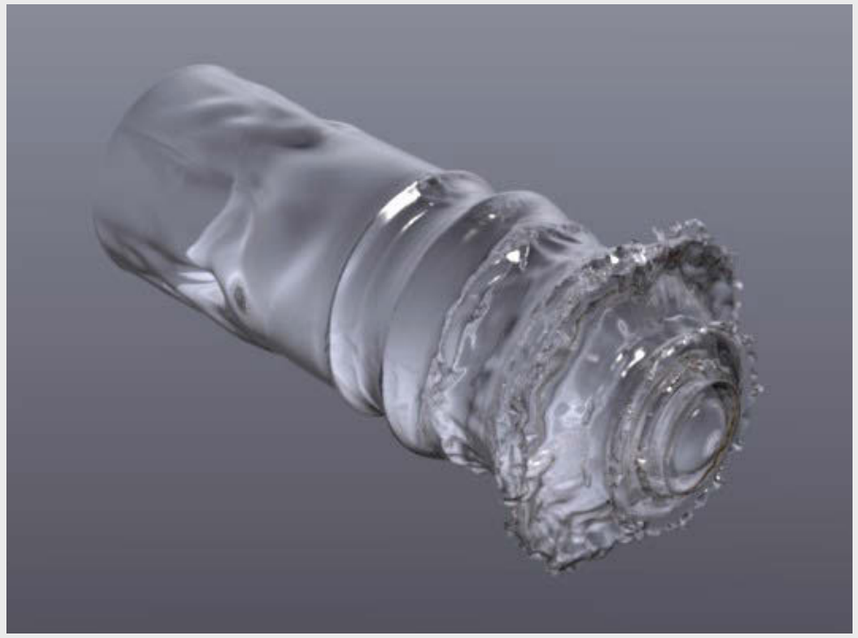
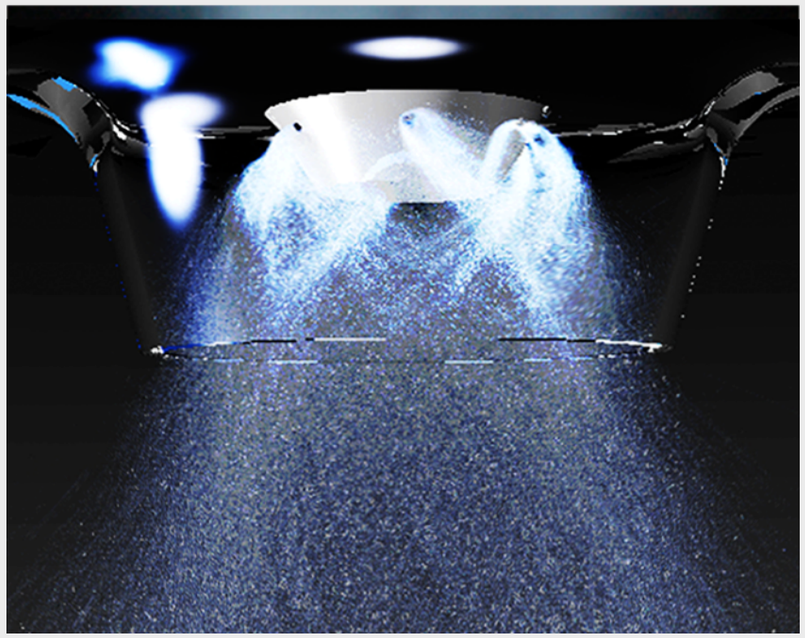
High Fidelity Simulations of Liquid Fuel Atomization in Internal Combustion Engines and Complex Gas Turbine Injectors





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Motivation

- Fuel is typically injected as a liquid
- Combustion occurs only in the gas phase

  ⇒ atomize liquid to enhance evaporation

- Atomization process controls combustion:
  - local mixture composition ⇒ pollutant formation
  - combustion stability
  - turbulence generation

⇒ to optimize combustion, one needs to optimize the liquid fuel atomization

- However, fuel spray characterization as used in traditional CFD is highly calibrated, and thus not predictive

Motivation

- **Many details of liquid atomization in applications are still unknown**
  - experimental access is difficult or often impossible
  - even with optical access, spray drops obscure the atomization process
  - some new experimental techniques:
    - ballistic imaging (time gating photons)
    - phase contrast X-ray (Advanced Photon Source @ Argonne National Lab)

Diesel Spray (Helsinki University)

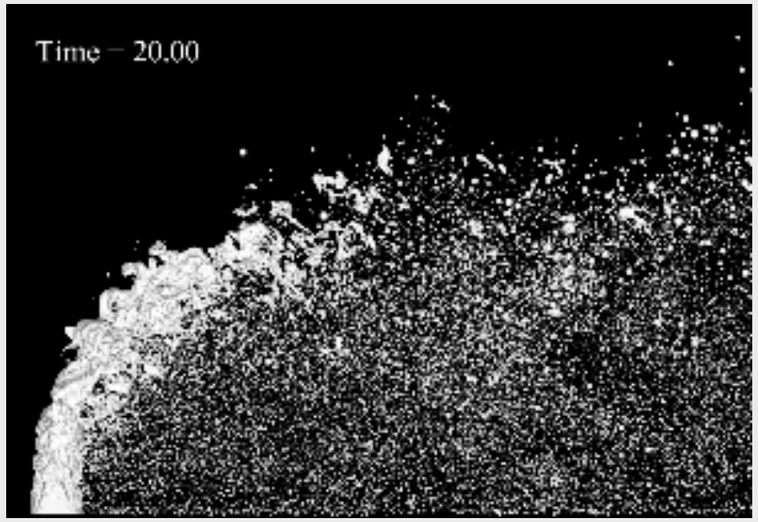
Diesel Spray (Spiekermann et al., 2007)

- **Can we use simulations (CFD) to study and predict atomization?**
  - need governing equations describing the flow $\Longrightarrow$ Navier-Stokes (continuum limit)
  - need numerical techniques to solve the governing equations
  - need computers to apply the numerical techniques and find solutions

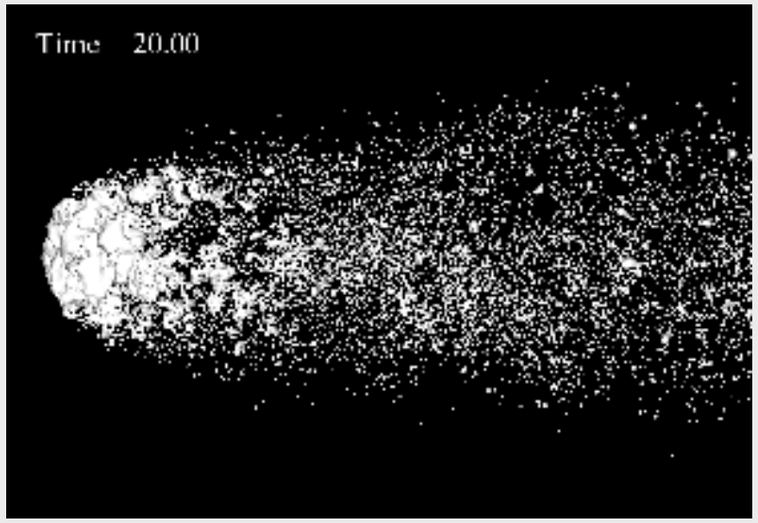
- **Goal: CFD as a first principle, predictive discovery tool**
  $\Longrightarrow$ no tuning parameters!

Motivation

- **Numerical Challenges for First Principle Predictive Simulations**
  - discontinuous material properties
  - singular surface tension forces
  - complex phase interface geometry
  - frequent topology changes
  - interaction with turbulence
  - inherently three dimensional
  - vast range of scales: from cm to μm ⇒ multi-scale

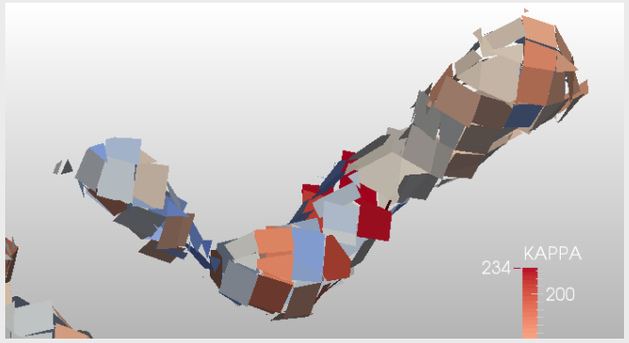


- **Multi-Scale Simulation Approach**
  - split atomization into primary & secondary atomization
  - track the complex phase interface geometry during primary breakup ⟹ resolve all scales
  - assume simple phase interface geometry for secondary breakup and use Lagrangian spray models
  - couple both



Primary Breakup Phase Interface Treatment

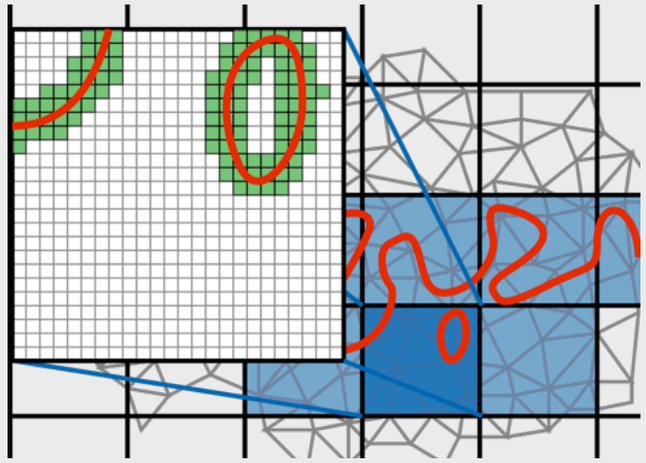
- Resolve interface dynamics during primary atomization
- Capture the phase interface by



- Volume of Fluid

- un-split geometric transport with PLIC interface reconstruction
  - arbitrary unstructured meshes
  - fully conservative and bounded

OR



- Level Set

- overset high resolution meshes (Refined Level Set Grid method)
  - high-order finite difference
  - non-conservative
  - resolved interface scale independent of resolved flow scale
  - unstructured flow solver meshes

- Topology changes occur automatically
  - inherent breakup length scale ~ grid size
- Hypothesis:
  - local flow mesh resolution sufficient so topology change initiation is physics driven
  - interface mesh resolution sufficient so numerical breakup doesn't impact resulting drop sizes

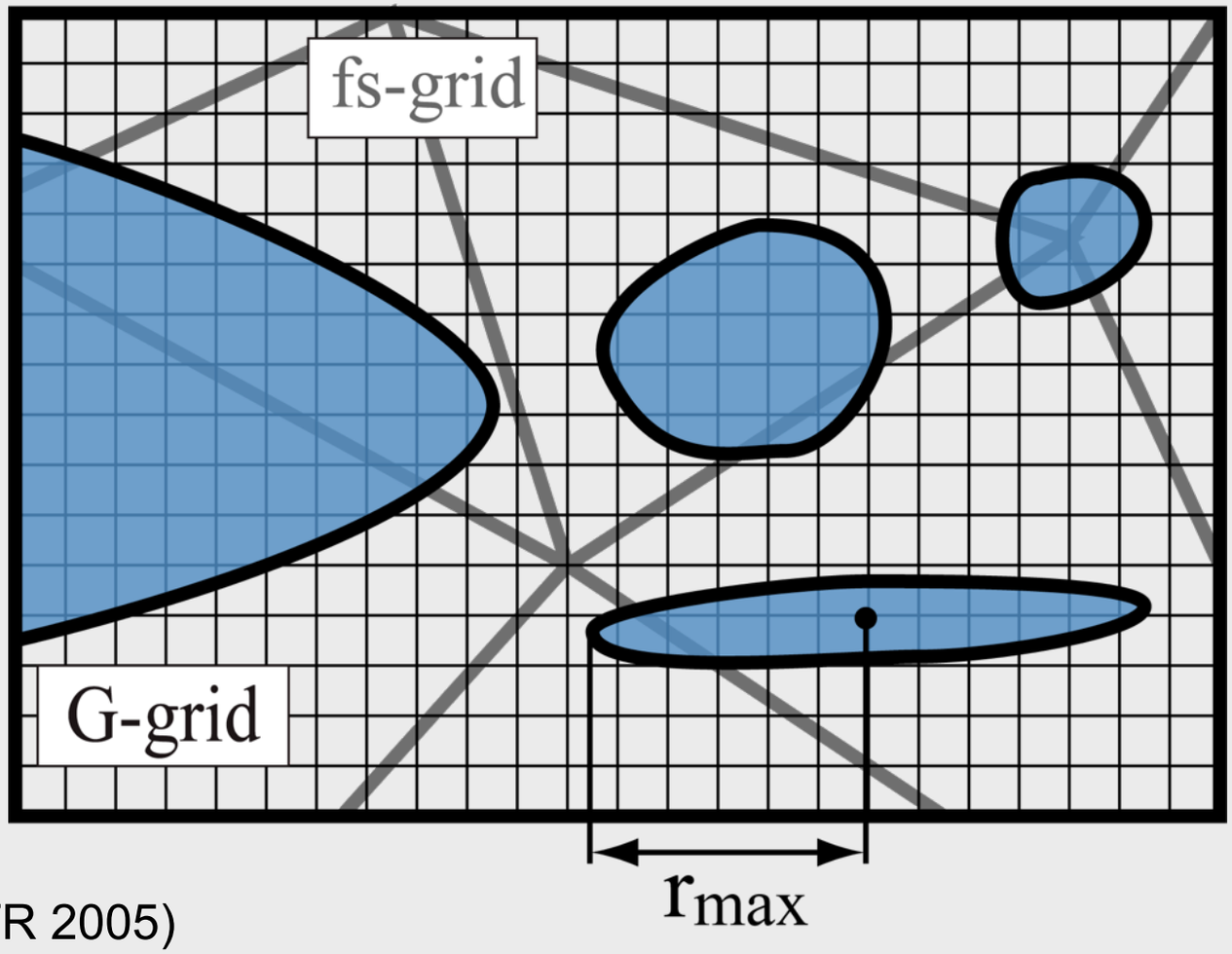
➡ But: Due to range of scales in primary atomization, one never resolves all the scales one would like ⇒ notoriously under-resolved

Secondary Breakup & Small Drops

- Small drop flow physics typically not resolved by local flow solver mesh
- Lagrangian approach more appropriate
  - full two-way coupling of momentum based on drag laws
    - assumes simple shape: spheres
    - point particle approximation: drop volume << cell volume
  - stochastic secondary atomization model (Apte et al. 2003)
- Requires coupling procedure = Drop transfer algorithm

Drop Transfer

- Identify all separated liquid structures with
  - $V_D < \alpha \Delta V_{\text{fs}}$
  - $r_{max} < \beta \left(\frac{3}{4\pi} V_D \right)^{1/3}$
- Insert into Lagrangian spray model preserving position, mass, and momentum



(for details see JCP, 229, pp. 745–759, 2010 & CTR 2005)

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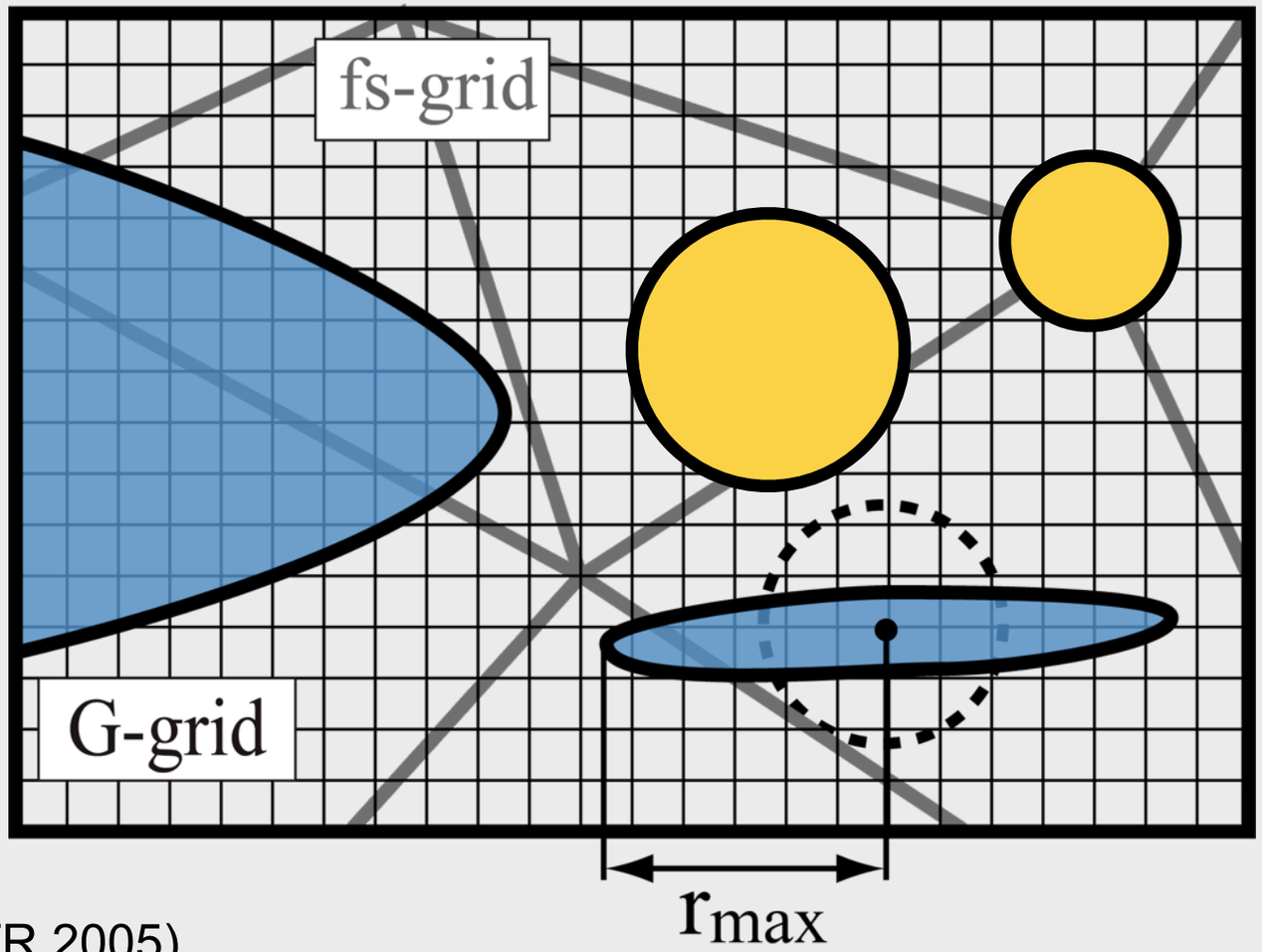

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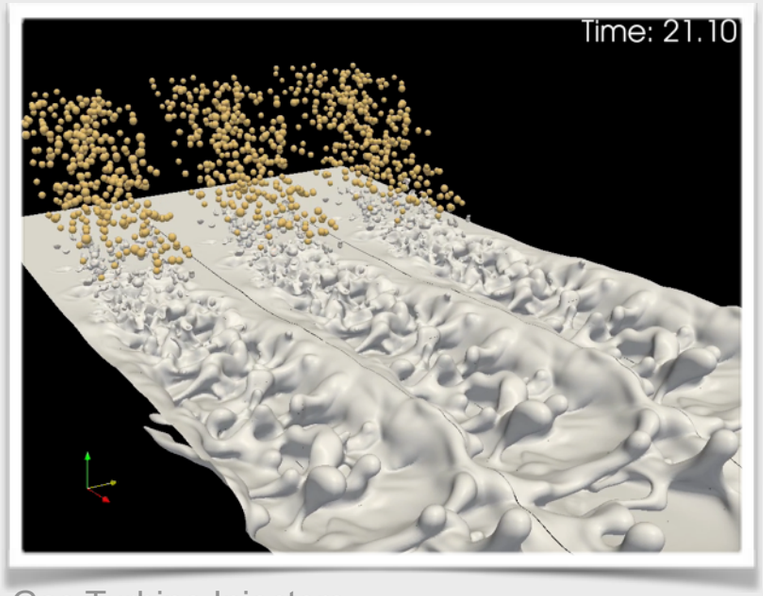
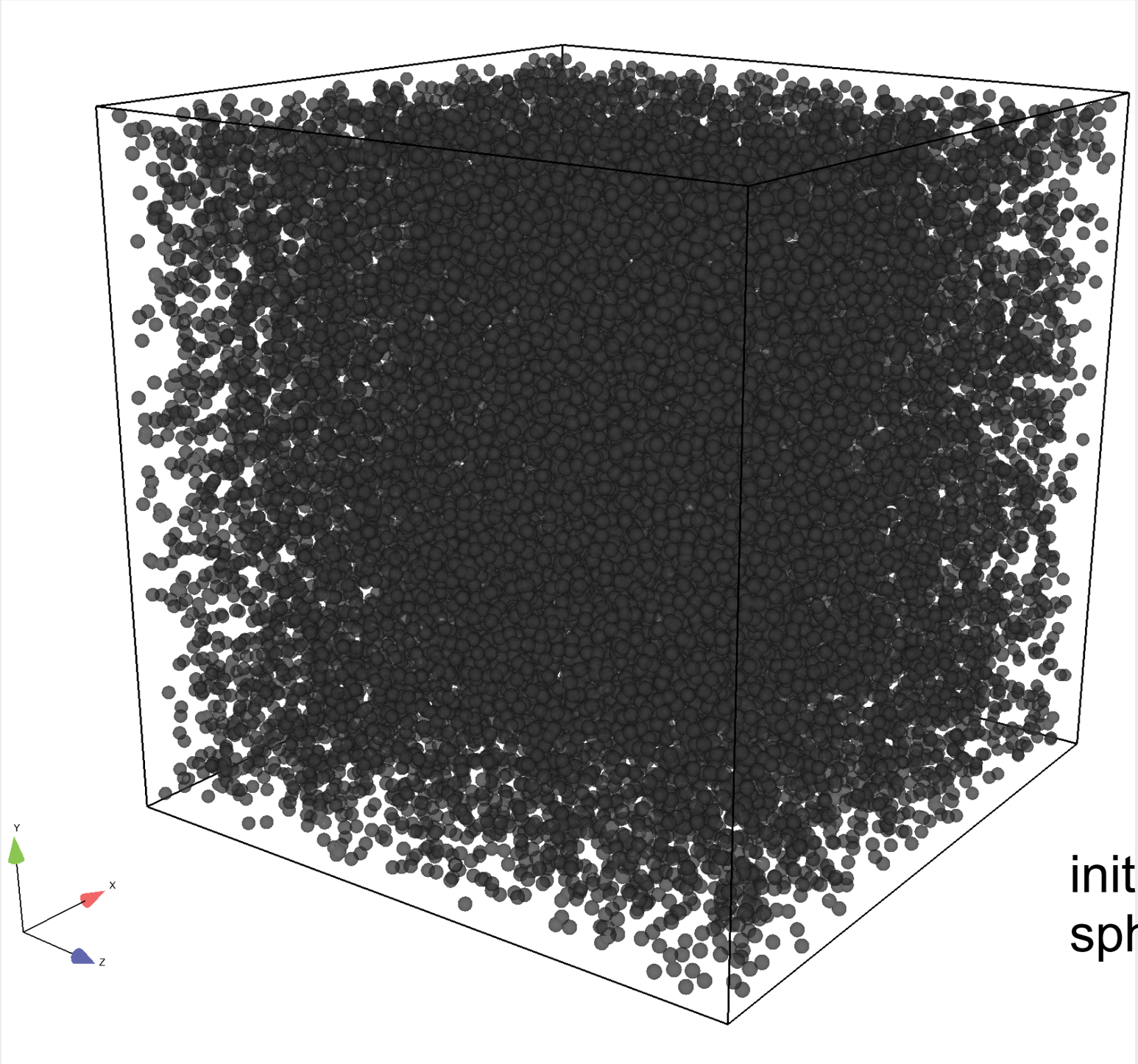
- re-transfer from Lagrangian to Eulerian interface capturing if necessary



Parallel Drop Transfer Algorithm

- Example: 25,000 randomly placed, mono-disperse spheres
- grid size: 2048 x 2048 x 2048



initially seeded spheres

Parallel Drop Transfer Algorithm

- Example: 25,000 randomly placed, mono-disperse spheres
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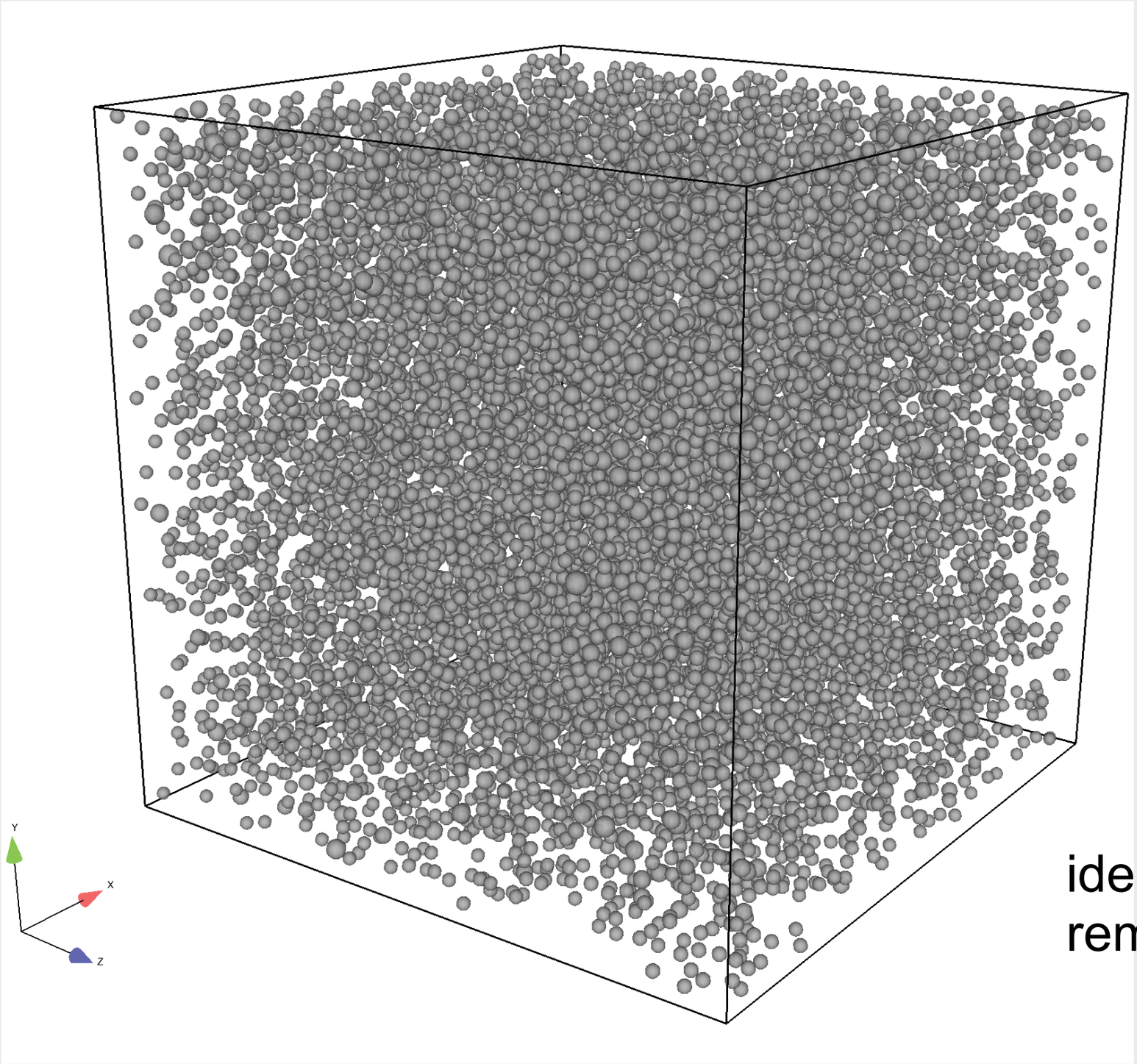

identified & removed drops

Parallel Drop Transfer Algorithm

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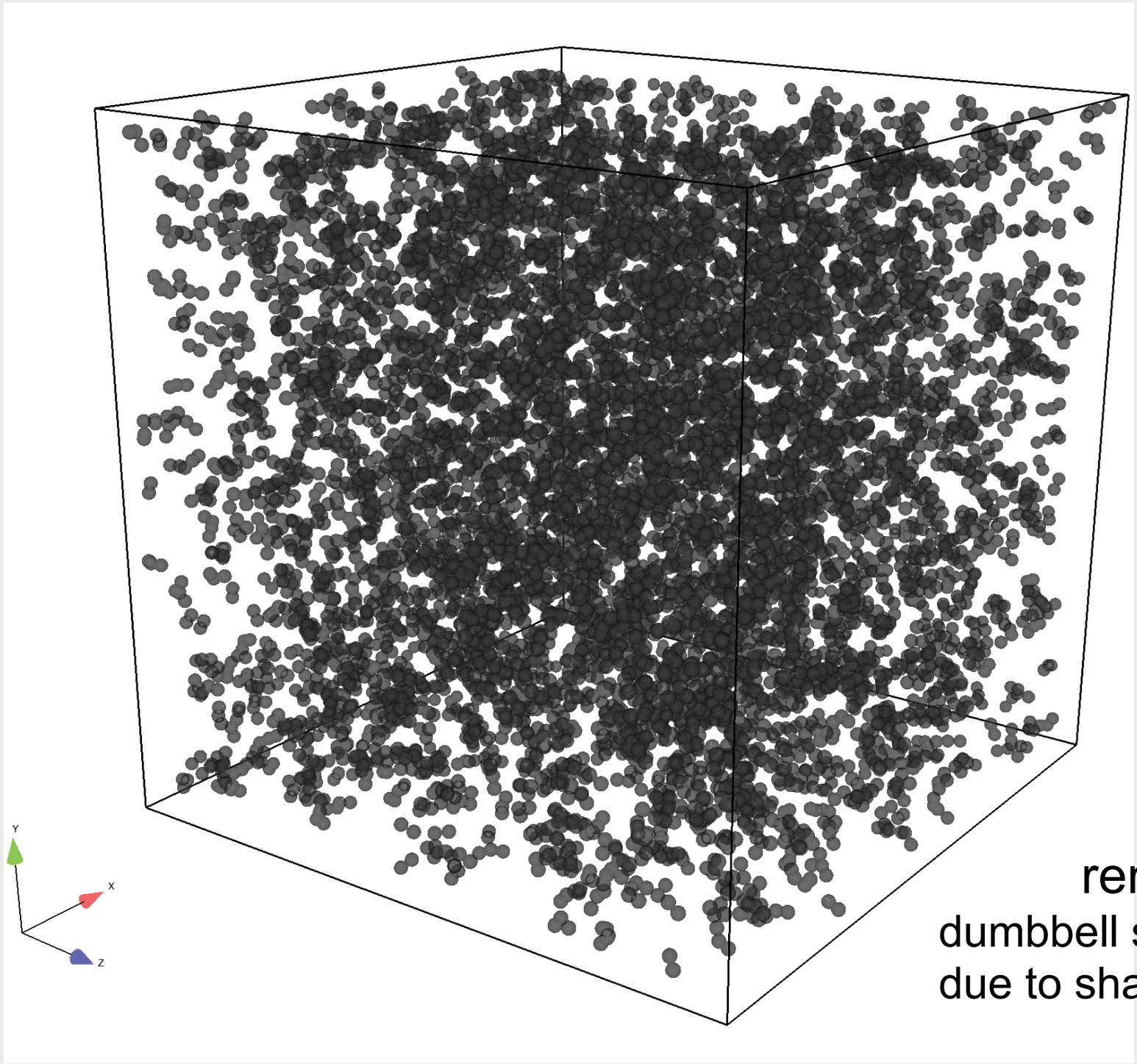
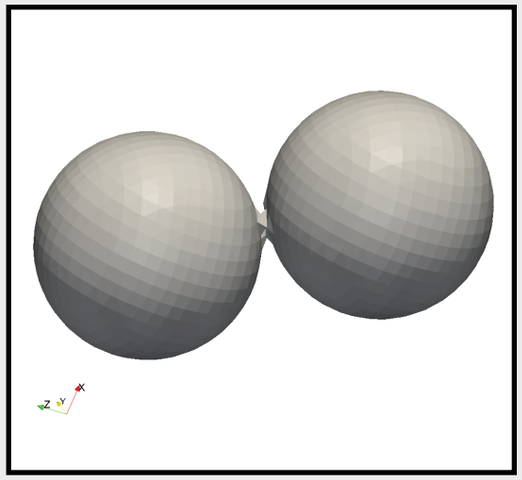
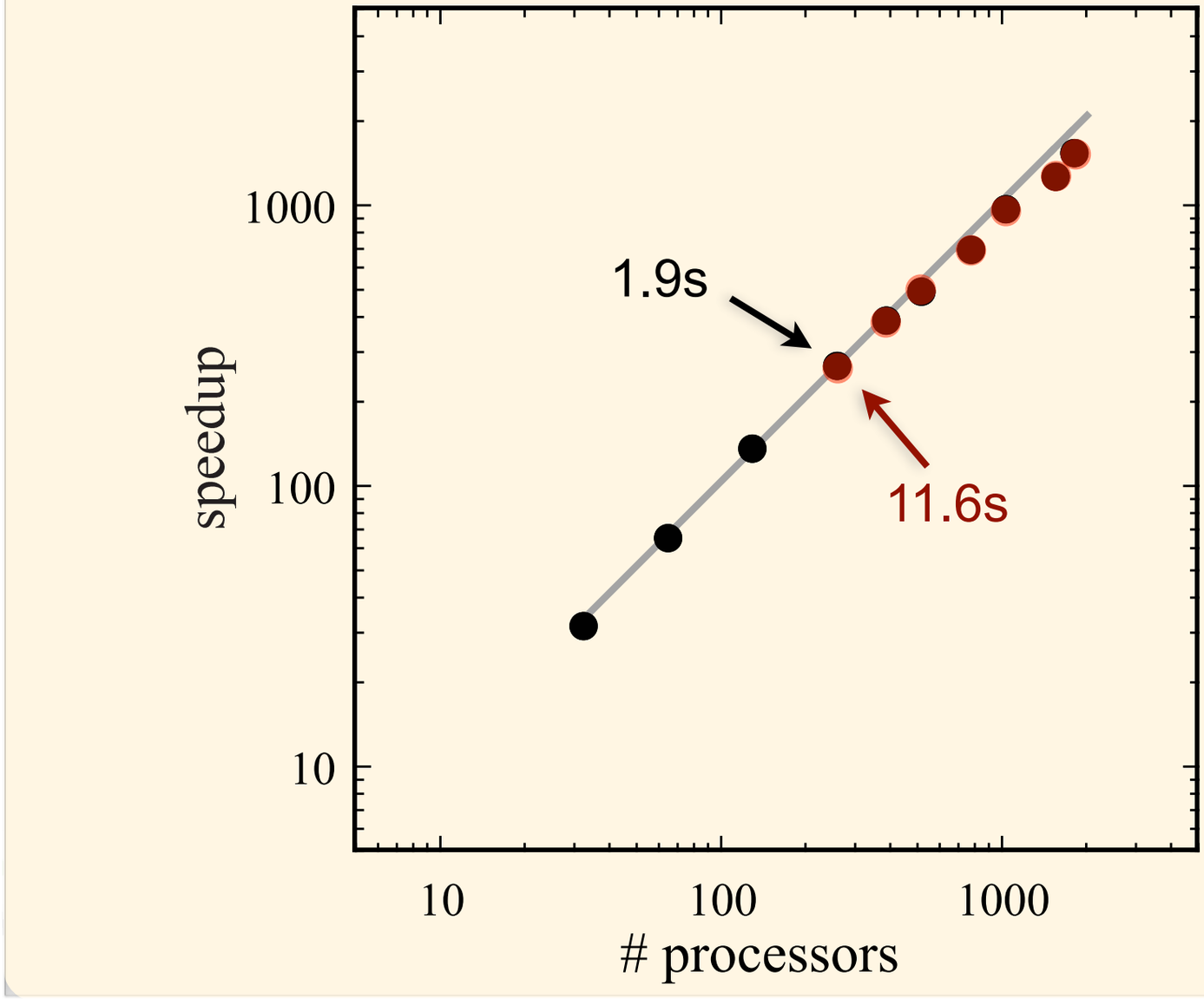




remaining drops:
dumbbell structures rejected due to shape criterium

Parallel Drop Transfer Algorithm

- Example: 25,000 randomly placed, mono-disperse spheres
- grid size: 1024 x 1024 x 1024 & 2048 x 2048 x 2048



ng drops:
res rejected
terium

Governing Equations

- Navier-Stokes equations for two-phase, incompressible flows in non-conservative form:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot \mu \nabla \boldsymbol{u} + \boldsymbol{g} + \frac{1}{\rho}\boldsymbol{T}_\sigma$$

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

$\boldsymbol{T}_\sigma$: surface tension force

- For finite volume Navier-Stokes solver control volume *cv*:

$$\rho_{cv} = \psi_{cv}\rho_l + (1 - \psi_{cv})\,\rho_g$$

$$\mu_{cv} = \psi_{cv}\mu_l + (1 - \psi_{cv})\,\mu_g$$

$\rho_l,\ \mu_l$: liquid density, viscosity

$\rho_g,\ \mu_g$: gas density, viscosity

- Surface tension force $\boldsymbol{T}_\sigma$ by Continuum Surface Force (CSF): [Brackbill et al. 92]

$$\boldsymbol{T}_\sigma = \sigma\kappa\delta\boldsymbol{n} = \sigma\kappa\frac{\nabla c}{[[c]]}$$

σ : surface tension coeff.

κ : surface mean curvature

c : marker function

G : level set scalar

ψ : volume fraction

Balanced Force Method

$$\mathbf{T}_\sigma = \sigma\rho_c\left(\frac{\kappa_{c\to f}}{\rho_{c\to f}}\nabla\psi(G)\right)_{f\to c}$$

(see M. Francois et al. 2006)

Flow Solver

- Results from two different flow solvers

- **NGA** ***(Desjardins et al. 2008)***

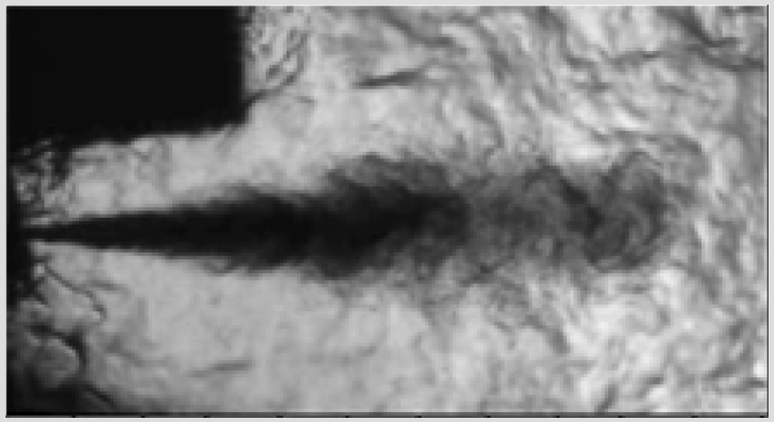
  - structured Cartesian or cylindrical
  - 2nd order finite volume
  - discretely kinetic energy conserving
  - balanced force surface tension force
  - phase interface remains discontinuity
  - dynamic Smagorinsky LES in the single phase regions
  - Lagrangian spray drop/parcel model with full two-way coupling and stochastic secondary atomization model *(Apte et al. 2003)*
  - interface capturing by RLSG level set on high-resolution overset mesh
  - drop identification and transfer algorithm

- **CLIFF** ***(Cascade Technologies)***

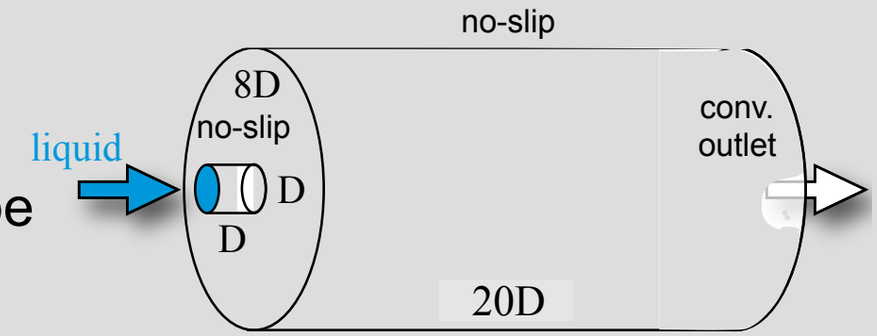
  - unstructured arbitrary polyhedra
  - 2nd order finite volume
  - discretely kinetic energy conserving
  - balanced force surface tension force
  - phase interface remains discontinuity
  - dynamic Smagorinsky LES in the single phase regions
  - Lagrangian spray drop/parcel model with full two-way coupling and stochastic secondary atomization model *(Apte et al. 2003)*
  - interface capturing by geometric unspilt VoF on flow solver mesh
  - drop identification and transfer algorithm

Diesel Jet Atomization

- Conditions:
  - Injector diameter: D = 100 μm
  - Injection velocity: 100 m/s
  - Density ratio: 850 / 25
  - Viscosity ratio: $1.70 \cdot 10^{-3}$ / $1.78 \cdot 10^{-5}$
  - Surface tension coeff.: 0.05 N/m
  - Characteristic numbers: Re = 5000, We = 17000
  - Inlet profile: DNS of Re = 5000 turbulent pipe
  - Domain size: 20D x 8D x 2π
  - Drop transfer D_{max}: 16.8μm
  - Lagrangian description: no secondary atomization, no collisions
  - Grid type: cylindrical (flow solver) & Cartesian (RLSG)
  - Flow solver resolution: Δx_{min} = D/50 = 2μm, D/100 = 1μm, D/200 = 0.5μm
  - RLSG resolution: Δx_G = D/64 = 1.56μm, D/128 = 0.78μm, and D/256 = 0.39μm
  - Maximum grid sizes: 210 million (flow solver) & 5 billion w/ 390 million active (RLSG)
  - Cost: 14/40 days on 256 cores (1.8 teraflops total)



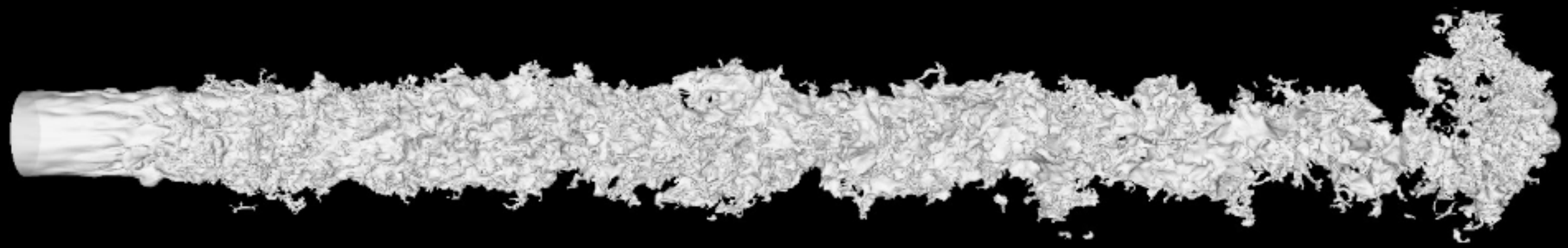
Experiment: Spiekermann et al. (2007)



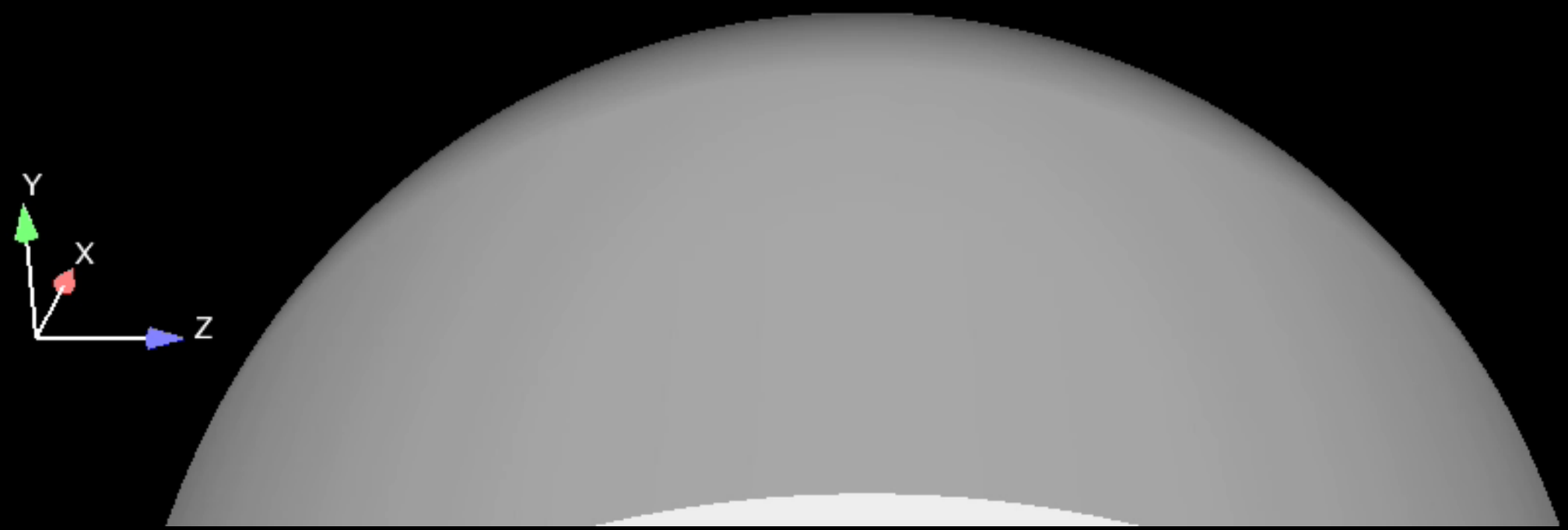
Time = 0.00 μs

Time = 0.00 μs

Time = 18.00 μs



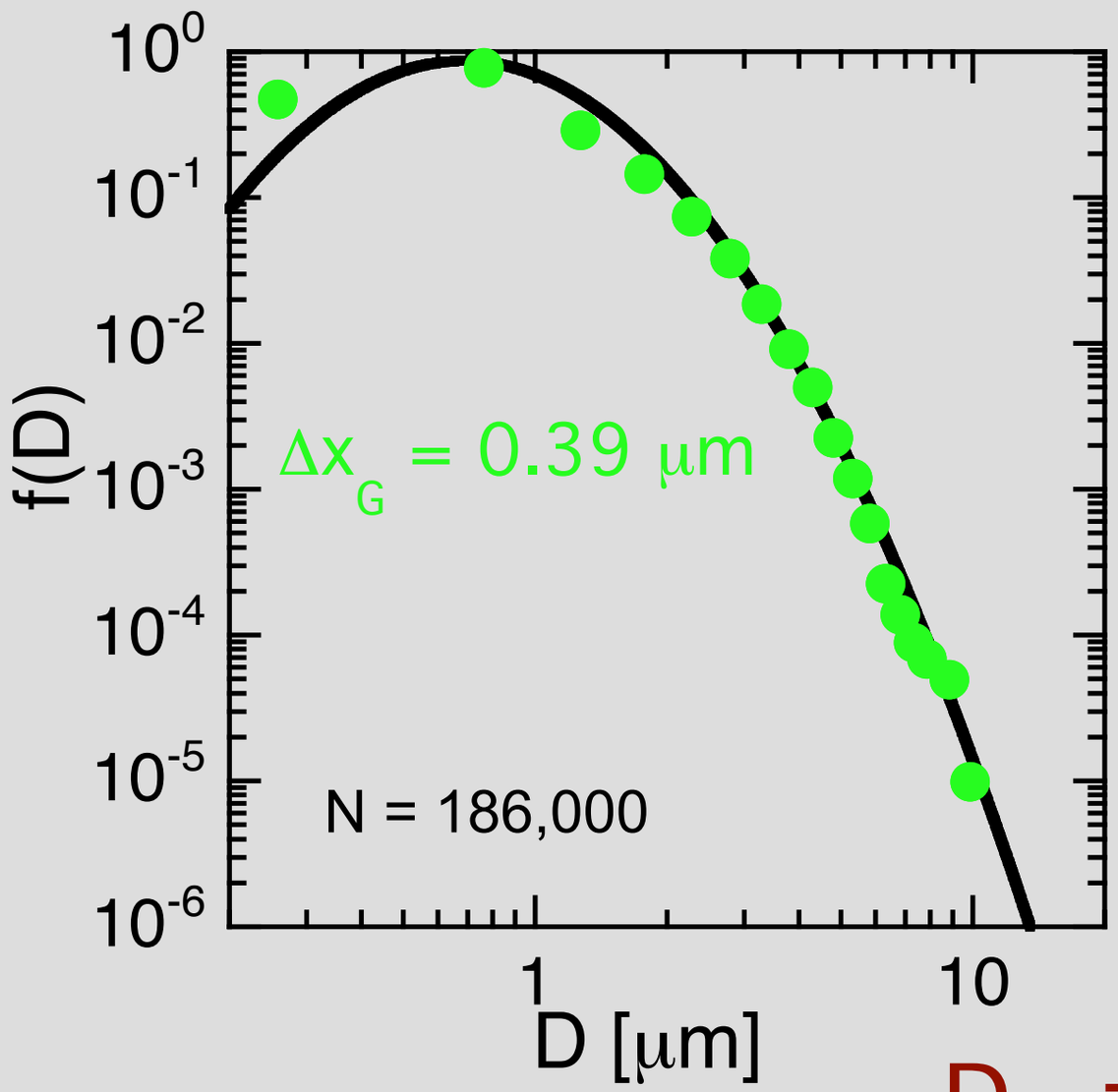
Time = 0.00 μs

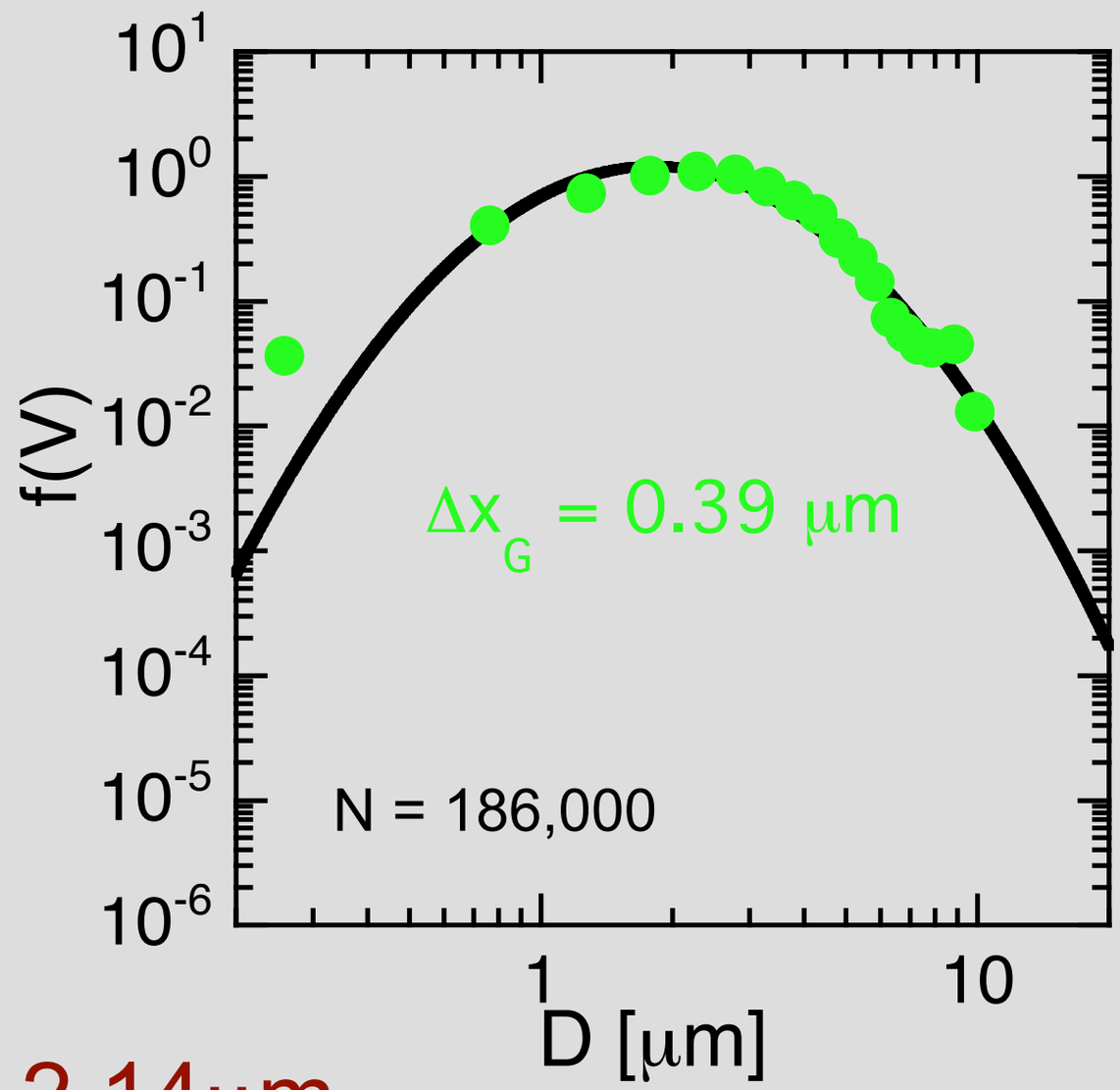


Diesel Injection: Drop Size Distributions

Drops resulting from primary atomization

line: log-normal fit



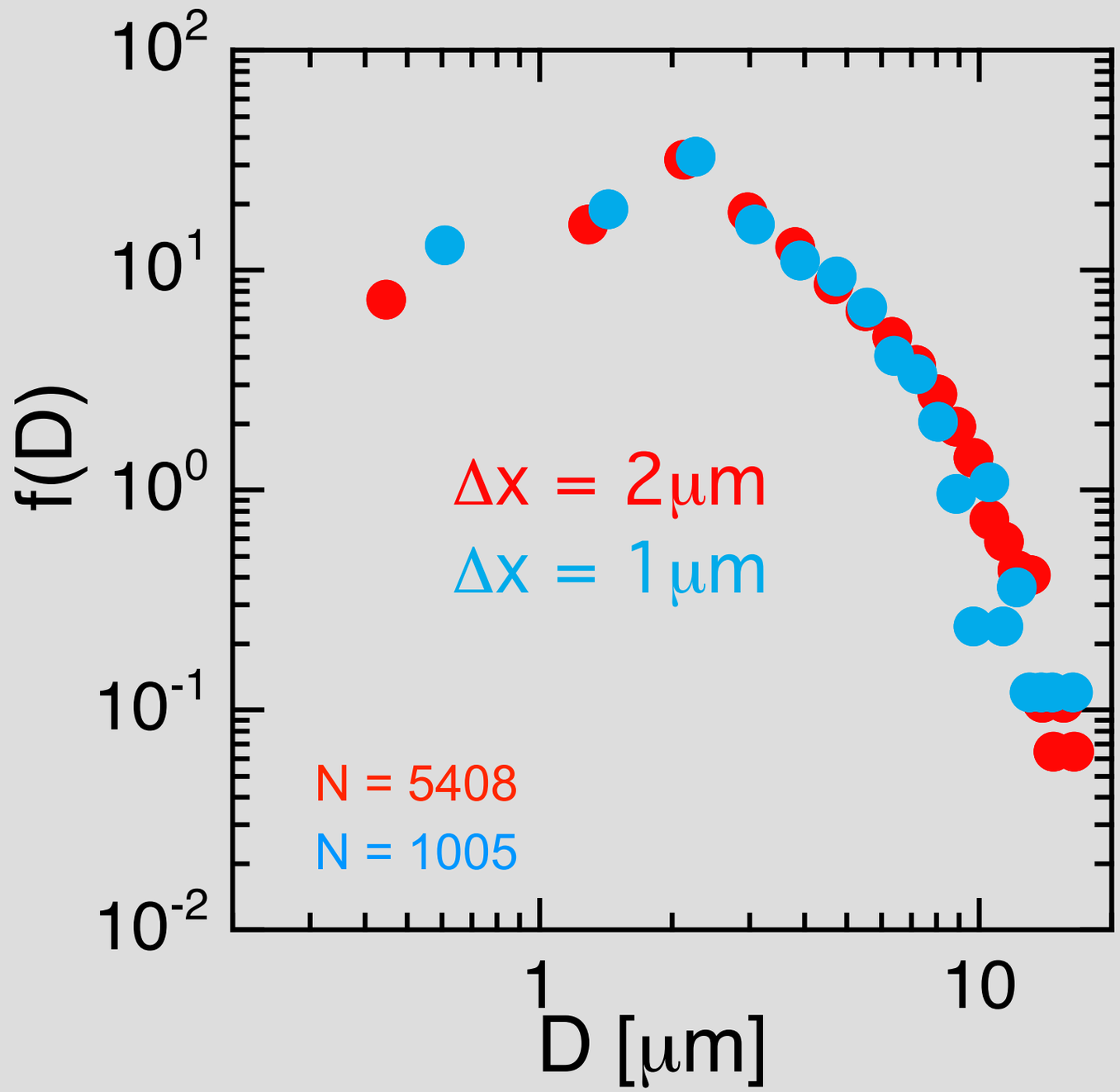


D_{32} = 2.14μm

flow solver: Δx_{min} = 1μm

Flow Solver Grid Impact on Distributions

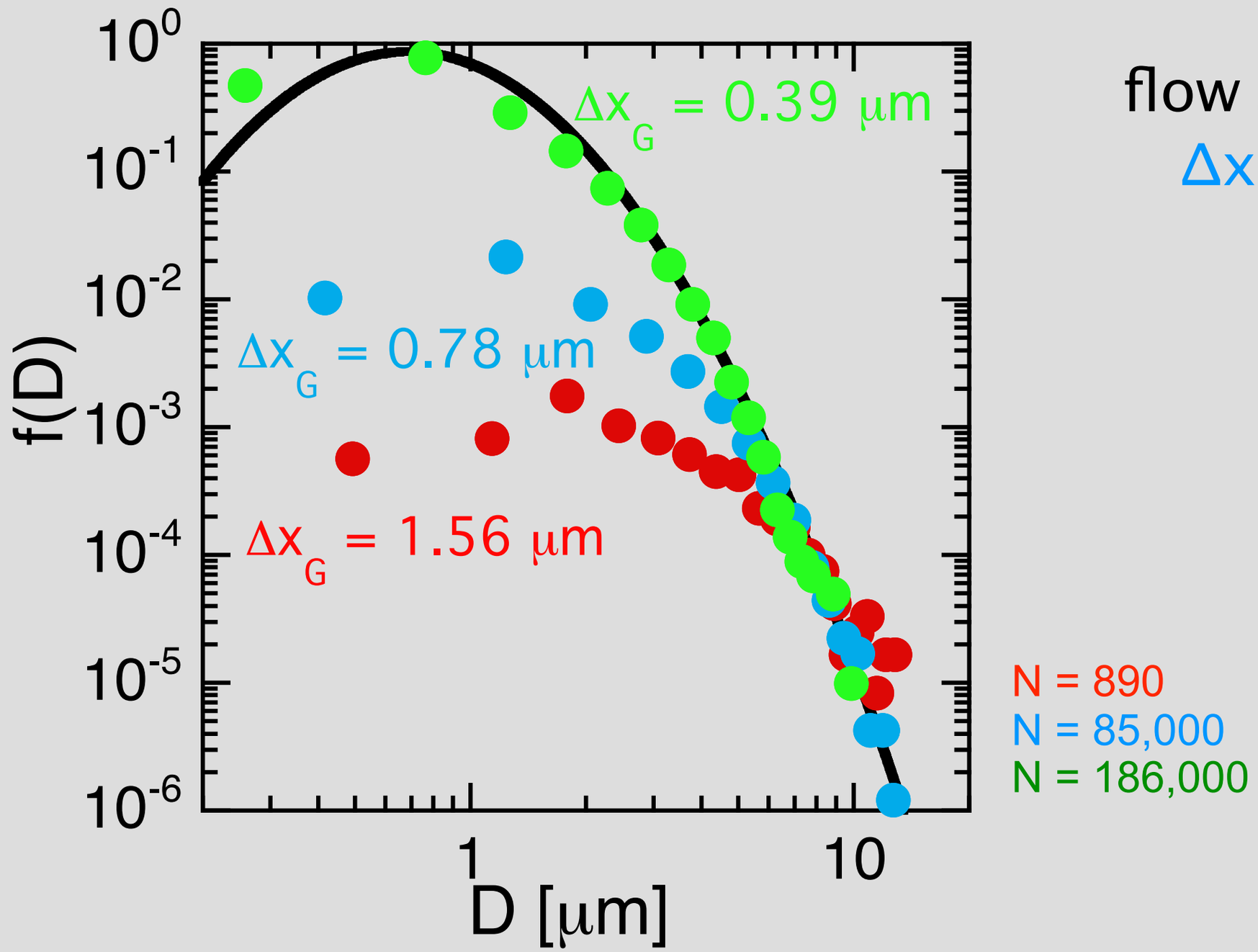
drops resulting from primary atomization



interface grid =
breakup length scale =
Δx_G = 1.56 μm

Breakup Length Scale Impact on Distributions

drops resulting from primary atomization



flow solver grid:

Δx_{min} = 1μm

Breakup Length Scale Impact on Distributions

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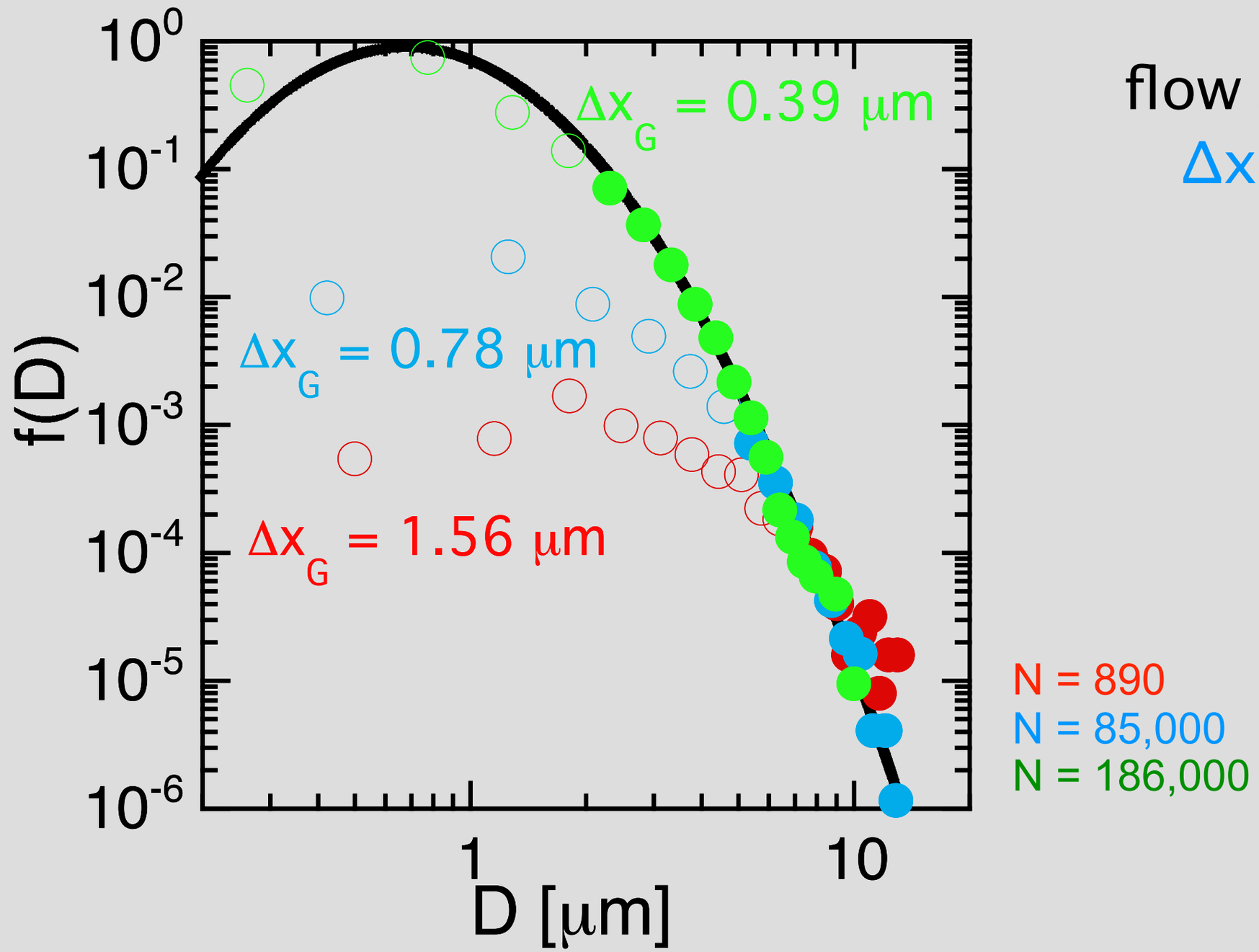
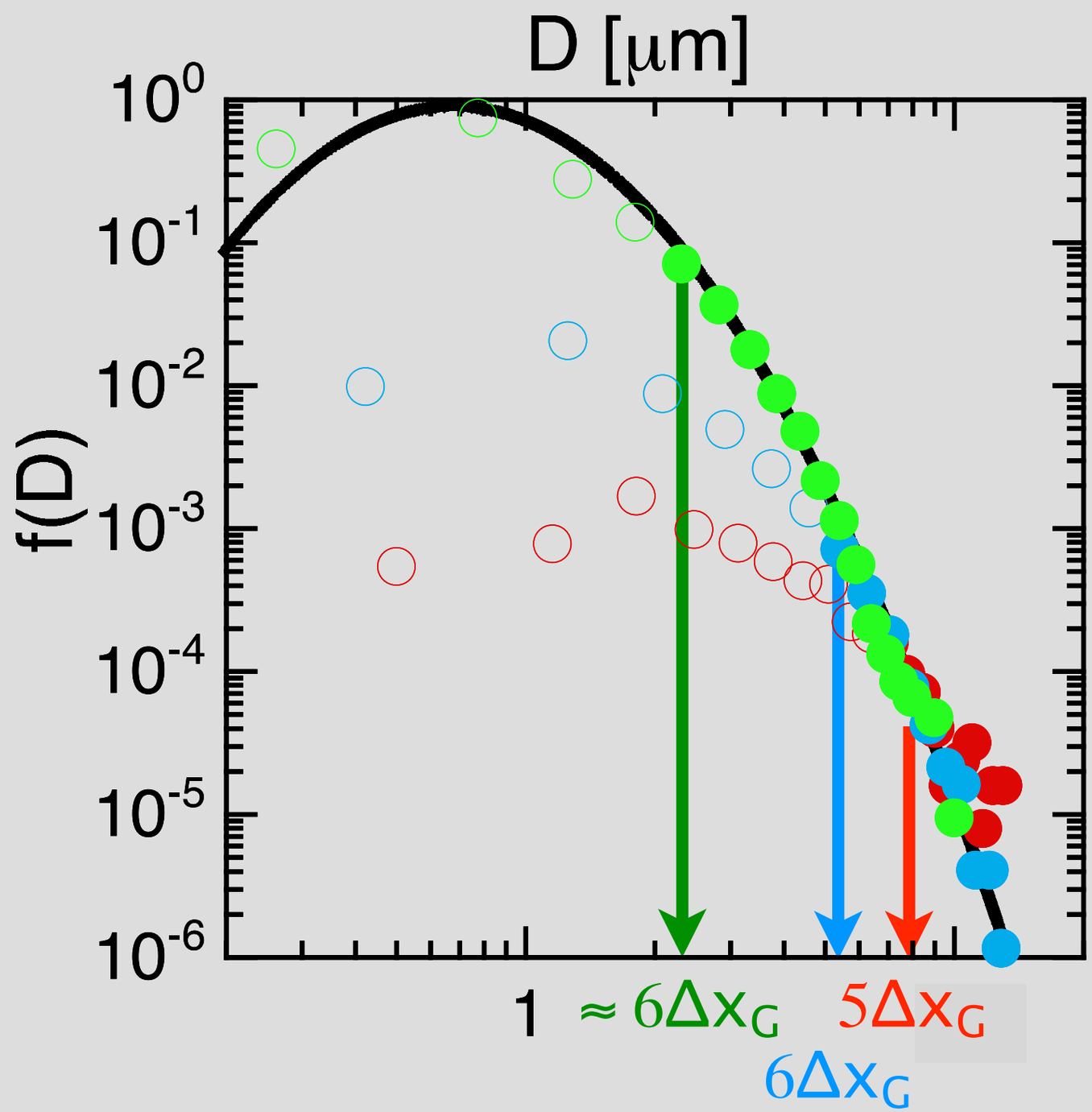


flow solver grid:

Δx_{min} = 1μm

Breakup Length Scale Impact on Distributions

drops resulting from primary atomization



flow solver grid:

$\Delta x_{min} = 1\mu m$

required interface grid resolution for grid independence:

$\Delta x_G = D/6$

all smaller drops are likely numerical artifacts