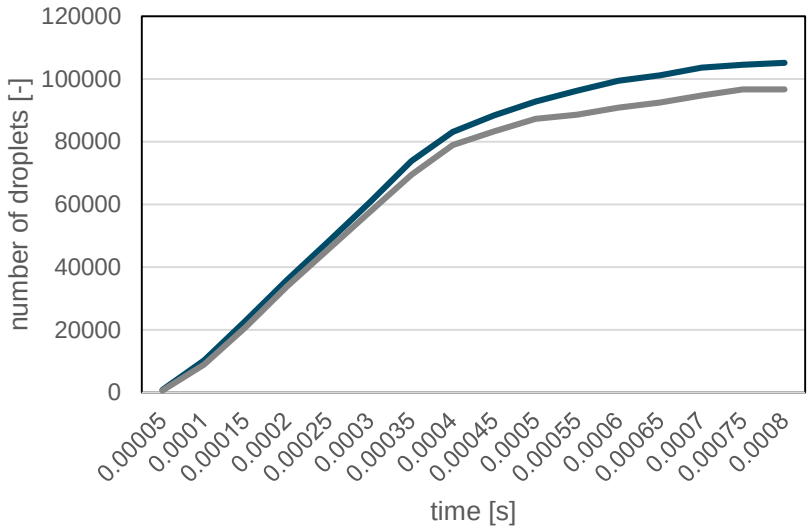




Atomisation of a liquid jet in crossflow with basilisk

compare jet A1/HEFA fuels, fuel sensitivity

- Maximum level of refinement 12, minimum cell size 8,9 µm
- Final time at stationarity 0,85 ms, 16 d computation on 1152 cores.



Jet A1

$\rho_l = 789\ kg\ m^{-3}$

$\boldsymbol{\mu_l = 1,42.10^{-3} kg\ m^{-1}\ s^{-1}}$

$\sigma = 2{,}57.10^{-2}\ N\ m^{-1}$

$\boldsymbol{SMD(correlations) = 3,0.10^{-5} m}$

HEFA

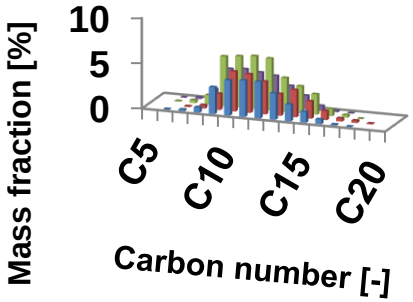
$\rho_l = 783\ kg\ m^{-3}$

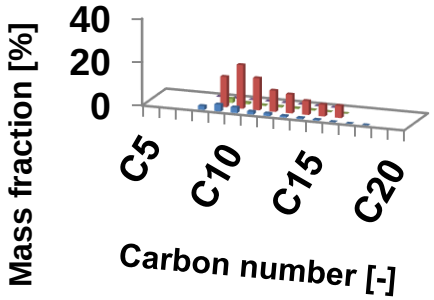
$\boldsymbol{\mu_l = 2,67.10^{-3} kg\ m^{-1}\ s^{-1}}$

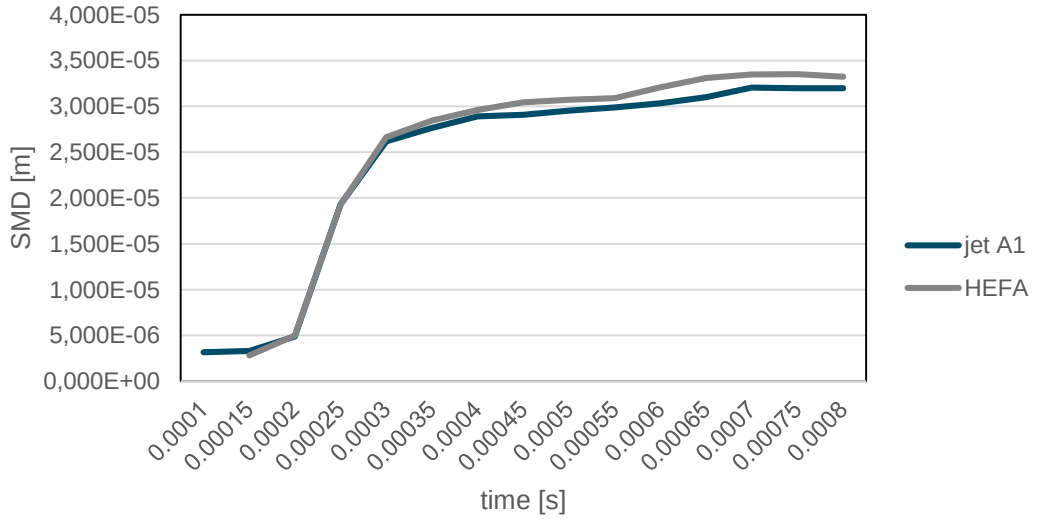
$\sigma = 2{,}53.10^{-2}\ N\ m^{-1}$

$\boldsymbol{SMD(correlations) = 3,5.10^{-5} m}$

$N\ m^{-1}$





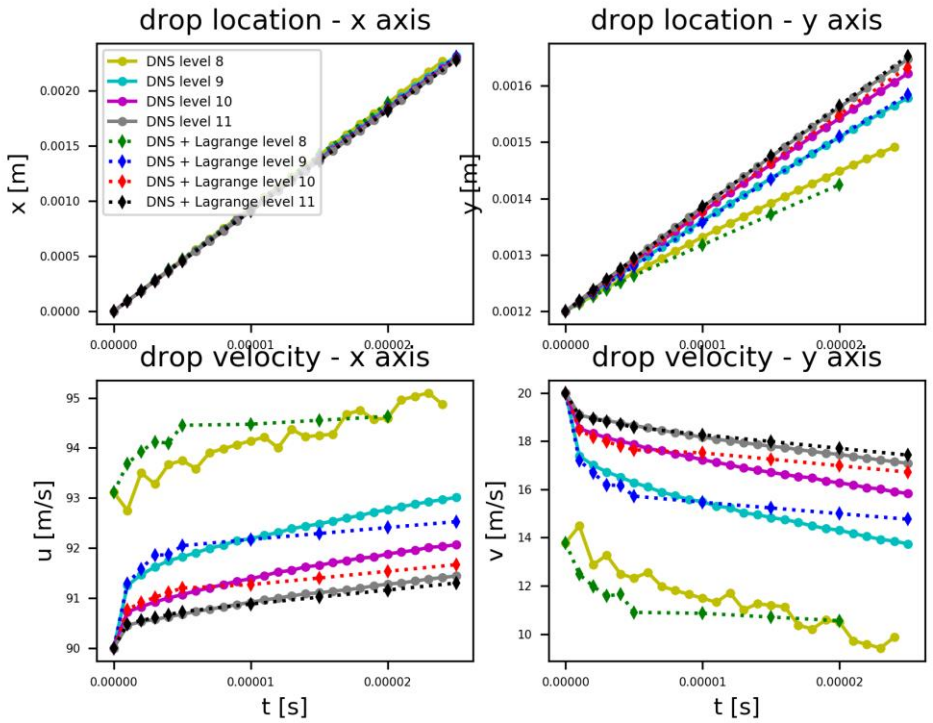


n-alkanes iso-alkanes cyclo-alkanes aromatics

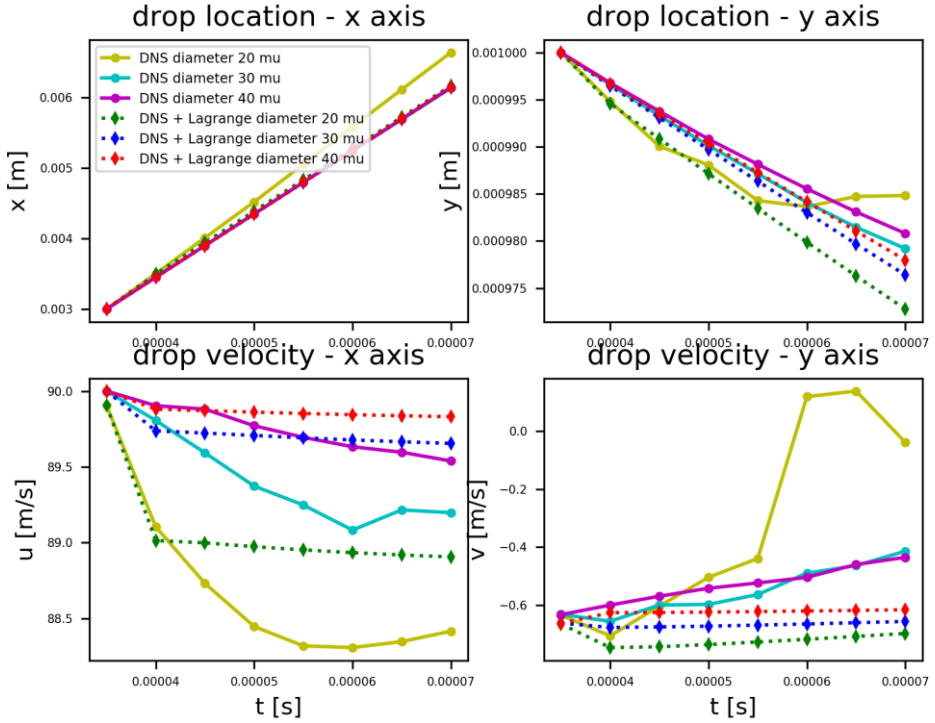
Simulation of a liquid jet in crossflow with basilisk

Validation of the Lagrange solver

- Single drop $30\mu m$ in air flow for different resolutions



- Single drop downstream of the liquid jet of different sizes

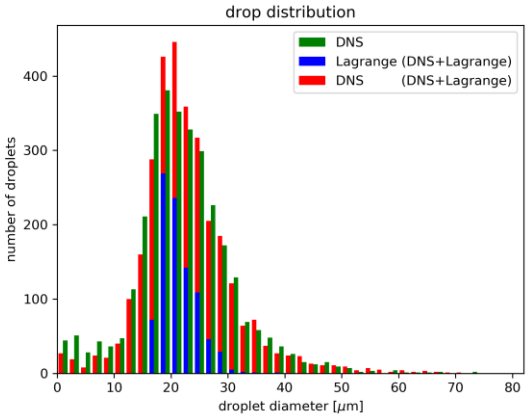


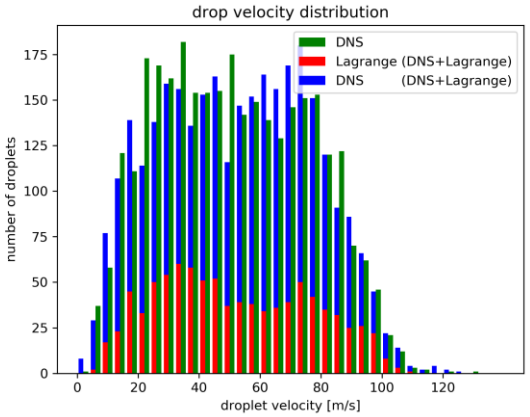
Simulation of a liquid jet in crossflow with basilisk

Validation of the Lagrange solver

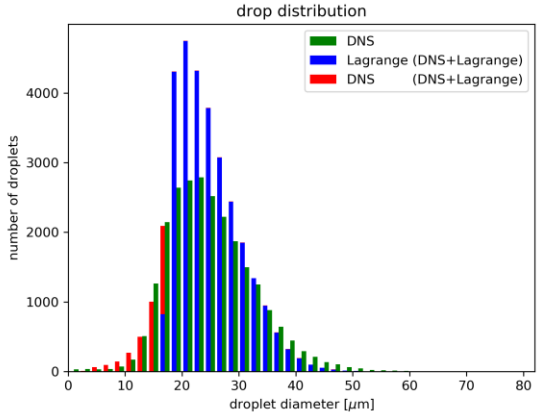
- Compare distributions for DNS alone and coupled with Lagrange near and far from jet injection for $t = 0{,}85\ ms$

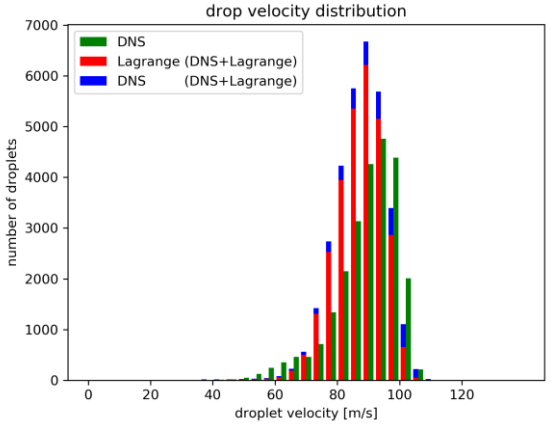
0.002 < x < 0.003





0.02 < x < 0.03

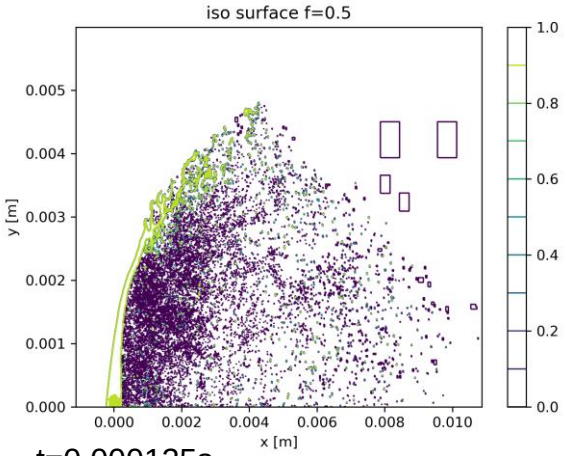




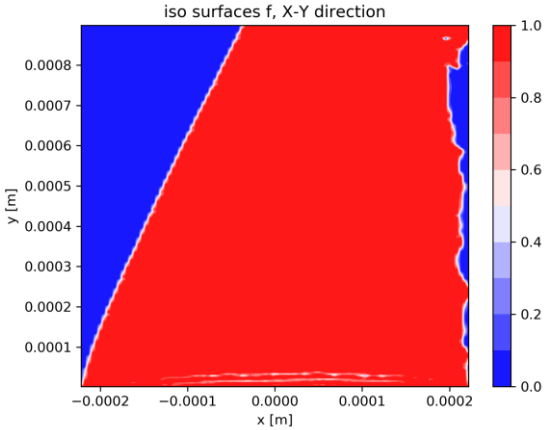
Atomisation of a liquid jet in crossflow with basilisk

compare jet A1/HEFA fuels, fuel sensitivity

- Half computation domain at same maximum level of refinement: **inclusion of gas phase**

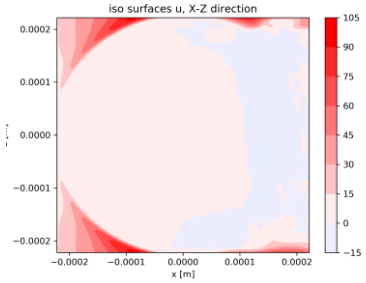


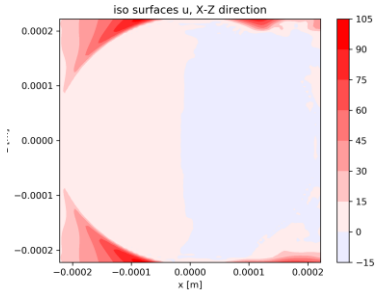
t=0.000125s



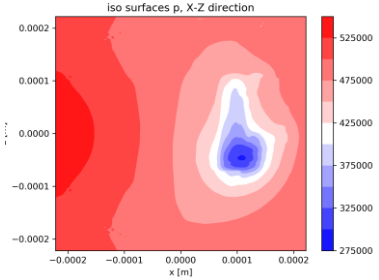
t=0.000122s

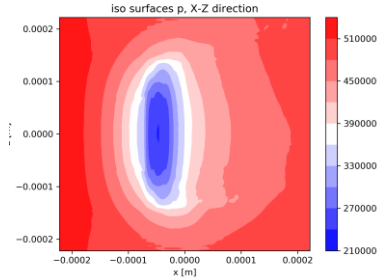
velocity u





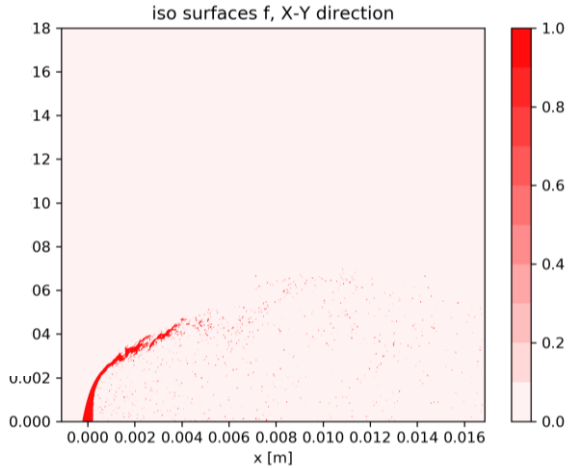
pressure



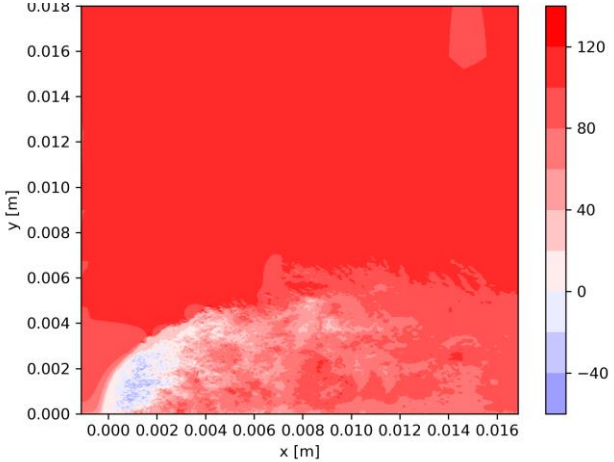


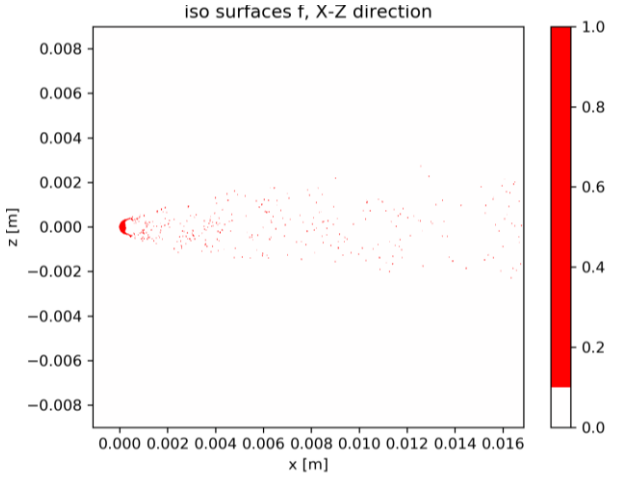
Refine more, smaller computation domain

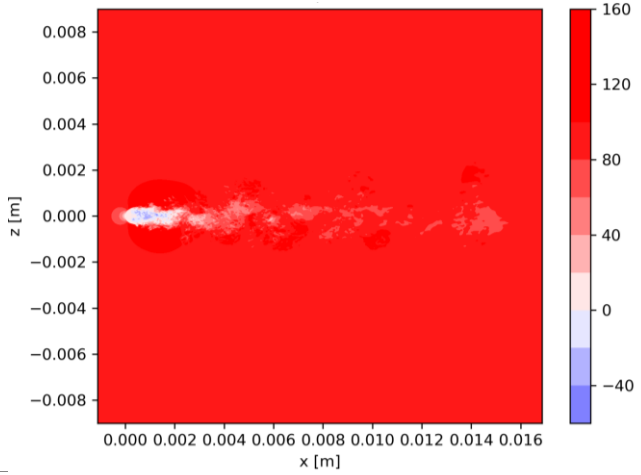
- Determine backflow region with simulations in big domain, length 0,036 m.



Iso surface u



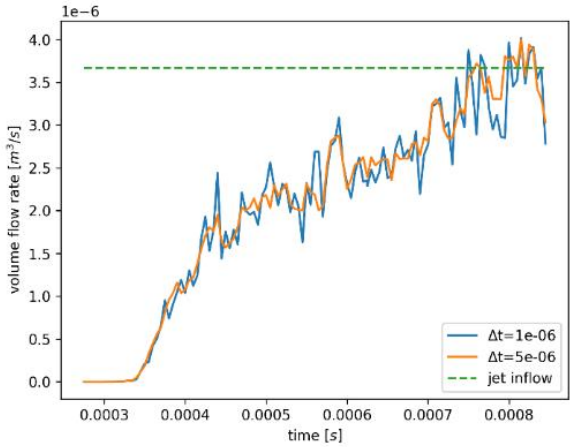




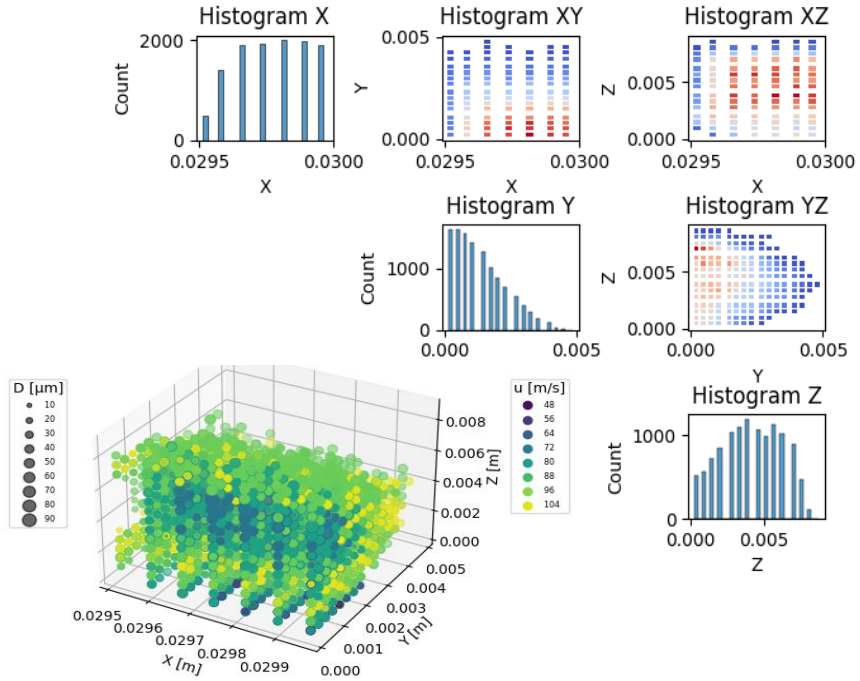
Simulation of a liquid jet in crossflow with basilisk

Coupling basilisk DNS with theta/spraysim: very first step

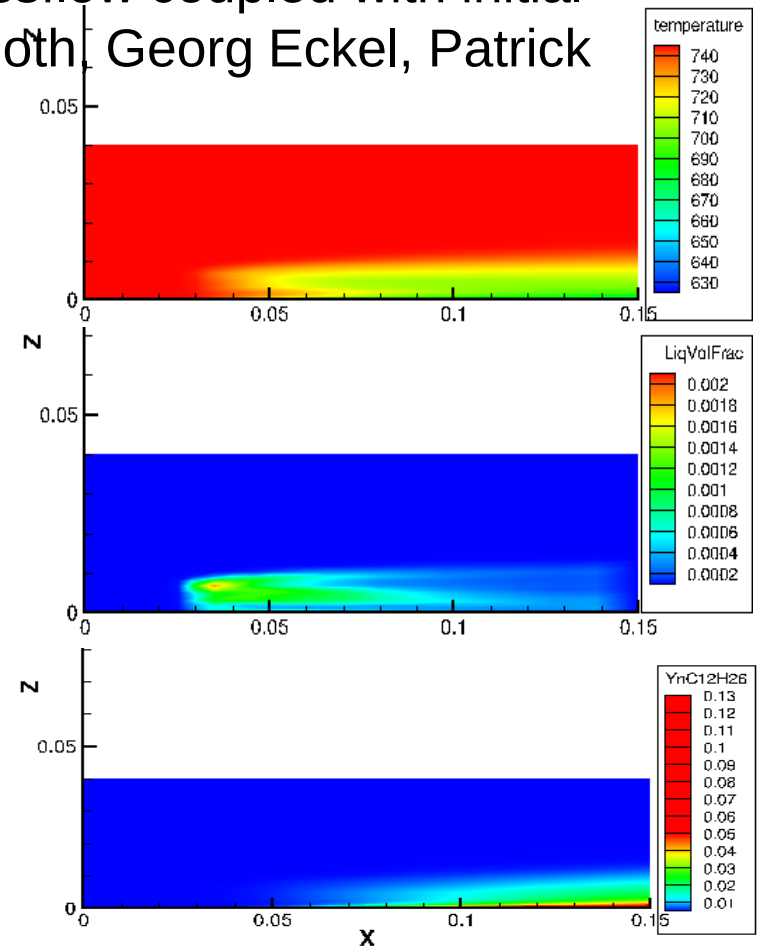
ILASS 2023 conference: Lagrangian simulations of a liquid jet in crossflow coupled with initial spray conditions from Direct Numerical Simulations, Corine Kieffer-Roth, Georg Eckel, Patrick Le Clercq.



Volume flow rate from the droplets with velocity high enough to cross the plane located at $x = 0.03\,m$ during a given time slot Δt.



Collect all the droplets able to cross $x = 0.03\,m$ for 12 last Lagrange time steps. Compute distributions, droplets in the defined intervals (position and velocity components, diameter) are the parcels for spraysim.



Steady simulations with theta/spraysim, wall temperature 750 K

Simulation of a pressure swirl atomizer with basilisk

- Embedded boundaries for the injector geometry, coupled with Lagrange solver.

STL file with triangles at injector surface from CAD

„distance“ function, works only in serial

Centered distance field to triangles, mesh adapted until threshold error is reached

interpolation

distance field at vertices Φ

„fraction“ function

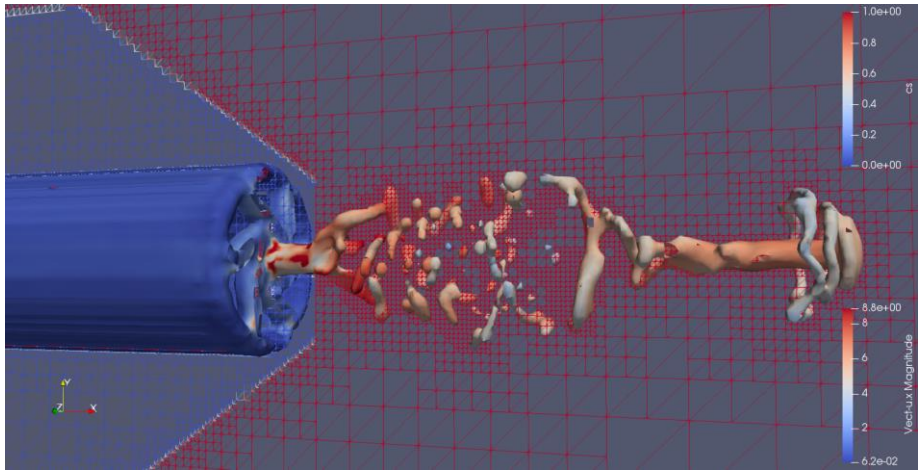
Volume fraction solid phase c_s describing the injector

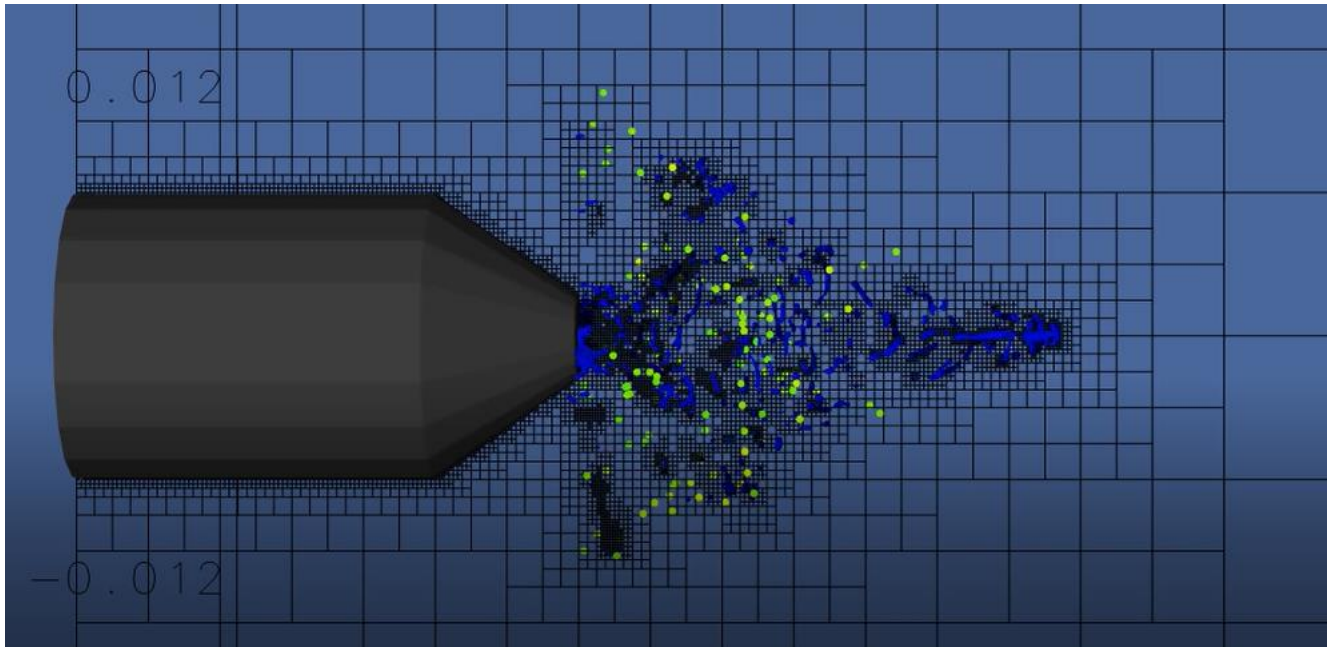
In parallel, restart from Φ, stored separately, as vertex fields cannot be dumped

Vertex indices and Φ stored for the serial run, test with „is_vertex“ and assign Φ for restart in parallel

⇒ works fine for free slip boundary conditions (neumann, all derivatives 0) and serial

$u_{in} = 0{,}5\ m/s,\ p_{out} = 1\ bar$





Thank you for your attention!