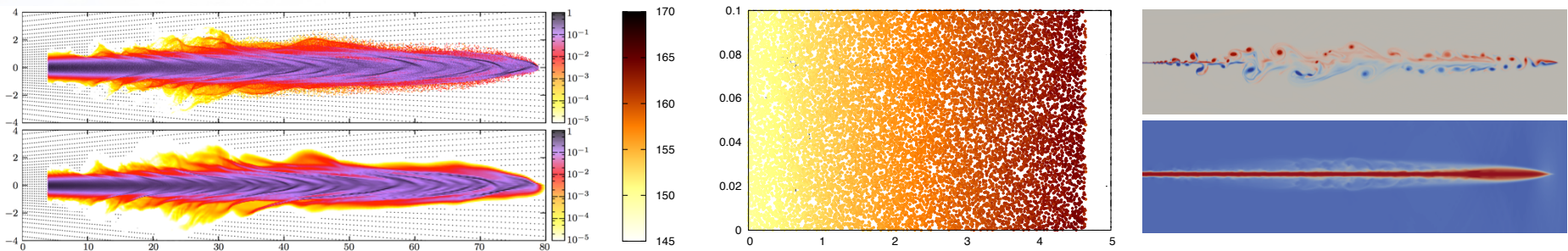


An Eulerian strategy for disperse phase flows

F. Doisneau, M. Arienti, J. Oefelein

Combustion Research Facility

Sandia National Laboratories, Livermore, CA 94551



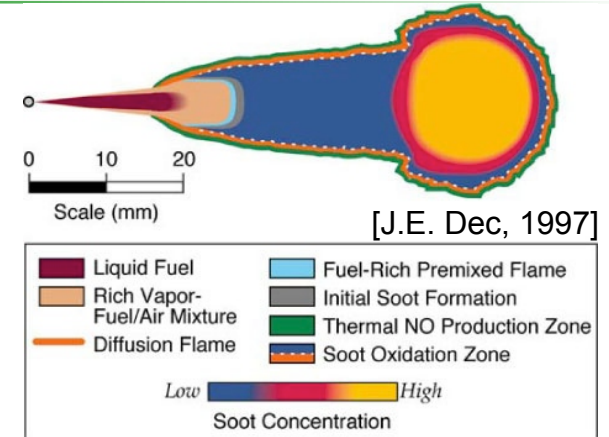
Support by Sandia National Laboratories' LDRD program
LDRD – Laboratory Directed Research and Development
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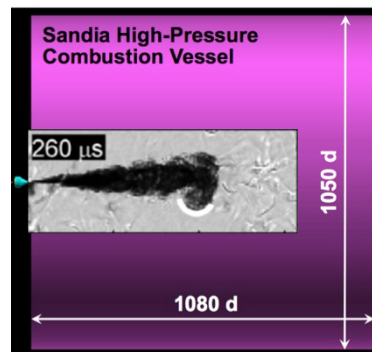
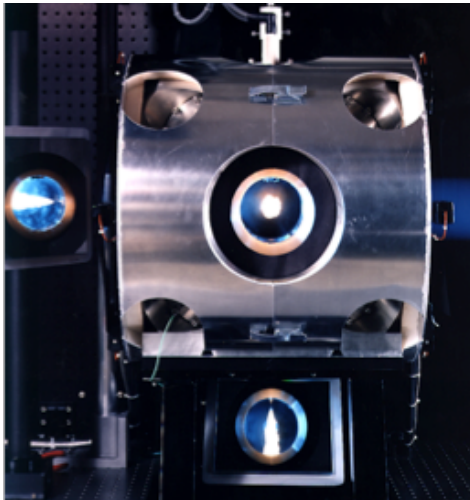
MOTIVATION 1 – Liquid fuel injection

In Diesel and Gasoline engines

- Inlet is turbulent (+ cavitation)
 - $Re \sim 10^5$, $d = 90\mu m$
- High pressure chamber and sonic flow
 - $p = 60bar$, $u_i = 600m/s$
- Atomization process not understood
 - $We \sim 10^4$, $1\mu m < r_i < 100\mu m$



➔ **MULTI-SCALE&MULTI-PHYSICS** drive **MIXING&COMBUSTION**



Experimental background
High pressure vessels
[Pickett 2010, Skeen 2014]

Need for a
High Fidelity Simulation
that is **affordable**

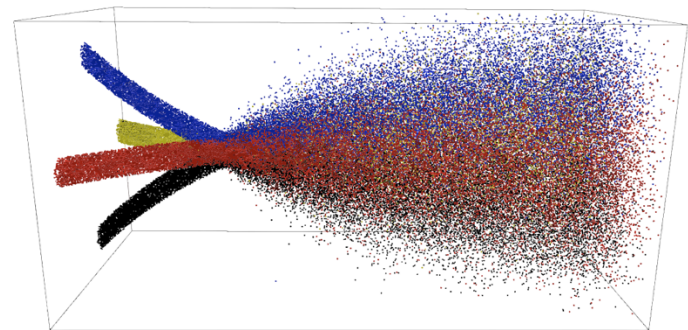
MOTIVATION 2 – Kinetic problems

Versatility of coupled Boltzmann equation

- Kinetic equations
 - Boltzmann
 - Vlasov
 - Williams
- With many applications
 - gases
 - plasmas
 - sprays
 - astrophysics
- and possibly coupled
 - multicomponent Boltzmann
 - Maxwell or subset
 - Navier-Stokes

Kinetic theory to translate **non-equilibrium**/unknown equilibrium

- Complex **behavior**
- Large **dimensionality**
- Strong **couplings**
- Requires a **dedicated approach**



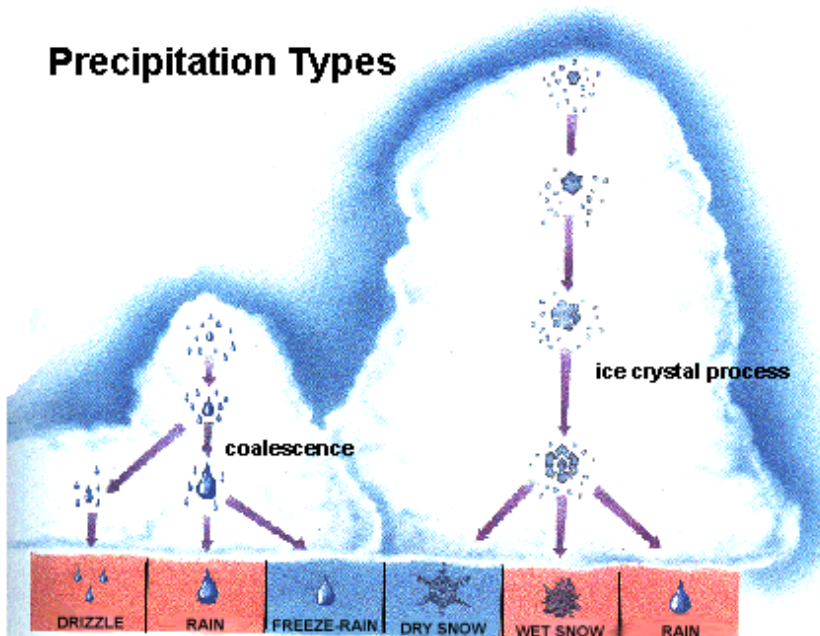
MOTIVATION 3 – Rain formation

Atmospheric sciences

- Raindrop formation/fall depends on:
 - Thermodynamics
 - Turbulence
 - Coalescence dynamics
- Empirical models not accurate enough



Precipitation Types



- Need for **detailed+large scale** computations

State of the art – Particle solvers

Transport for out-of-equilibrium systems

- **Direct Simulation Monte-Carlo (aka stochastic Lagrangian)**
 - straightforward equations
 - can handle any correlations
 - converges as $n^{1/2}$
 - noise
 - unexpected errors related to non-linearity
 - load-balancing problem
 - coupling to a Eulerian fluid difficult
- **Eulerian resolution (aka Moment Methods)**
 - deterministic
 - coupling to Eulerian fluids straightforward
 - predictable load
 - solves for some moments
 - requires assumptions/presumed pdfs
 - unexpected errors related to the assumptions
 - requires a dedicated numerical scheme (realizability, robustness)
 - **Kinetic** [Bouchut 2003, de Chaisemartin 2009]
 - **MUSCL** [Le Touze 2012, Vie 2015]
 - **Semi-Lagrangian** [Cheng 1976, Besse 2003]
 - **Discontinuous Galerkin** [Sabat 2014]

MODEL – Kinetic theory for sprays

A high-fidelity description

Point particles with velocity $\mathbf{c}$, temperature θ , surface S

Number density function **NDF** : describes the disperse phase

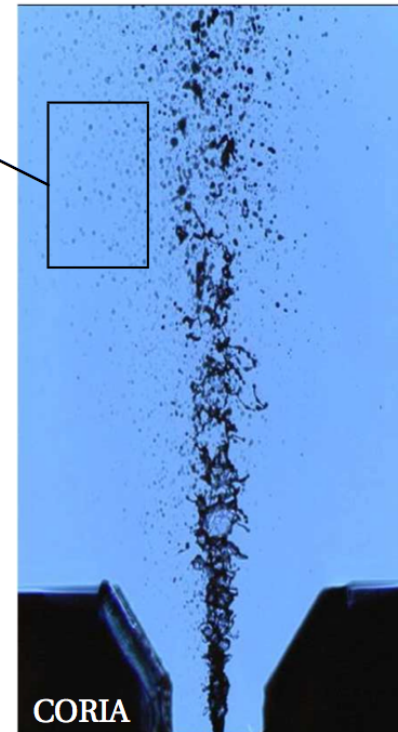
$$dN = f(t, \mathbf{x}, \mathbf{c}, S, \theta) d\mathbf{x} d\mathbf{c} dS d\theta$$

NDF satisfies a Boltzmann-like PDE [Williams, 1958]

$$\partial_t f + \partial_{\mathbf{x}} \cdot (\mathbf{c}f) + \partial_{\mathbf{c}} \cdot (\mathbf{F}f) + \partial_{\theta} (\mathbf{H}f) = \mathfrak{B} + \mathfrak{C}$$

Closures : all the physical modeling job

- Drag force $\mathbf{F}$
- Heat transfer $\mathbf{H}$
- Break-up $\mathfrak{B}$
- Collisions $\mathfrak{C}$



MODEL – Kinetic theory for sprays

A high-fidelity description

Inertial droplet coalescence :

$$\mathcal{E}^+ = \frac{1}{2} \int_{\mathbf{c}^\star} \int_{v^\star \in [0, v]} f(t, \mathbf{x}, \mathbf{c}^\diamond, v^\diamond) f(t, \mathbf{x}, \mathbf{c}^\star, v^\star) \mathcal{K}_{\text{coal}} J dv^\star d\mathbf{c}^\star$$

$$\mathcal{E}^- = \int_{\mathbf{c}^\star} \int_{v^\star} f(t, \mathbf{x}, \mathbf{c}, v) f(t, \mathbf{x}, \mathbf{c}^\star, v^\star) \mathcal{K}_{\text{coal}} dv^\star d\mathbf{c}^\star$$

Coalescence source term

- integral
- quadratic
- multivariate kernel
- non-linear kernel

Balistic coalescence kernel modeling

$$\mathcal{K}_{\text{coal}} = \pi (r^\diamond + r^\star)^2 \|\mathbf{u} - \mathbf{u}^\star\| \mathcal{E}(\dots)$$

Efficiency $\mathcal{E}$ models

- collision efficiency [Langmuir, 1948, Beard and Grover, 1974]
- coalescence efficiency [Brazier-Smith et al., 1972, Ashgriz and Poo, 1990]

⇒ **closed**



MODEL – Kinetic theory for sprays

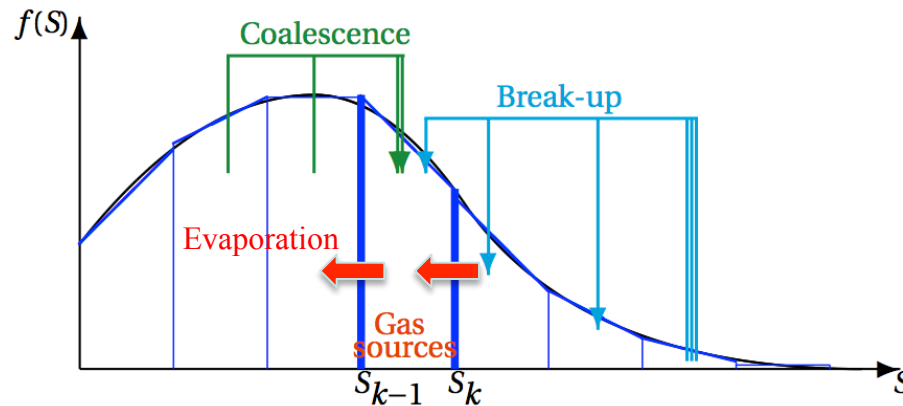
A high-fidelity description

- Reduction of kinetic theory is
 - **Crucial**
 - **Problem dependent**
- Two approaches considered
 - Lagrangian (Direct simulation Monte-Carlo)
 - Eulerian Multi-Fluid (Sectional)
- Objectives
 - Numerical strategy for strongly coupled massively parallel simulations
 - Hybrid approach for wide spectrum of droplet sizes

MODEL – Sectional method (EULERIAN)

A cost-efficient way to capture polydispersity

- Various drop sizes are treated as a continuum:
Multi-Fluid [Laurent 2001, Doisneau 2013]



$$\begin{aligned}
 N_{\text{sec}} \text{ systems } \left\{ \begin{aligned} \partial_t n_k + \partial_{\mathbf{x}} \cdot (n_k \mathbf{u}_k) &= {}^2C_k^n + {}^2B_k^n + {}^2E_k^n \\ \partial_t m_k + \partial_{\mathbf{x}} \cdot (m_k \mathbf{u}_k) &= {}^2C_k^m + {}^2B_k^m + {}^2E_k^m \\ \partial_t (m_k \mathbf{u}_k) + \partial_{\mathbf{x}} \cdot (m_k \mathbf{u}_k \otimes \mathbf{u}_k) &= m_k \mathbf{F}_k + {}^2C_k^u + {}^2B_k^u + {}^2E_k^u \\ \partial_t (m_k h_k) + \partial_{\mathbf{x}} \cdot (m_k h_k \mathbf{u}_k) &= m_k \mathbf{H}_k + {}^2C_k^h + {}^2B_k^h + {}^2E_k^h \end{aligned} \right. \quad \Longleftrightarrow \quad \text{Navier-Stokes with sources}
 \end{aligned}$$

...many integral source terms to compute

MODEL – Sectional method (EULERIAN)

A cost-efficient way to capture polydispersity

Coalescence terms : quadratic sums of 2D elementary integrals

$${}^2C_k^{n+} = \sum_{i=1}^k \sum_{j=1}^{i-1} Q_{ijk}^n$$

$${}^2C_k^{m+} = \sum_{i=1}^k \sum_{j=1}^{i-1} (Q_{ijk}^{\star} + Q_{ijk}^{\diamond})$$

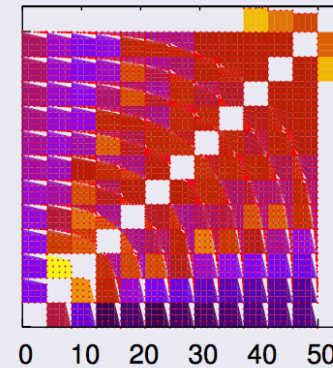
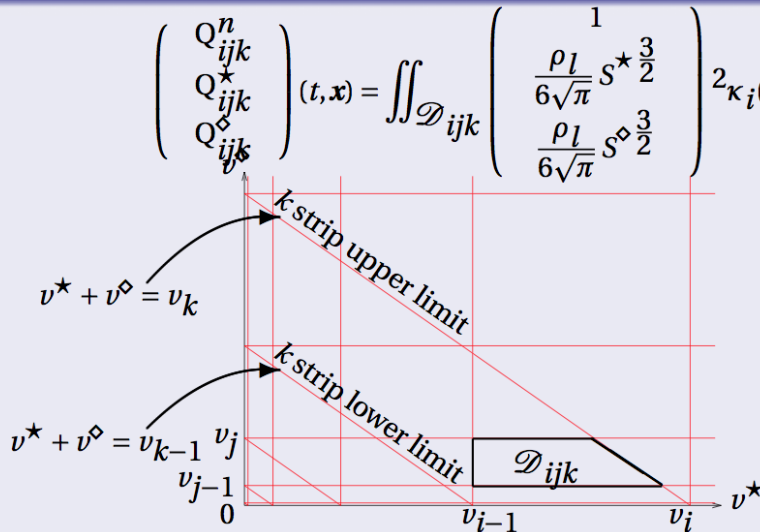
$${}^2C_k^{u+} = \sum_{i=1}^k \sum_{j=1}^{i-1} (u_i Q_{ijk}^{\star} + u_j Q_{ijk}^{\diamond})$$

$${}^2C_k^{n-} = \sum_{i=1}^N \sum_{j=1}^N Q_{kji}^n$$

$${}^2C_k^{m-} = \sum_{i=1}^N \sum_{j=1}^N (Q_{kji}^{\star} + Q_{kji}^{\diamond})$$

$${}^2C_k^{u-} = u_k \cdot {}^2C_k^{m-}$$

Elementary integrals



Relative error of integrals for Exp-TSM with (NC5) 13 sections, sizes in radius (μm) ; + quadrature nodes.

If one size moment $\Rightarrow$ size dependency factorization and **precalculation**

General case $\Rightarrow$ **integration at all times !**

MODEL – Sectional method (EULERIAN)

A cost-efficient way to capture polydispersity

- The coupled NS-PGD system

$$\left\{ \begin{array}{l}
 \partial_t \rho_g Y_f + \partial_x \rho_g Y_f \mathbf{u}_g = \omega_f + \sum_k E_k^{m-g} \\
 \partial_t \rho_g Y_i + \partial_x \rho_g Y_i \mathbf{u}_g = \omega_i, \quad i \in \llbracket 1; N_{\text{species}} \rrbracket, i \neq f \\
 \partial_t \rho_g \mathbf{u}_g + \partial_x \rho_g \mathbf{u}_g \otimes \mathbf{u}_g = -\partial_x p + \sum_k \left(-\mathbf{F}_k + \mathbf{u}_k E_k^{m-g} \right) \\
 \partial_t \rho_g e_g + \partial_x \rho_g e_g \mathbf{u}_g = -p \partial_x \mathbf{u}_g + \sum_k \left(-H_k + \mathbf{F}_k (\mathbf{u}_g - \mathbf{u}_k) + h_k E_k^{m-g} \right) \\
 \left. \begin{array}{l}
 \partial_t m_k + \partial_x m_k \mathbf{u}_k \\
 \partial_t m_k \mathbf{u}_k + \partial_x m_k \mathbf{u}_k \otimes \mathbf{u}_k \\
 \partial_t m_k h_k + \partial_x m_k h_k \mathbf{u}_k
 \end{array} \right\} = \left\{ \begin{array}{l}
 E_{k+1}^m + B_k^{m+} + C_k^{m+} - (E_k^m + E_k^{m-g} + B_k^{m-} + C_k^{m-}) \\
 \mathbf{F}_k + \mathbf{u}_{k+1} E_{k+1}^m + \mathbf{B}_k^{u+} + \mathbf{C}_k^{u+} - \mathbf{u}_k (E_k^m + E_k^{m-g} + B_k^{m-} + C_k^{m-}) \\
 H_k + h_{k+1} E_{k+1}^m + B_k^{h+} + C_k^{h+} - h_k (E_k^m + E_k^{m-g} + B_k^{m-} + C_k^{m-})
 \end{array} \right\} \quad k \in \llbracket 1; N_{\text{sec}} \rrbracket
 \end{array} \right.$$

pressureless

sections

Needs to be closed

- Key parameter: number of **sections**

MODEL – DS Monte-Carlo (LAGRANGIAN)

A reference for particle resolution

- The coupled NS-parcel system

$$\left\{ \begin{array}{l} \partial_t \rho_g Y_f + \partial_x \rho_g Y_f \mathbf{u}_g = \omega_f + \sum_k E_k^{m-g} \\ \partial_t \rho_g Y_i + \partial_x \rho_g Y_i \mathbf{u}_g = \omega_i, \quad i \in [1; N_{\text{species}}], i \neq f \\ \partial_t \rho_g \mathbf{u}_g + \partial_x \rho_g \mathbf{u}_g \otimes \mathbf{u}_g = -\partial_x p + \sum_k \left(-\mathbf{F}_k + \mathbf{u}_k E_k^{m-g} \right) \\ \partial_t \rho_g e_g + \partial_x \rho_g e_g \mathbf{u}_g = -p \partial_x \mathbf{u}_g + \sum_k \left(-H_k + \mathbf{F}_k (\mathbf{u}_g - \mathbf{u}_k) + h_k E_k^{m-g} \right) \end{array} \right.$$

$$d_t \mathbf{X}_k = \mathbf{u}_k; \quad d_t \mathbf{u}_k = \mathbf{F}_k; \quad c_{p,l} d_t \theta_s = H_k; \quad d_t r_k = R_k.$$

- Collision step is split
- Key parameter: number of **parcels**

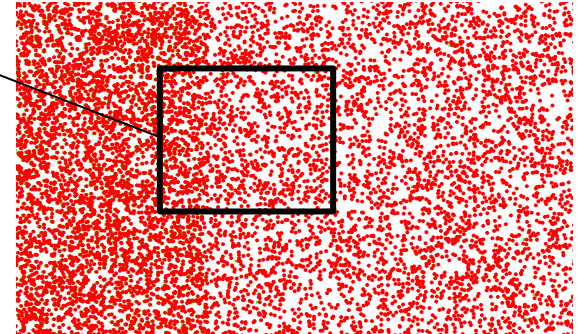
MODEL – DS Monte-Carlo (LAGRANGIAN)

A reference for particle resolution

- **Stochastic Lagrangian coalescence step**
 - **Pick N/2 random pairs in a control volume**
 - **Collision probability**

$$P(\nu_p) = \frac{\lambda_{12}^{\nu_p}}{\nu_p!} \exp(-\lambda_{12})$$

with $\lambda_{12} = \frac{n_{p1}(N_J - 1)\Delta t}{\mathcal{V}(C_J)} \mathcal{K}_{\text{coal}}(|\mathbf{u}_{p1} - \mathbf{u}_{p2}|, r_{p1}, r_{p2})$

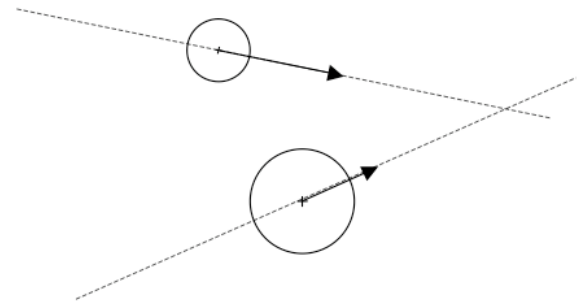


- **Variable update**

$$n'_{p1} = n_{p1} - n_{p2}$$

$$v'_{p2} = v_{p2} + \nu_p v_{p1}$$

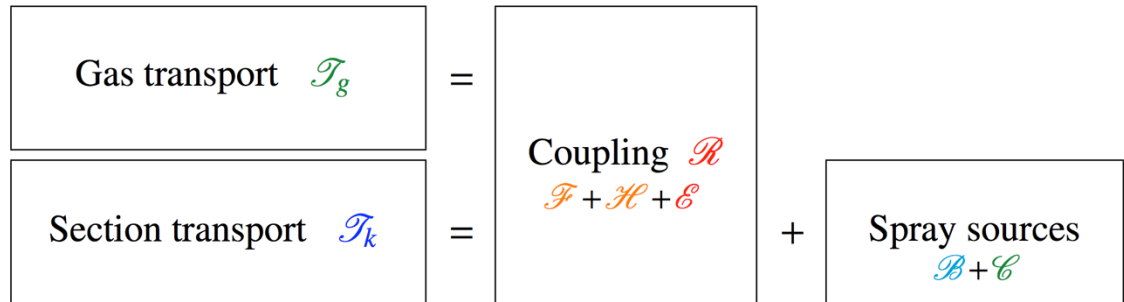
$$\mathbf{u}'_{p2} = \frac{v_{p2}\mathbf{u}_{p2} + \nu_p v_{p1}\mathbf{u}_{p1}}{v_{p2} + \nu_p v_{p1}}$$



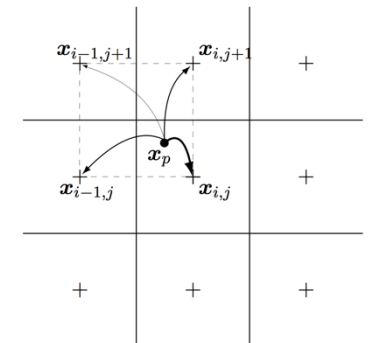
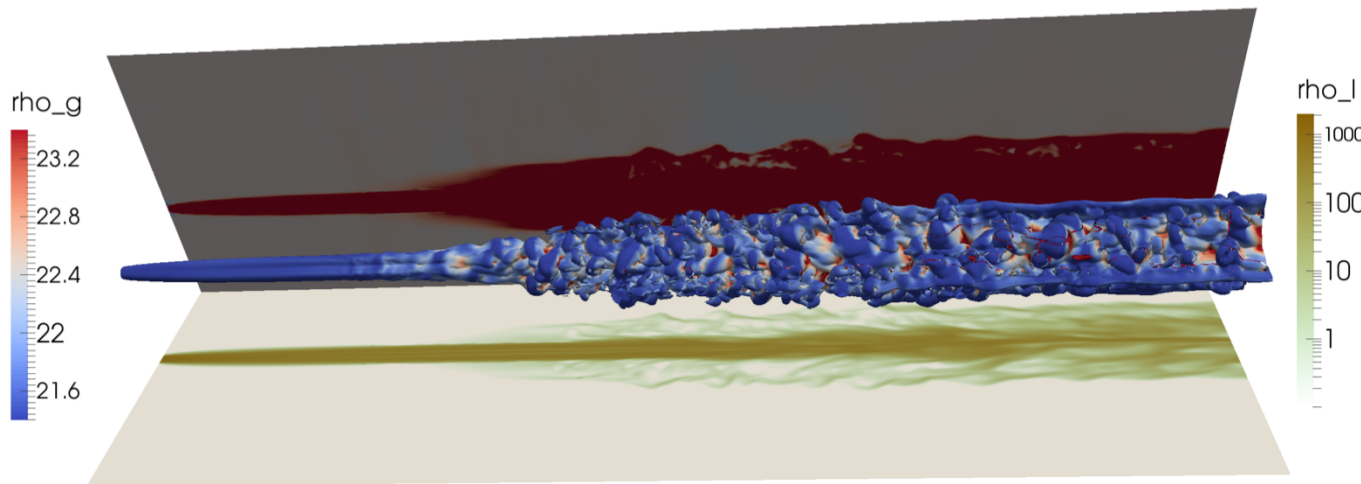
NUMERICS – Euler-Euler coupling needs

Effort on numerical methods for multi-scale coupled flows

- 1) Time integration tailored **splitting**

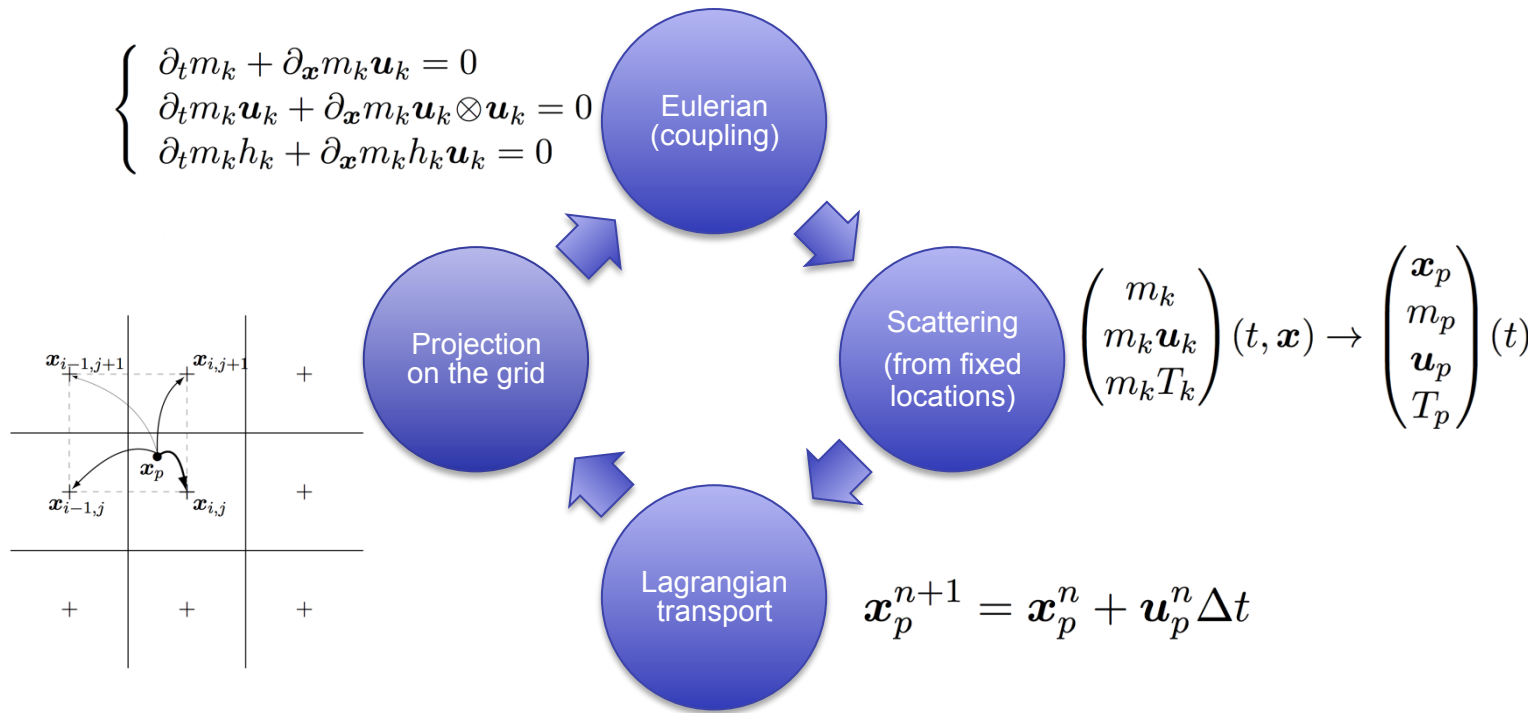


- 2) Space transport novel **semi-Lagrangian scheme**



NUMERICS – PGD transport

A robust and accurate answer to PGD peculiarities

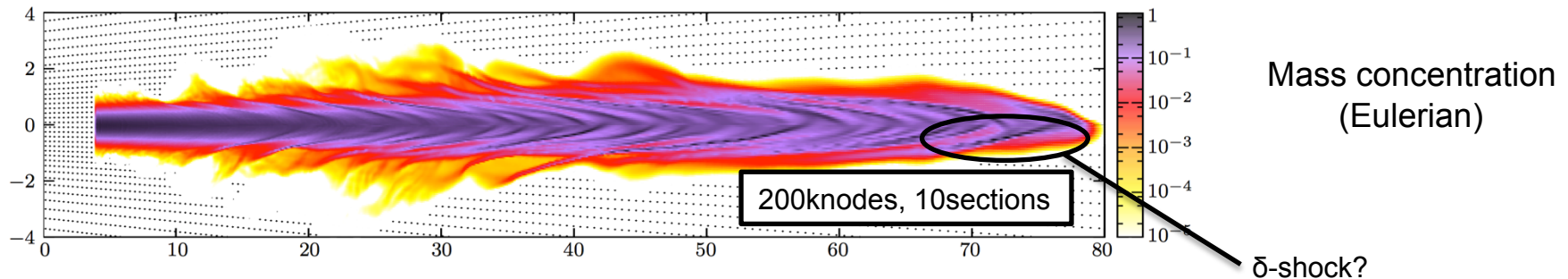


- **Novel semi-Lagrangian PGD transport scheme**
 - **Deterministic: no noise**
 - **Localizes spray info at mesh nodes: good for coupling**
 - **Easier load balancing**
 - **No fluxes to be computed: reduce cost and numerical diffusion**

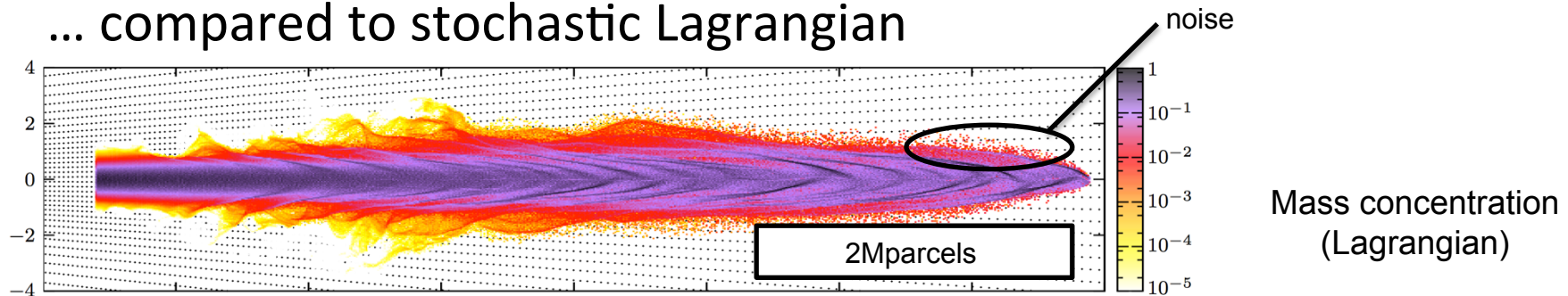
NUMERICS – PGD transport

2D test with prescribed flow field

- Obtained **cost-efficient** and **accurate** results



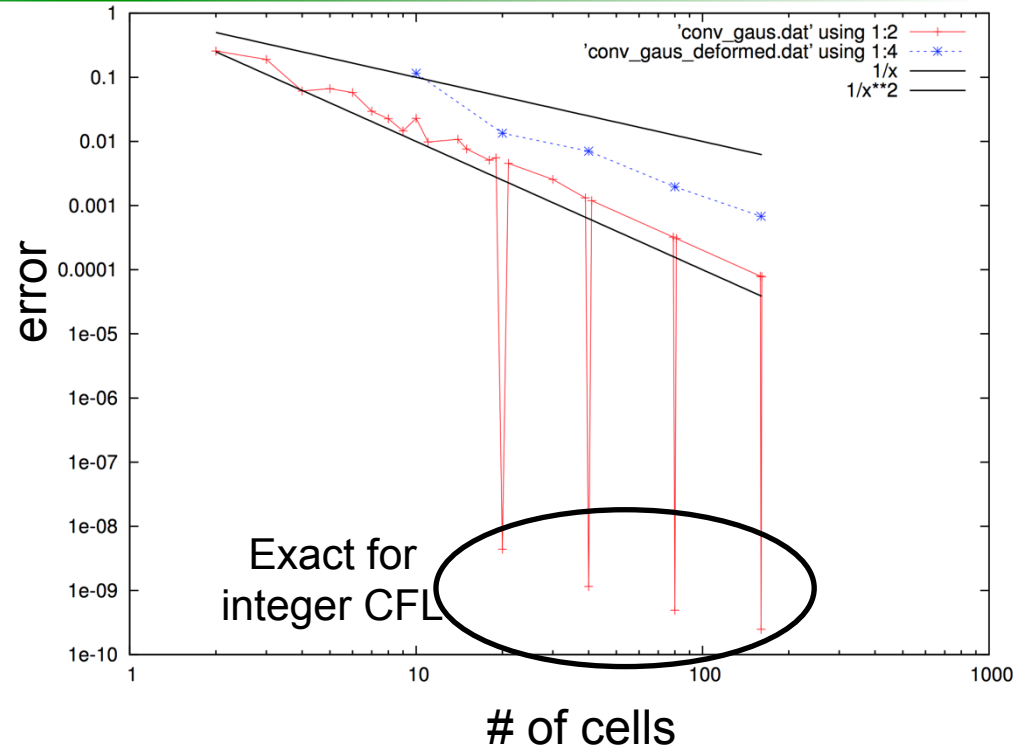
... compared to stochastic Lagrangian



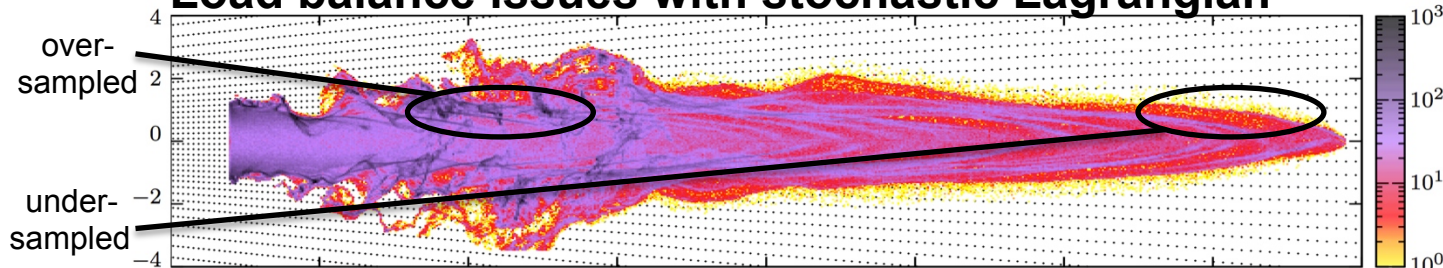
NUMERICS – PGD transport

Transport is 2nd order in space

- **No CFL constraint**
(unconditionally stable)
- **Handles vacuum**
- **Handles δ -shocks**
- **Predictable load**



Load balance issues with stochastic Lagrangian



Number of
numerical parcels
(Lagrangian)



APPLICATIONS

- 1) Test cases for fuel injection**
- 2) Coalescence studies**

TEST 1 – Momentum Coupling

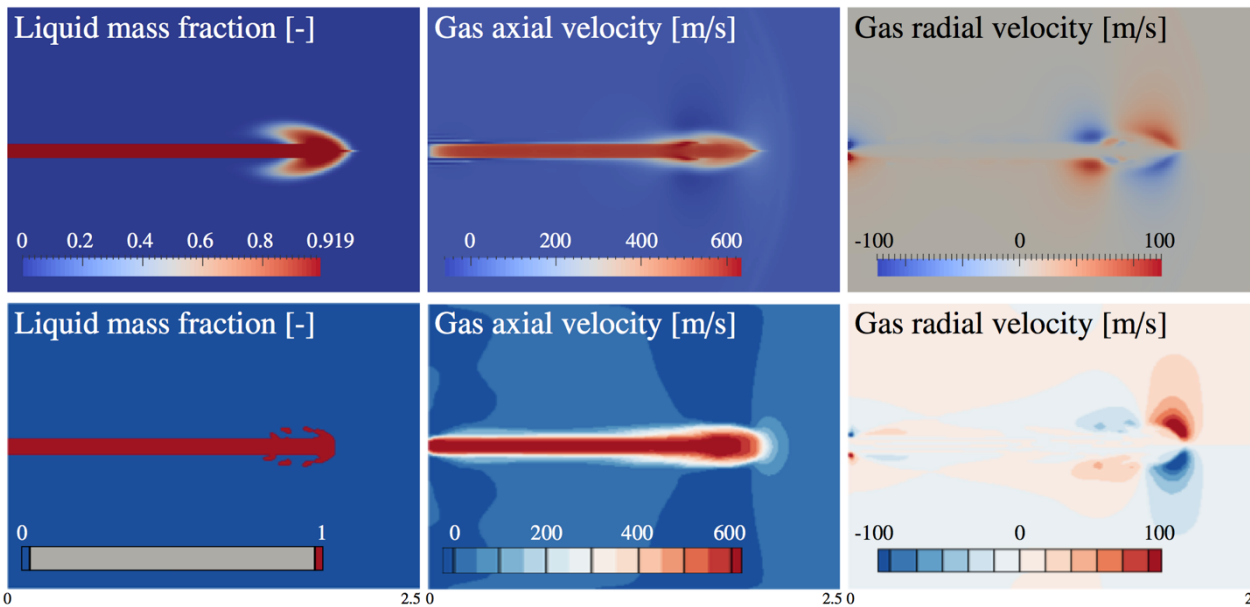
Comparison between E-ES and CLSVOF

✓ Supersonic dense injection (toy problem)

- Large liquid/gas loading ratio (35/1)
- velocity plug-flow boundary
- no thermal transfer
- $T_{\text{end}} = 4\mu\text{s}$

Raptor E-ES

$\Delta x = 12.5 \mu\text{m}$, $\Delta t = 8 \text{ ns}$



CLSVOF

$\Delta x = 13.3 \mu\text{m}$, $\Delta t \sim 6 \text{ ns}$

✓ Agreement on **gas entrainment**

✱ Liquid density discrepancy from **pressureless** assumption

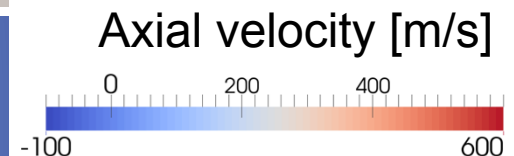
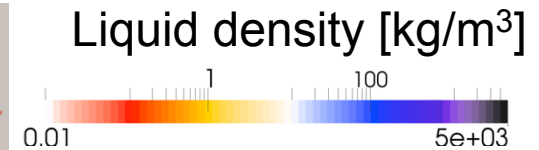
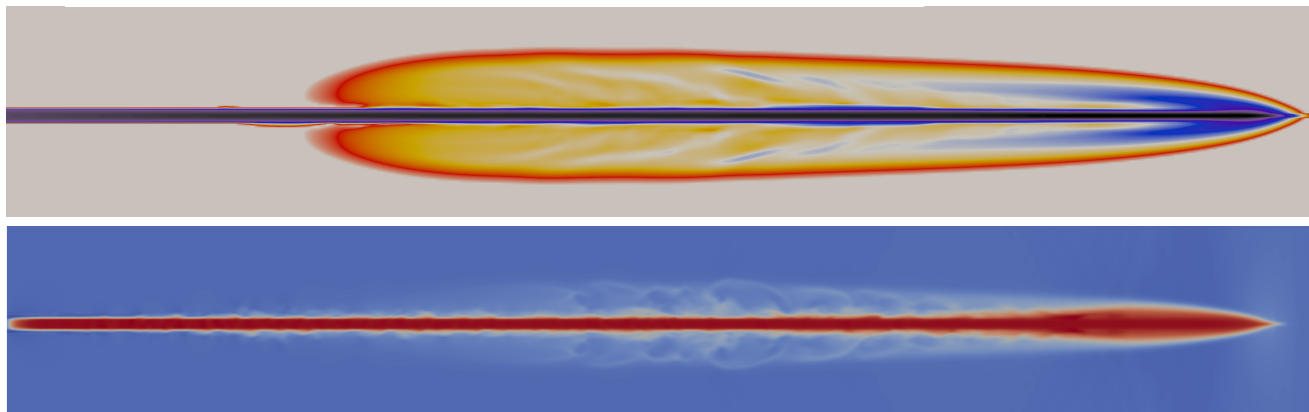
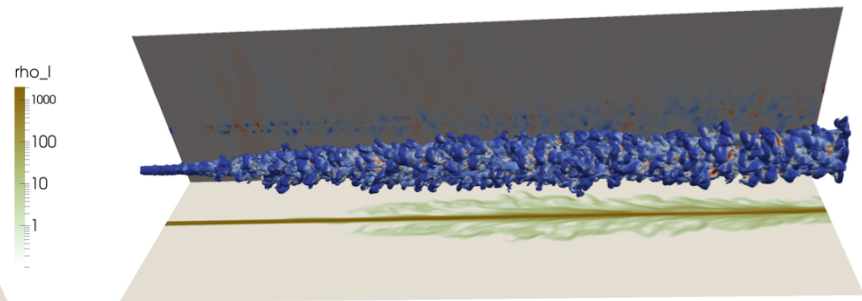
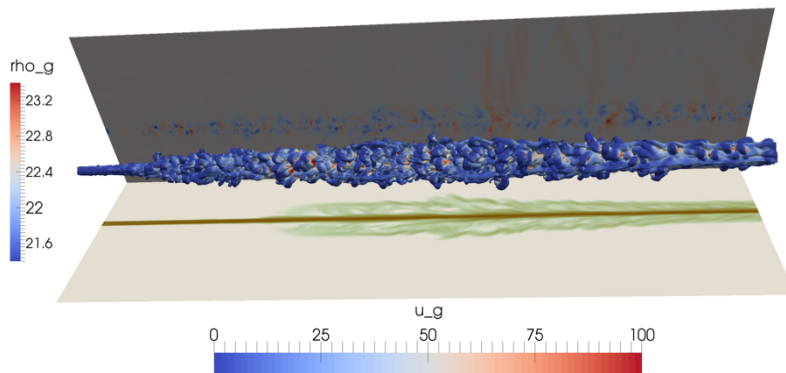
✱ Jet tip is different because of **lack of surface tension**

TEST 2 – Induced turbulence

Entrainment and induced turbulence by jet injection

- Executed with **RAPTOR E-ES**

- Box 3x3x10mm
- $d_{inj}=90\mu\text{m}$, $T_{end}=40\mu\text{s}$
- quiescent gas at 60bar, 900K
- n-dodecane at 702kg/m^3 , 600m/s
- 50Mcells (cartesian mesh)
- $\Delta x=12.5\mu\text{m}$, $\Delta t=8\text{ns}$, $T_{end}=40\mu\text{s}$
- 1 section (prescribed initial size)
- PGD transport (δ -shocks)

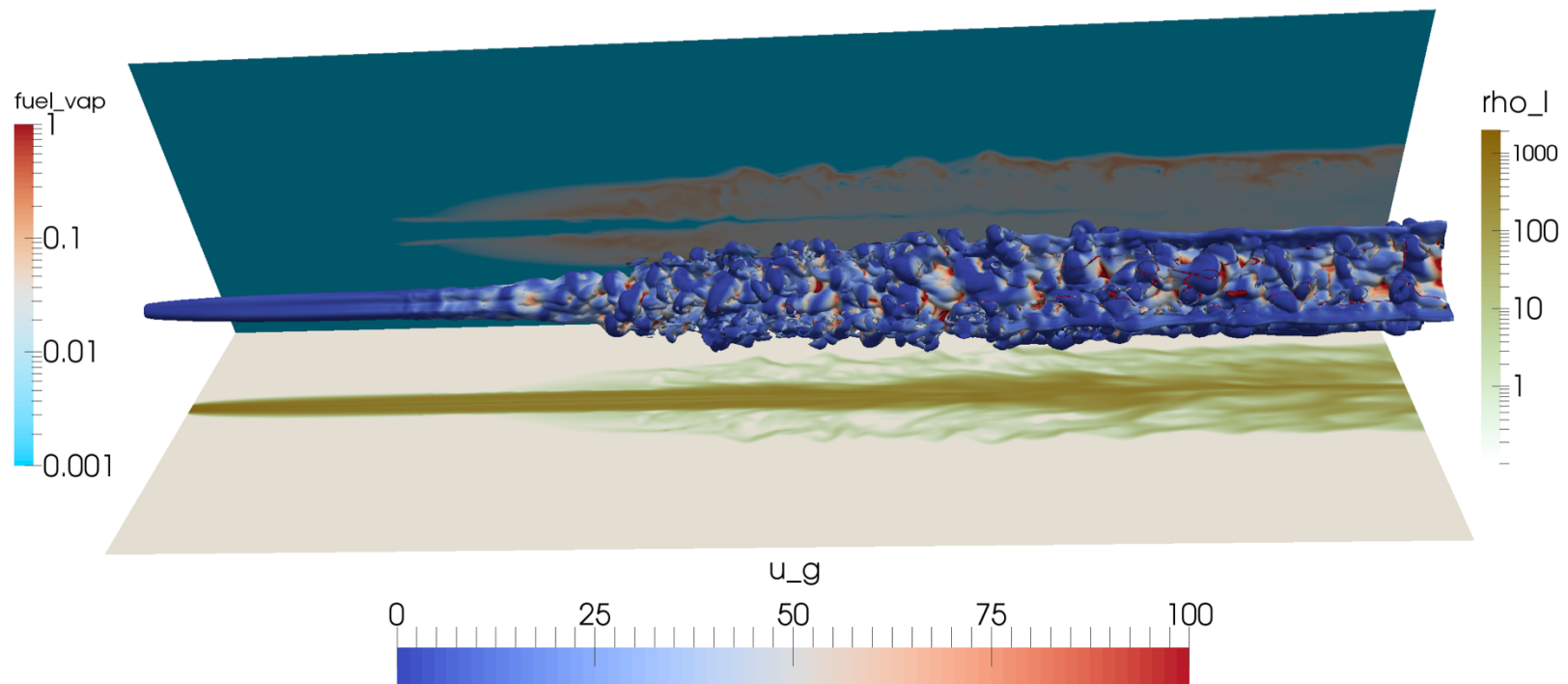


TEST 3 – Fuel vaporization

Fuel vapor footprint

- Executed with **RAPTOR E-ES**

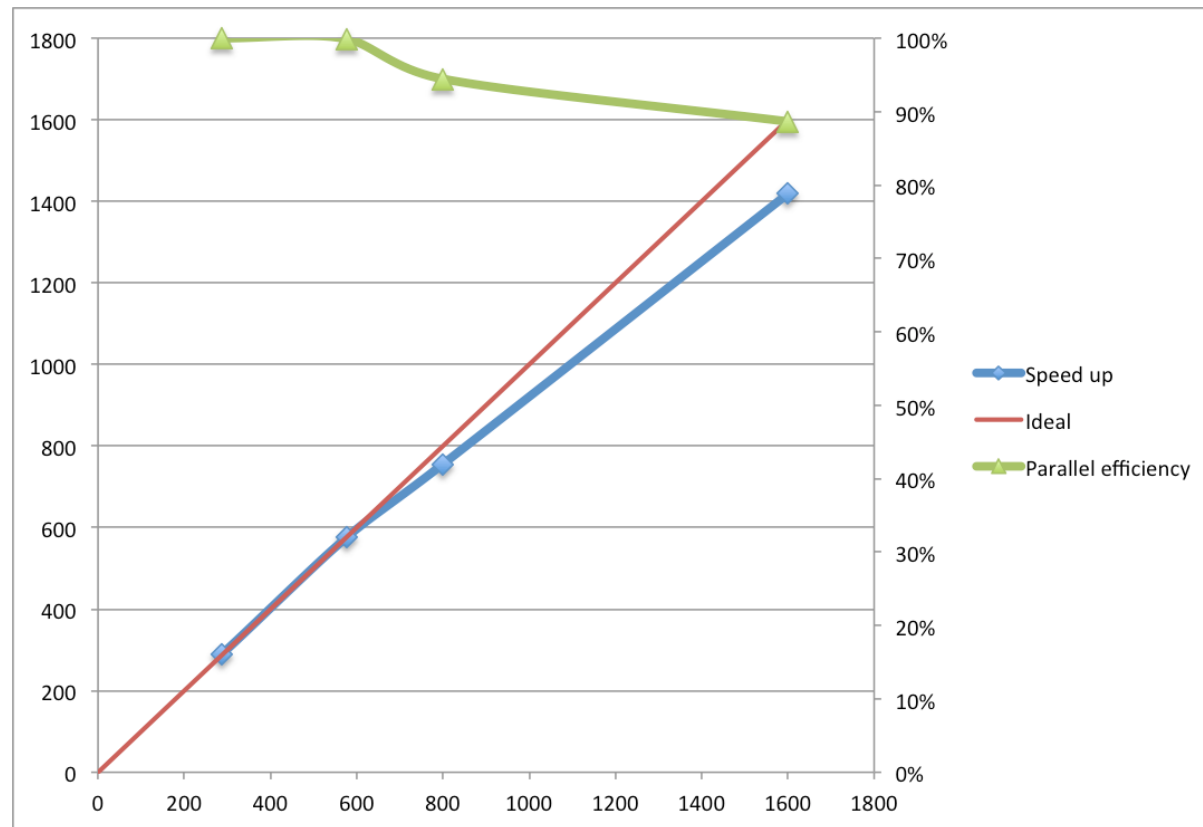
- Box 3x3x10mm
- $d_{inj}=90\mu\text{m}$, $T_{end}=40\mu\text{s}$
- quiescent gas at 60bar, 900K
- n-dodecane at 702kg/m³, 600m/s
- 50Mcells (cartesian mesh)
- $\Delta x=12.5\mu\text{m}$, $\Delta t=8\text{ns}$, $T_{end}=40\mu\text{s}$
- 1 section (prescribed initial size)
- PGD transport (δ -shocks)
- d²-law



TEST 4 – Weak scaling

Towards massively parallel computations

- Executed with **RAPTOR E-ES**
 - Injection case, 50Mcells
 - resolution of the full length of the jet (maximum number of “particles”)
 - including I/O





APPLICATIONS

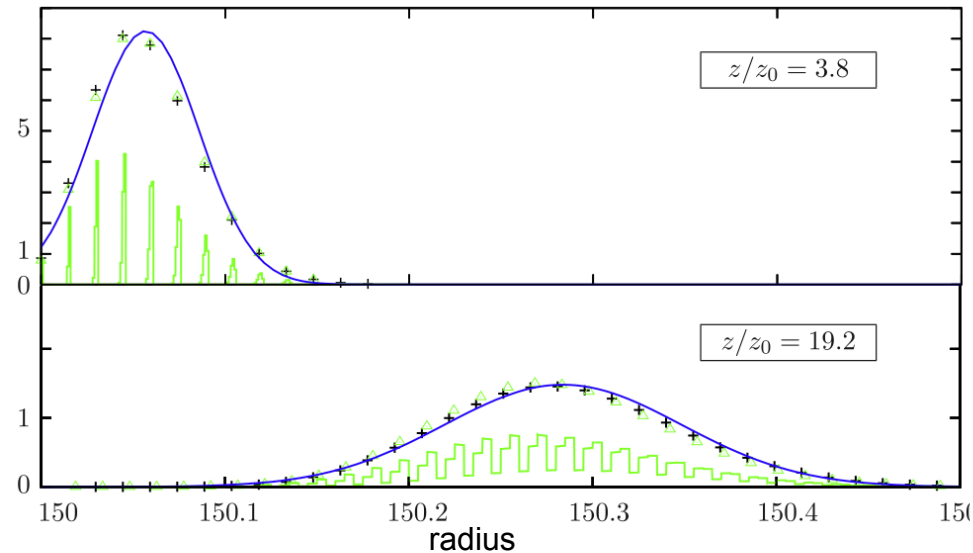
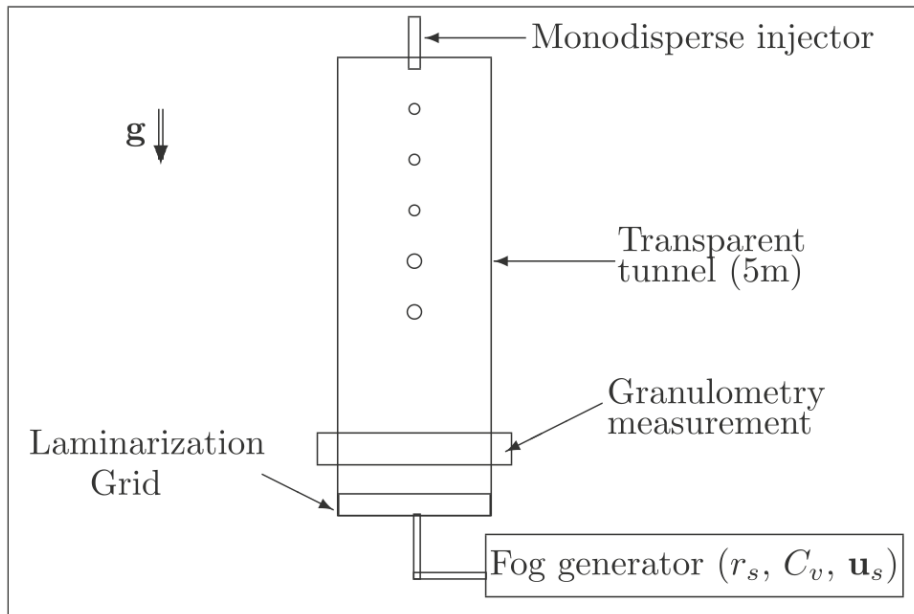
- 1) Test cases for fuel injection
- 2) Coalescence studies**

The D'Herbigny coalescence problem

A benchmark for coalescence

- **Linearized coalescence problem**

- **Big drops (150 μ m) falling**
- **Mist of small drops (3 μ m)**
- **No auto-coalescence**
- **Analytical solutions for various regimes [Doisneau 2013]**
 - Early (exact poisson)
 - Linear increase of radius and dispersion
 - Variation of cross-section

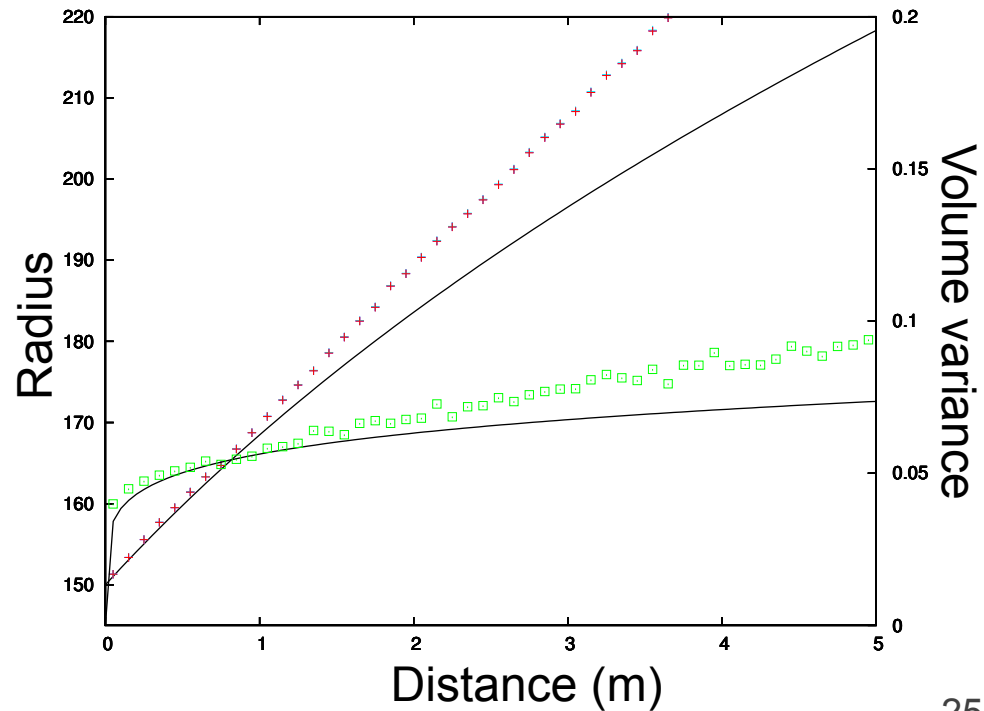
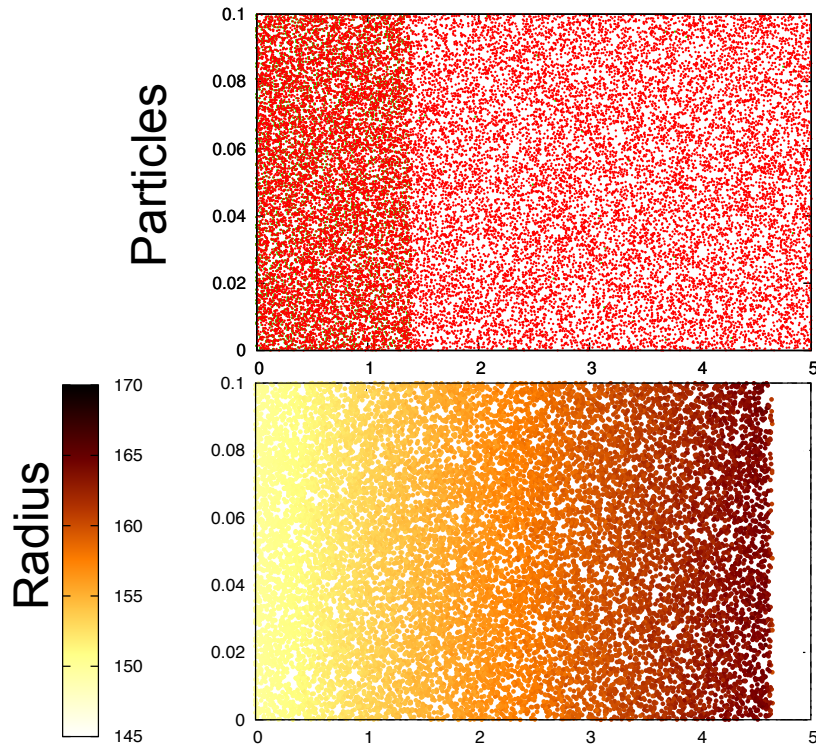


Transition from Poisson to Gaussian and refined sectional approximation (200 sections)

D'Herbigny – Stochastic Lagrangian

A costly approach

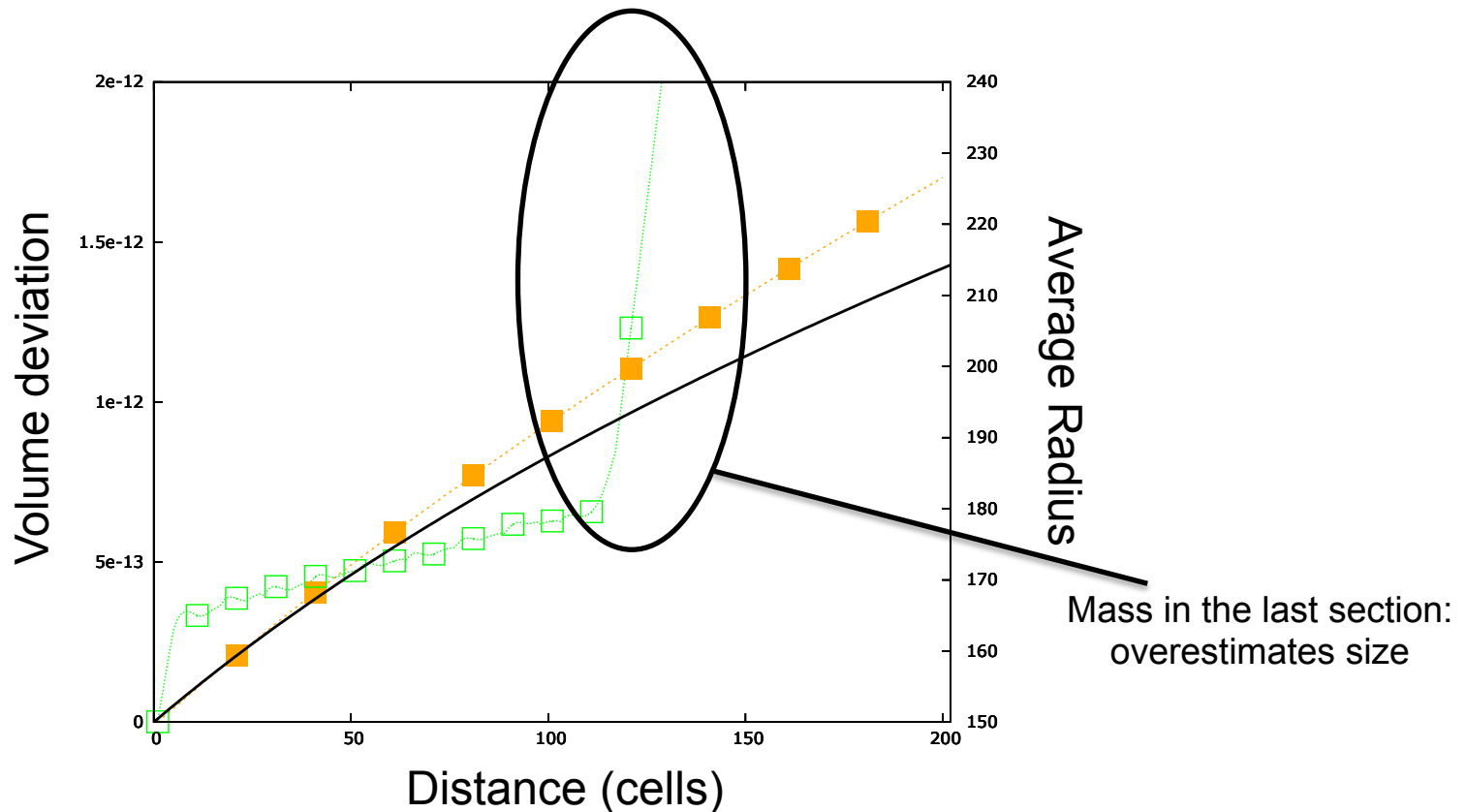
- Executed with in-house code
 - $C_v = 60$ ppm, $L = 5$ m
 - Random pair algorithm $\sim O(n)$
 - 2x20,000 parcels
 - ~ 400 parcels/collisional cell
 - Algorithm verified



D'Herbigny – Deterministic sectional

Efficient approach for low inertia droplets

- Executed with **RAPTOR E-ES**
 - $C_v = 60$ ppm, $L = 5$ m
 - Cartesian mesh (200 cells)
 - 11 sections
 - Standard sectional approach
 - Code verified



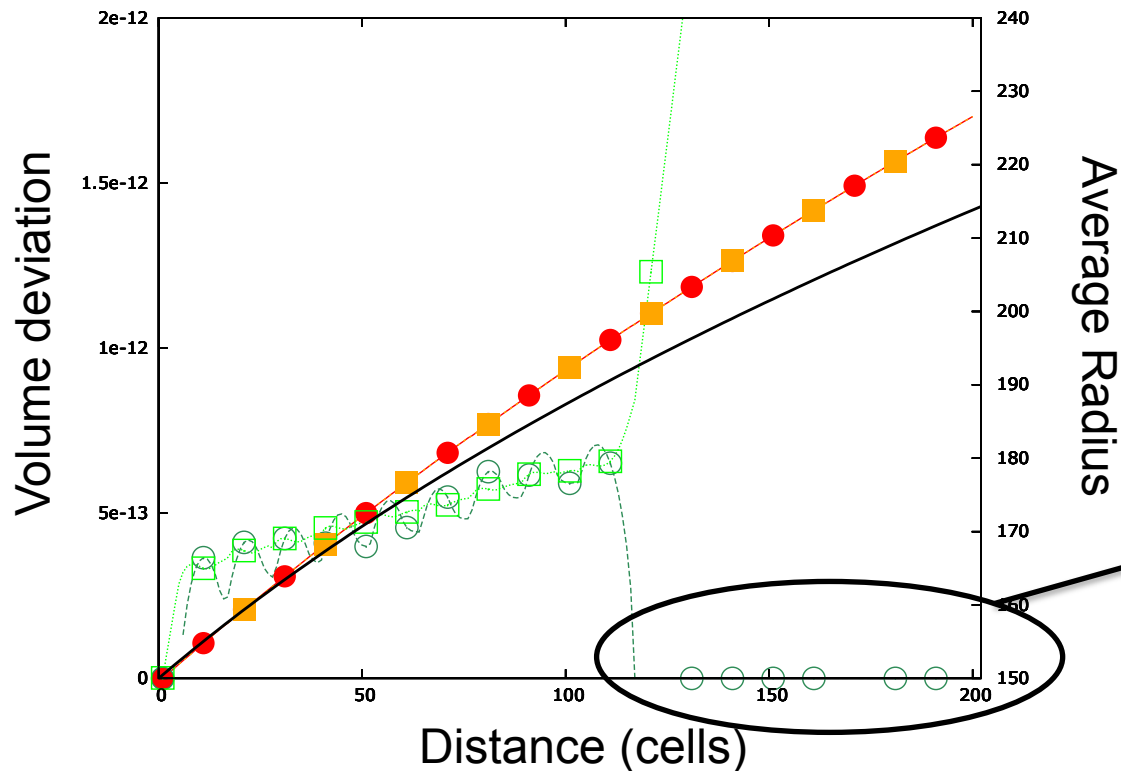
D'Herbigny – Hybrid Sectional-Lagrangian

A versatile method

- Executed with **RAPTOR E-ES**

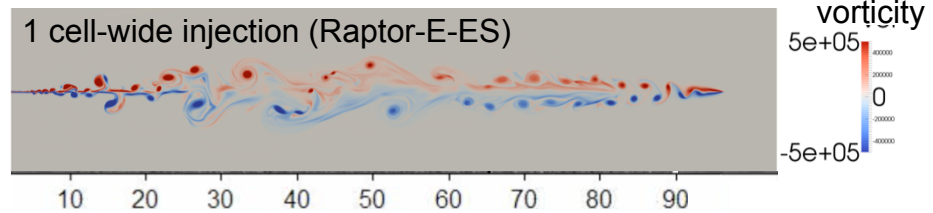
- When mass **outflows the last section**, it is injected in the cell as a cloud of **stochastic parcels**

- Good agreement on average radius
- Needs more parcels for dispersion



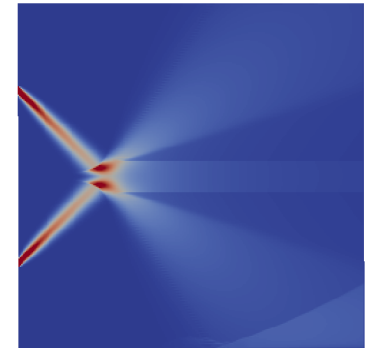
1 parcel injected:
kills size dispersion

CONCLUSION



- The semi-Lagrangian formalism is efficient for two-way coupled LES

- Provides all **qualities of Eulerian solvers**
- Robust at **high liquid/gas density ratio**
- Provide **fluctuating** data to avoid relying on RANS models



AG-QMOM with RAPTOR

- Flexibility

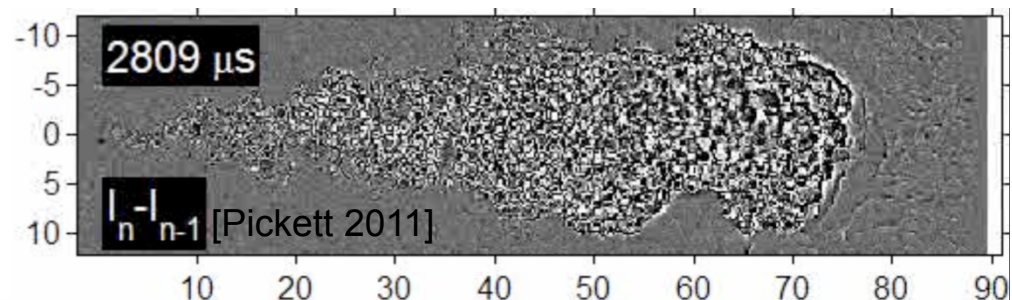
- Can host **spray models** (here coalescence)
- Dynamically **interfaced to Lagrangian** approach for inertial droplets
- Other **interfacings** possible (high order velocity moments)

Perspectives

- **Verification**

- vs CLSVOF
- vs stochastic Lagrangian
- vs Real-Gas solver

- **Validation** vs ECN results (spray A)



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