SAND2015-2924C

Modeling and simulation of a dense evaporating spray

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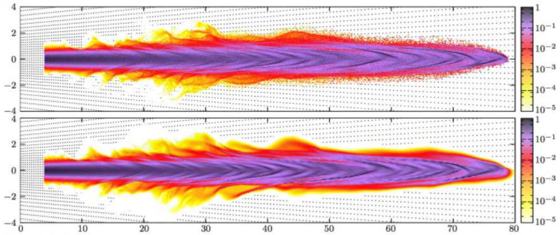
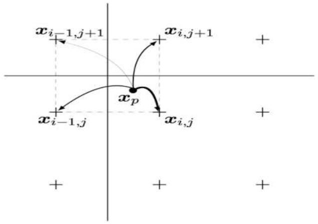
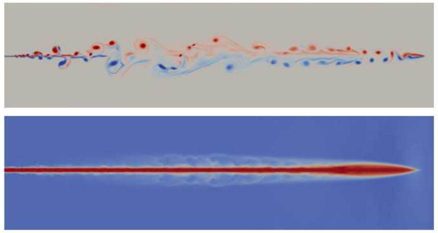




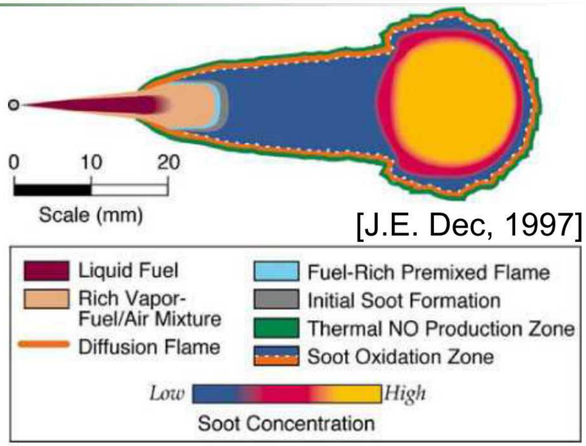


Support by Sandia National Laboratories' LDRD program
LDRD – Laboratory Directed Research and Development
Is gratefully acknowledged.

MOTIVATION – Liquid fuel injection

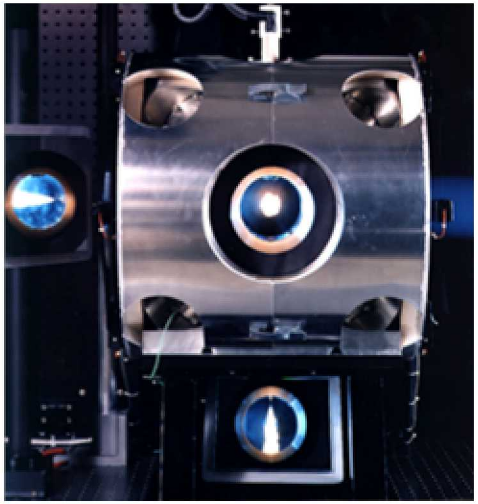
In Diesel and Gasoline engines

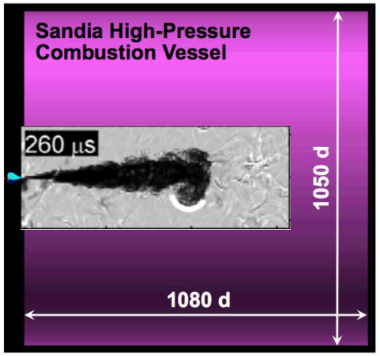
- **Inlet is turbulent** (+ cavitation)
  - Re ~ 10^5, d = 90µm
- **High pressure chamber and sonic flow**
  - p = 60bar, u_l = 600m/s
- **Atomization process not understood**
  - We ~ 10^4, 1µm < r_l < 100µm



[J.E. Dec, 1997]

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





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

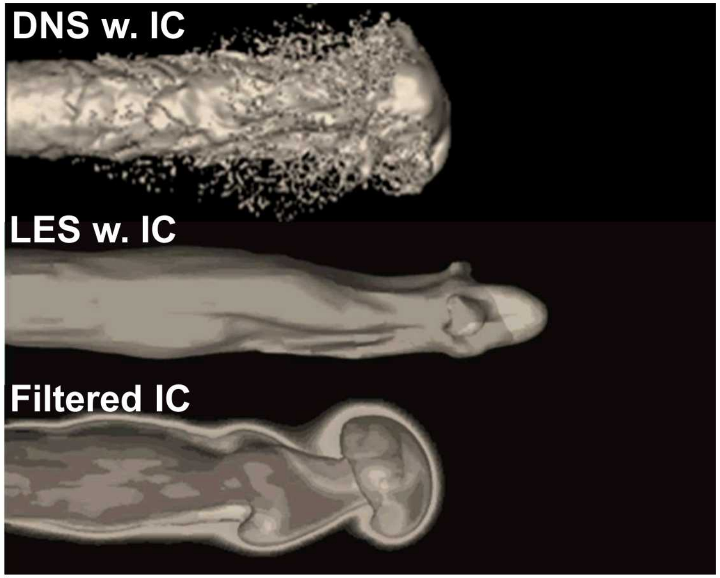
Need for a
High Fidelity Simulation
that is **affordable**

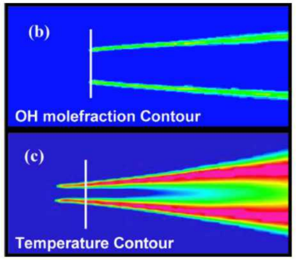
STATE OF THE ART – Injection simulation

No comprehensive simulation approaches

1 DNS with Interface Capturing
[Menard 2007; Desjardins 2010]
- **Accurate and insightful**
- **Intractably costly**

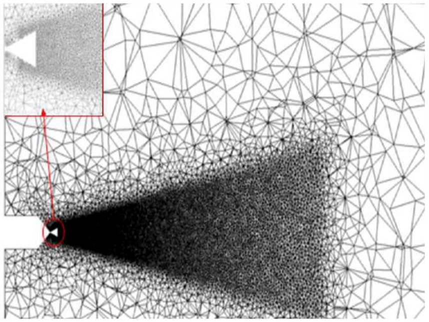
2 Filtered Interface Capturing
[Chesnel 2011]
- **Promising but empirical**

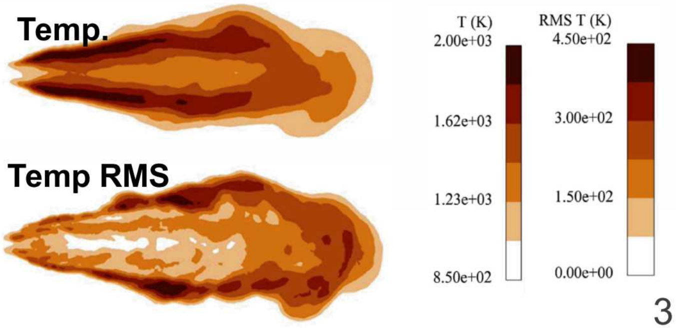




3 Extension of dilute spray with coarse AMR
[Som 2013]
- **Essential features missing**
- **Useful to investigate other physics** (e.g. complex chemistry)

1 Prescribed downstream boundary condition
[Tillou 2014]
- **Most applicable approach today**
- **Low predictibility**

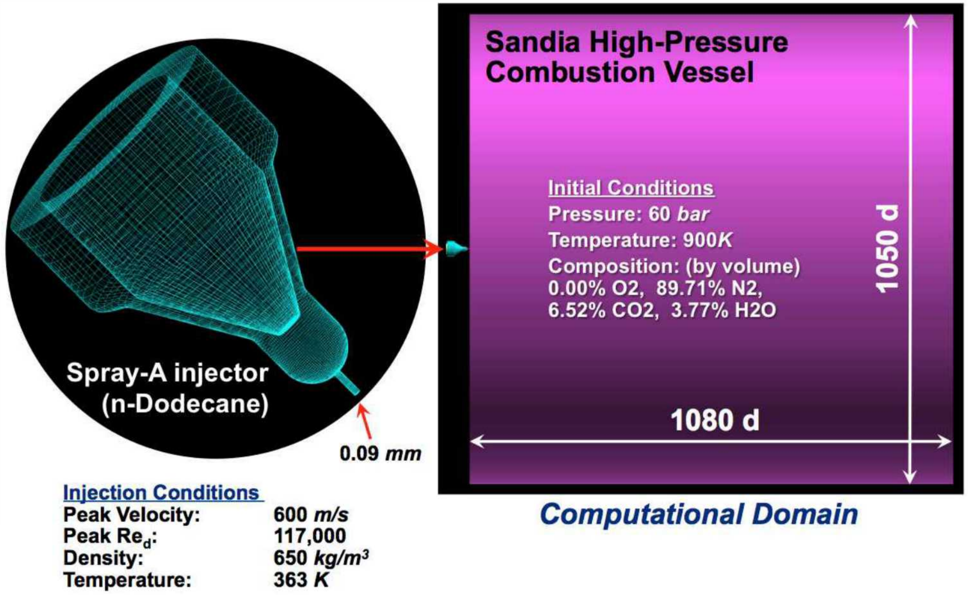




OBJECTIVE – Comprehensive simulation

From nozzle outlet to dilute spray

- **Sensitized to nozzle flow** (in an LES sense) O(1μm, 10ns)
  - **Re ~ 10^5, d = 90μm**
- **Robust to high pressures, velocities, and loadings**
  - **p = 60bar, u_l = 600m/s**
- **Compute the whole chamber** (with combustion) O (10^5μm, 10^6ns)
  - **with a billion points**



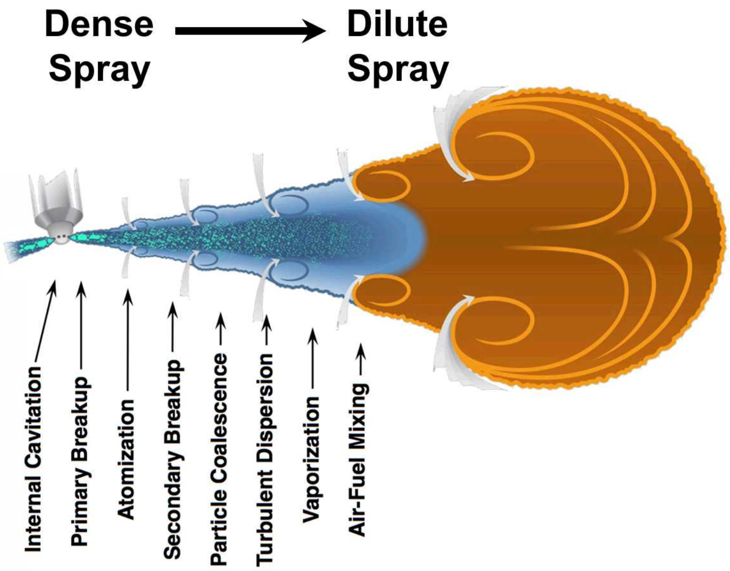
Computational Domain

We introduce a **Simplified Approach** of interface flows to describe more physical scales

MODEL – Two-phase approach

A simplified but promising approach

- **Coupled Eulerian-Eulerian** (gas and liquid moments) can **emulate at once**
  - **the inertial behavior of the dense liquid core**
  - **the break-up and dispersion of liquid blobs** (prescribes size of droplets)
  - **the dilute spray regime with droplets**



- Conservation for both **light** and **dense** phases
  - **no interface tracking**
  - **mesoscale-gradients handled more easily**
  - **as opposed to real gas approaches**
  - **but no built-in thermodynamics!**

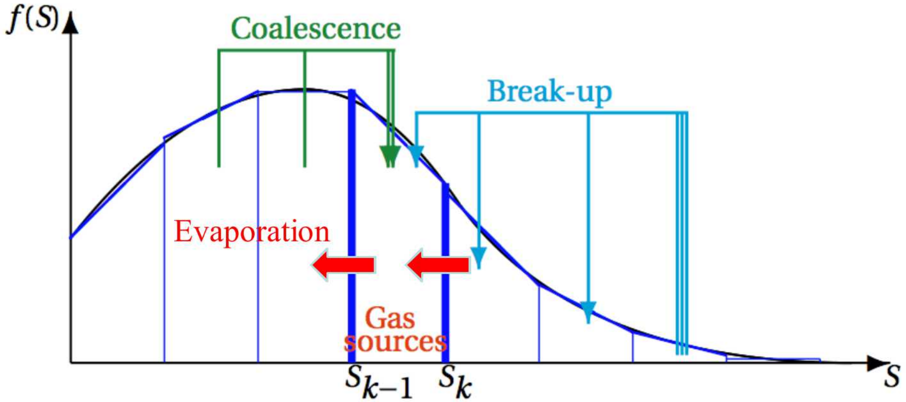
- …provided the transfers = need for **closures**!

MODEL – Sectional method

A cost-efficient way to capture polydispersity

- **Various drop sizes are treated as a continuum:**

  Multi-Fluid [Laurent 2001, Doisneau 2013]



$$N_{sec}\ \text{systems}\quad \begin{cases} \partial_t n_k + \partial_{\boldsymbol{x}}\cdot(n_k \boldsymbol{u}_k) = {}^2C^n_k + {}^2B^n_k + {}^2E^n_k \\ \partial_t m_k + \partial_{\boldsymbol{x}}\cdot(m_k \boldsymbol{u}_k) = {}^2C^m_k + {}^2B^m_k + {}^2E^m_k \\ \partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}}\cdot(m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k + {}^2\boldsymbol{C}^u_k + {}^2\boldsymbol{B}^u_k + {}^2E^u_k \\ \partial_t (m_k h_k) + \partial_{\boldsymbol{x}}\cdot(m_k h_k \boldsymbol{u}_k) = m_k H_k + {}^2C^h_k + {}^2B^h_k + {}^2E^h_k \end{cases} \rightleftharpoons \text{Navier-Stokes with } \textbf{sources}$$

…many integral source terms to compute

MODEL – Two-phase approach

Pressureless Gas Dynamics (PGD) decouples Lagrangian advection

- **The coupled NS-PGD* system**

$$
\left\{
\begin{aligned}
&\partial_t \rho_g Y_f + \partial_{\boldsymbol{x}} \rho_g Y_f \boldsymbol{u}_g &&= \omega_f + \sum_k \mathrm{E}_k^{m-g} \\
&\partial_t \rho_g Y_i + \partial_{\boldsymbol{x}} \rho_g Y_i \boldsymbol{u}_g &&= \omega_i \;, \qquad i \in [\![1; N_{\text{species}}]\!],\; i \neq f \\
&\partial_t \rho_g \boldsymbol{u}_g + \partial_{\boldsymbol{x}} \rho_g \boldsymbol{u}_g \otimes \boldsymbol{u}_g &&= -\partial_{\boldsymbol{x}} p + \sum_k \left(-\boldsymbol{F}_k + \boldsymbol{u}_k \mathrm{E}_k^{m-g} \right) \\
&\partial_t \rho_g e_g + \partial_{\boldsymbol{x}} \rho_g e_g \boldsymbol{u}_g &&= -p \partial_{\boldsymbol{x}} \boldsymbol{u}_g + \sum_k \left(-\mathrm{H}_k + \boldsymbol{F}_k (\boldsymbol{u}_g - \boldsymbol{u}_k) + h_k \mathrm{E}_k^{m-g} \right) \\
&\partial_t m_k + \partial_{\boldsymbol{x}} m_k \boldsymbol{u}_k &&= \mathrm{E}_{k+1}^{m} + \mathrm{B}_k^{m+} + \mathrm{C}_k^{m+} - \left(\mathrm{E}_k^{m} + \mathrm{E}_k^{m-g} + \mathrm{B}_k^{m-} + \mathrm{C}_k^{m-} \right) \\
&\partial_t m_k \boldsymbol{u}_k + \partial_{\boldsymbol{x}} m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k &&= \boldsymbol{F}_k + \boldsymbol{u}_{k+1} \mathrm{E}_{k+1}^{m} + \boldsymbol{B}_k^{u+} + \boldsymbol{C}_k^{u+} - \boldsymbol{u}_k \left(\mathrm{E}_k^{m} + \mathrm{E}_k^{m-g} + \mathrm{B}_k^{m-} + \mathrm{C}_k^{m-} \right) \\
&\partial_t m_k h_k + \partial_{\boldsymbol{x}} m_k h_k \boldsymbol{u}_k &&= \mathrm{H}_k + h_{k+1} \mathrm{E}_{k+1}^{m} + \mathrm{B}_k^{h+} + \mathrm{C}_k^{h+} - h_k \left(\mathrm{E}_k^{m} + \mathrm{E}_k^{m-g} + \mathrm{B}_k^{m-} + \mathrm{C}_k^{m-} \right)
\end{aligned}
\right.
\quad k \in [\![1; N_{\text{sec}}]\!]
$$

pressureless

sections

Needs to be closed

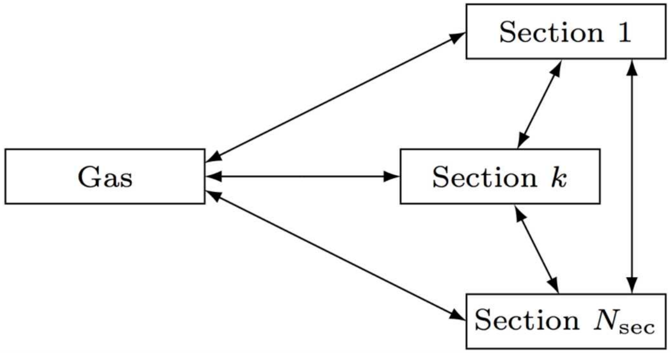
*obtained from kinetic theory or conservation principles

$$\partial_t f + \partial_{\boldsymbol{x}} \boldsymbol{c} f + \partial_{\boldsymbol{c}} \mathbf{F} f + \partial_\theta \mathrm{H} f + \partial_r \mathrm{E} f = \mathrm{B} + \mathrm{C}$$

MODEL – The closure problem

LES closures should respect dominant dynamics and equilibrium

- **Need the rate of exchange for**
  - **Momentum** (drag and dynamic subgrid model)
  - **Heat** (heating)
  - **Mass** (vaporization and combustion subgrid model)



- **Derivation from first principles is hard**
  - **All thermophysical properties needed**
  - **Subgrid knowledge needed too** (turbulent & atomizing)

- **Should enforce thermodynamics and equilibria**
  - **Multifluid models** by Saurel's team [D. Furfaro, 2015]

ANALYSIS – Two-way coupling

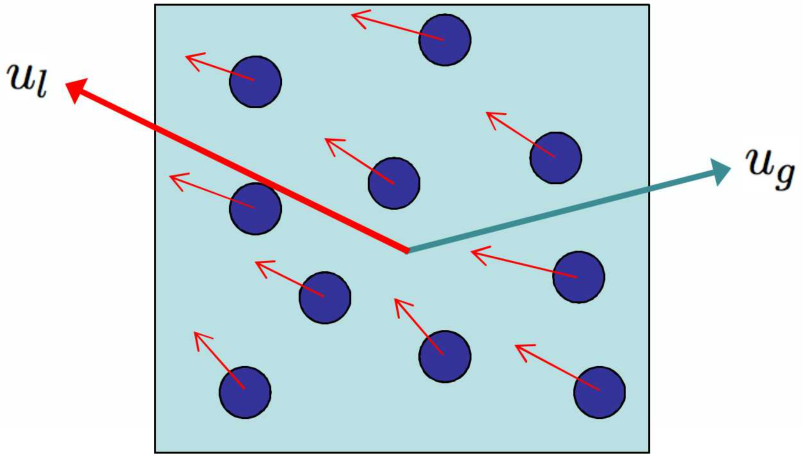
Two-way coupling as the main driver of characteristic times

- **Two-way coupling drives characteristic times** $C = \frac{m_l}{m_g}$
  - **Example for drag (0D):** [Doisneau, 2013]

$$\begin{cases} \partial_t(m_g u_g) = \frac{m_l}{\tau}(u_l - u_g) \\ \partial_t(m_l u_l) = -\frac{m_l}{\tau}(u_l - u_g) \end{cases} \Leftrightarrow \begin{cases} \partial_t(m_g u_g + m_l u_l) & = 0 \\ \partial_t(u_l - u_g) & = -\frac{1+C}{\tau}(u_l - u_g) \end{cases}$$

- **Correction factor can be large since C reaches** ~100

$$\tau^{\text{2-way}} = \frac{\tau}{1+C}$$



ANALYSIS – Two-way coupling

Two-way coupling as the main driver of characteristic times

- **Two-way coupling drives characteristic times**
  - **Drag**
  - **Same argument for heating**
  - **Vaporization is driven by heating**

$$C = \frac{m_l}{m_g}$$

$$\partial_t d^2 = -K$$

$$K = \frac{8\lambda_g}{\rho_l c_{p,g}} \log\left(1 + \frac{c_{p,g}(T_g - T_l)}{h_l}\right)$$

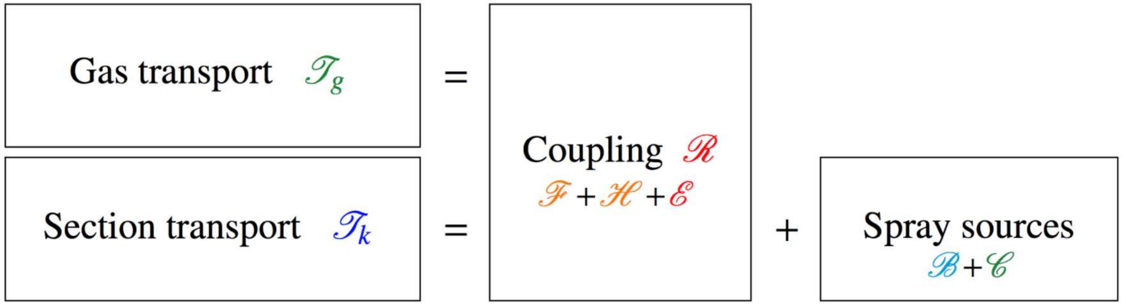
- **Correction factor can be large since C reaches** ~100

$$\tau^{\text{2-way}} = \frac{\tau}{1+C}$$

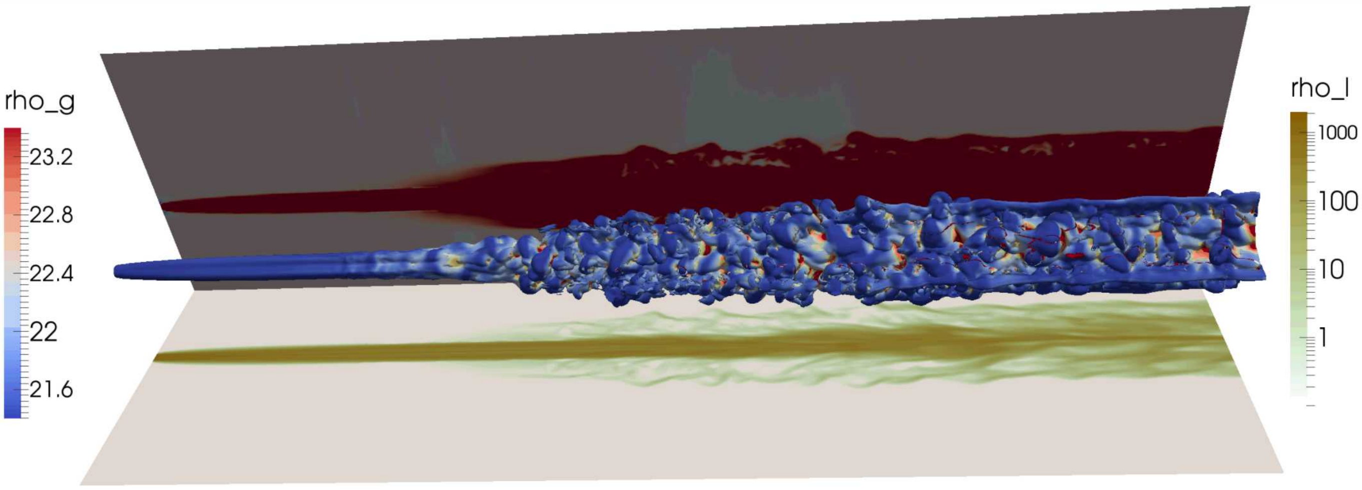
NUMERICS – Two-way coupling needs

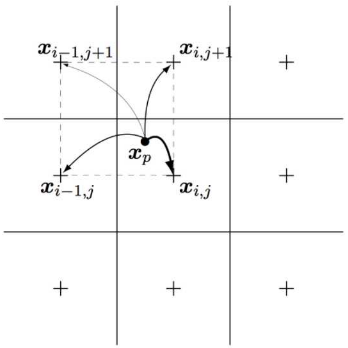
Effort on numerical methods for multi-scale coupled flows

- **1) Time integration tailored splitting**



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



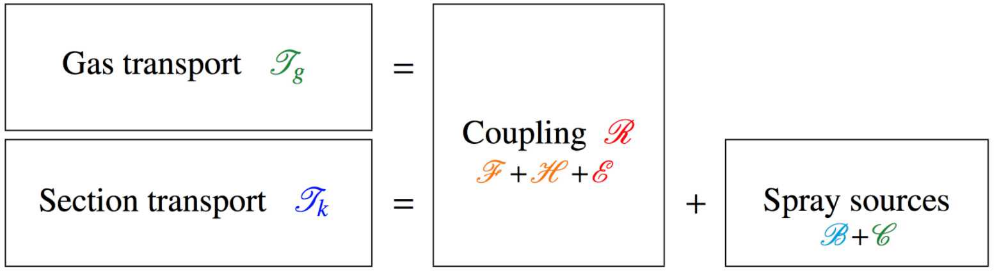


NUMERICS – Time integration

A Tailored Operator Splitting

Operator splitting

- Recycle legacy solvers
- Robust time integration
- Local properties enforced
- Adaptable accuracy



- **to integrate all phase exchange terms $\mathscr{R}$ at once (RK4)**
  - Realizability, conservativity, equilibrium
  - Strong couplings

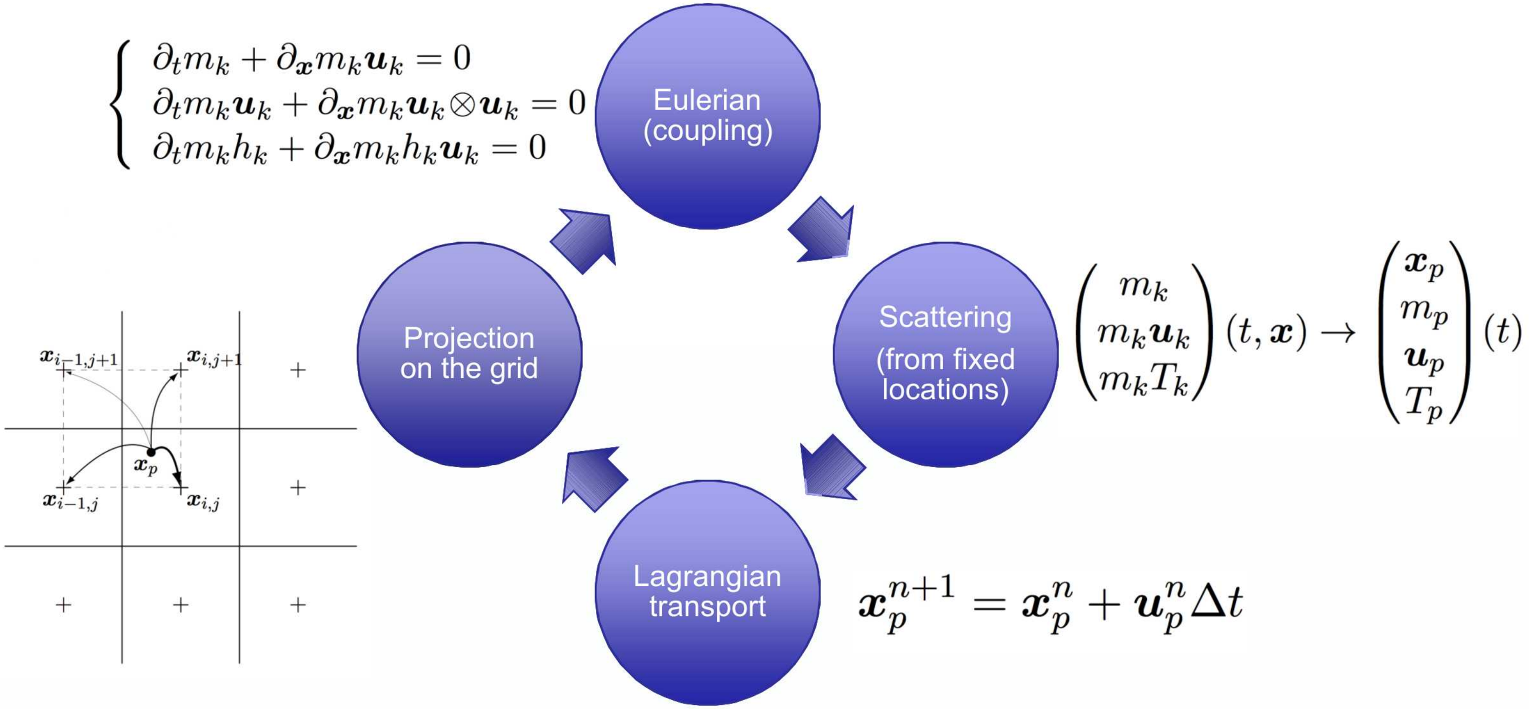
$$\boldsymbol{U}^{n+1} = \mathscr{R} \prod_{k=1}^{N_{\mathrm{sec}}} (\mathscr{T}_k) \; \mathscr{T}_g \; \boldsymbol{U}^n$$

- **to integrate spray sources $\mathscr{B}$ + $\mathscr{C}$**
  - Realizability and convergence
  - Strong particle-particle coupling

$$\boldsymbol{U}^n = \begin{pmatrix} \rho_g Y_i \\ \rho_g \boldsymbol{u}_g \\ \rho_g e_g \\ n_k \\ m_k \\ m_k \boldsymbol{u}_k \\ m_k h_k \end{pmatrix}^n$$

NUMERICS – PGD transport

A robust and accurate answer to PGD peculiarities

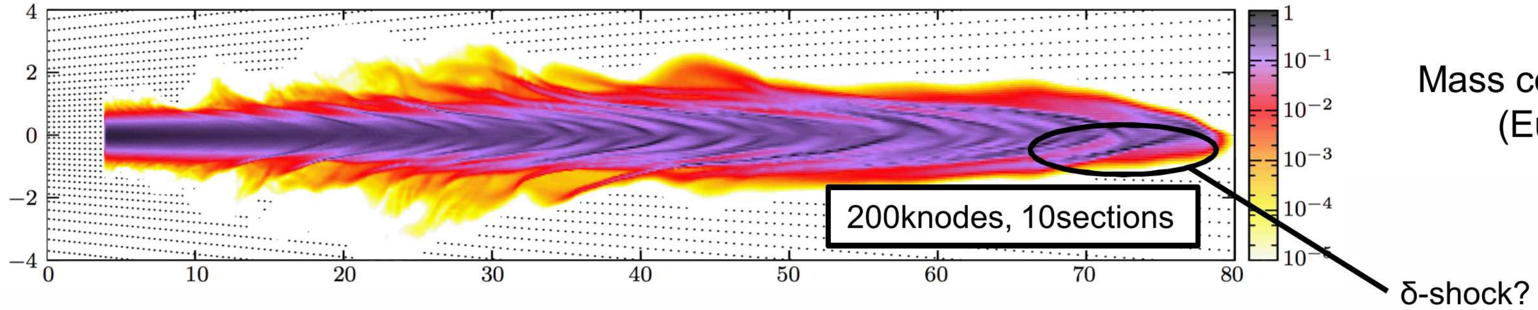


- **Novel semi-Lagrangian PGD transport scheme**
  - **Deterministic: no noise**
  - **Localizes spray info at mesh nodes: good for coupling**
  - **Easier load balancing**
  - **No fluxes to be computed: reduce cost and numerical diffusion**

NUMERICS – PGD transport

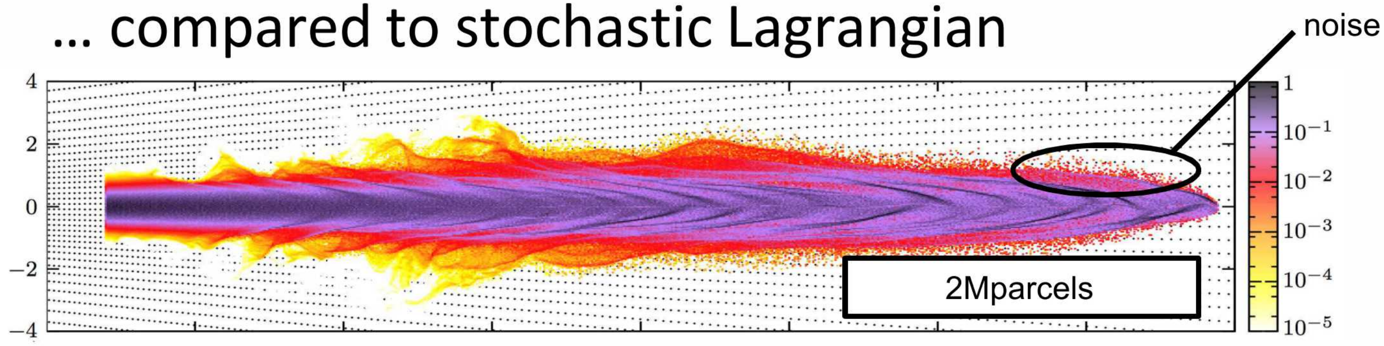
2D test with prescribed flow field

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



Mass concentration (Eulerian)

… compared to stochastic Lagrangian

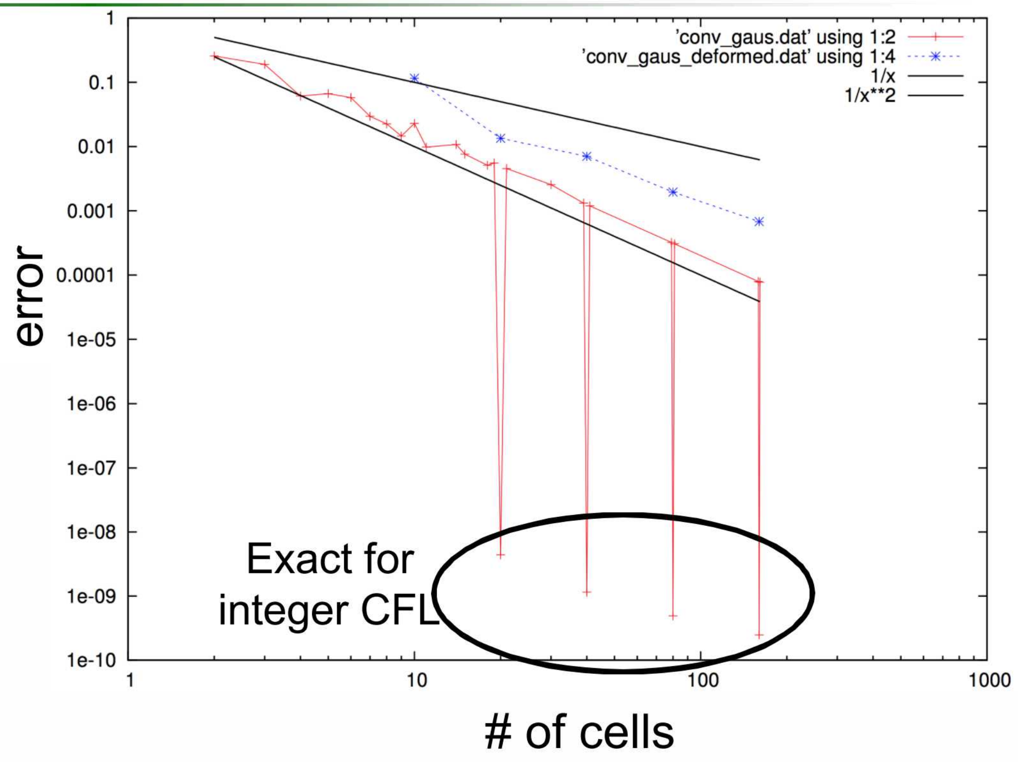


Mass concentration (Lagrangian)

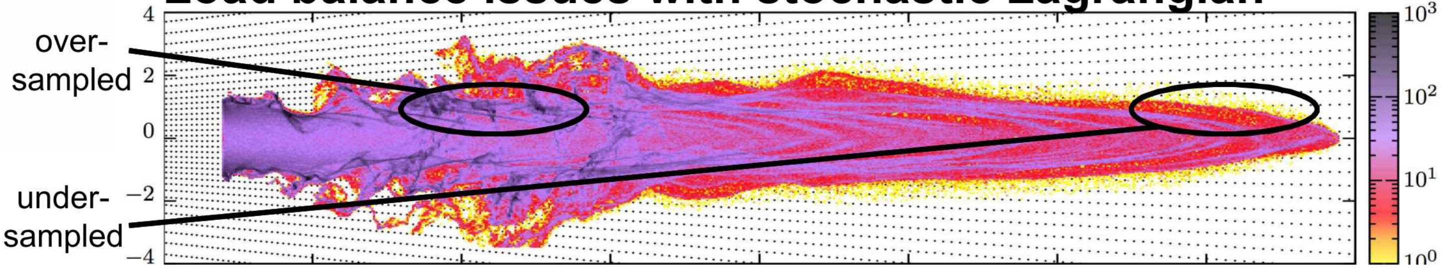
NUMERICS – PGD transport

Transport is 2nd order in space

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



Load balance issues with stochastic Lagrangian



TEST 1 – Momentum Coupling

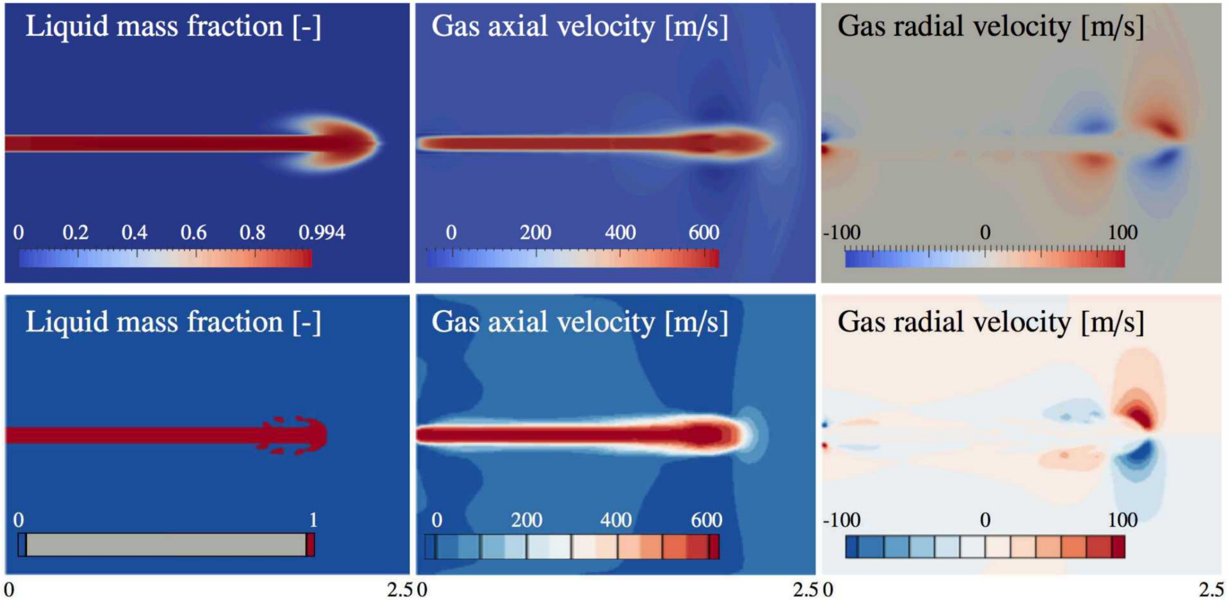
Comparison between E-ES and CLSVOF

✓ **Supersonic injection** (toy problem)

- velocity plug-flow boundary
- no thermal transfer
- T_{end} = 4μs

Raptor with E-ES

Δx = 12.5 μm, Δt = 8 ns



CLSVOF

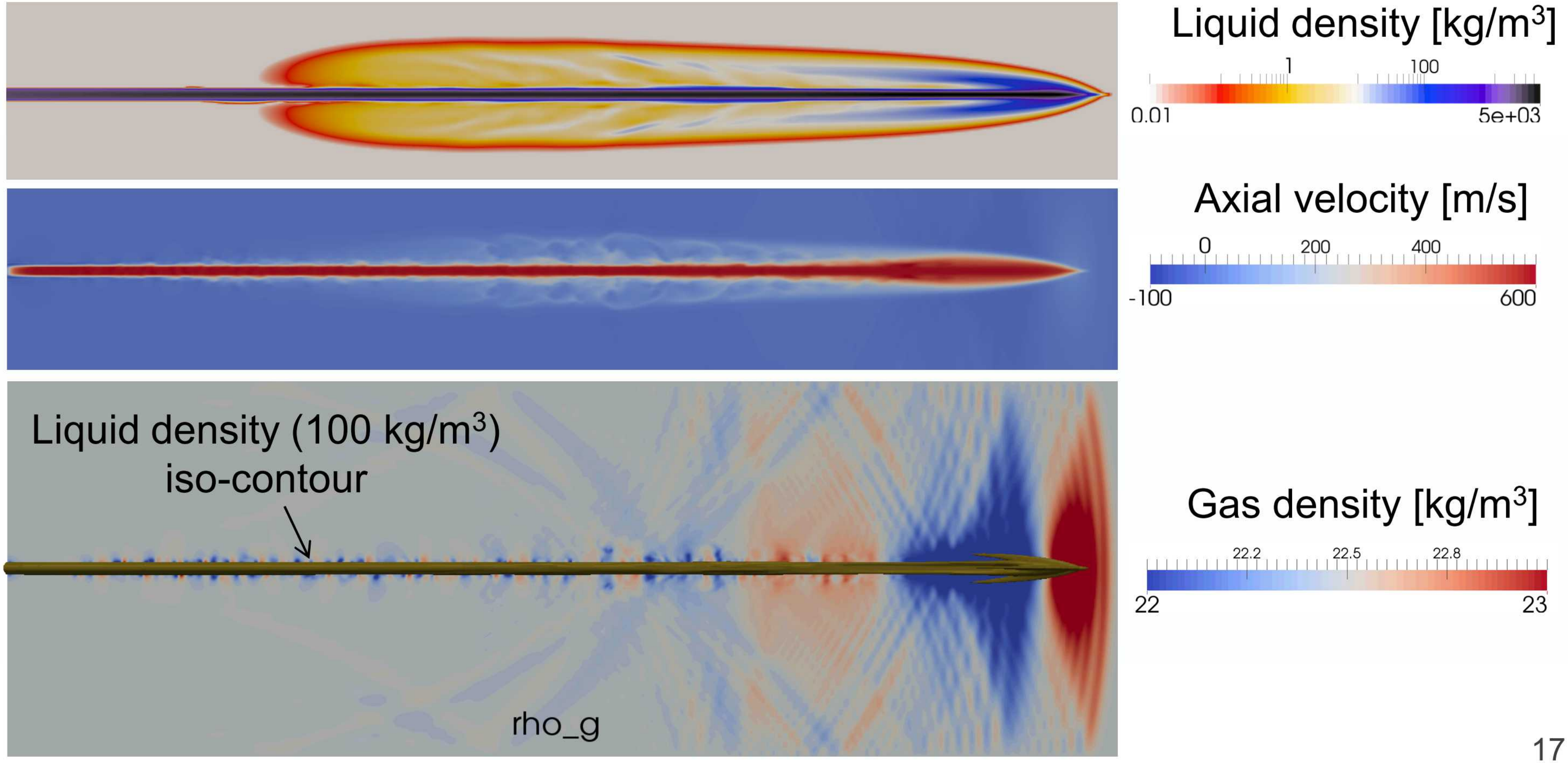
Δx = 13.3 μm, Δt ~ 6 ns

- ✓ 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

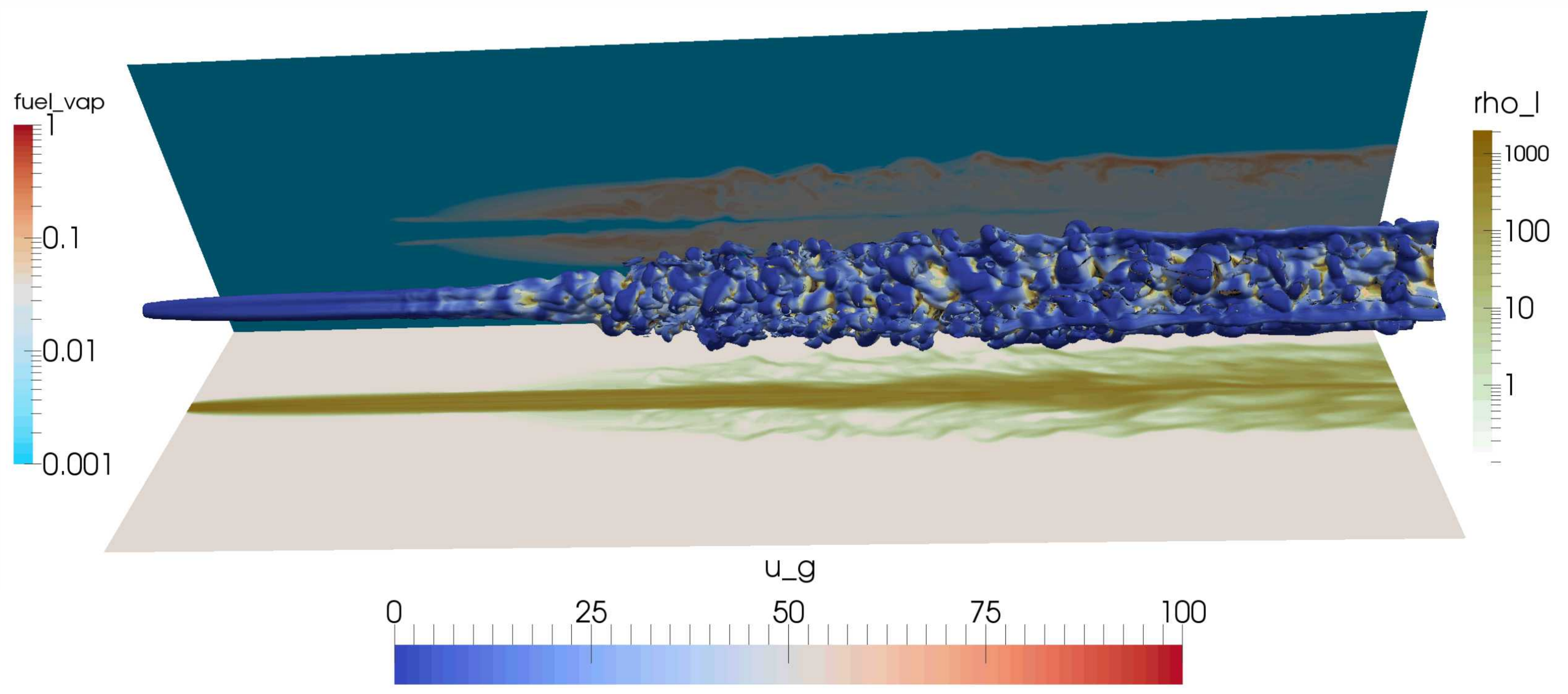
- Executed with **RAPTOR + E-ES**



TEST 3 – Fuel vaporization

Fuel vapor footprint

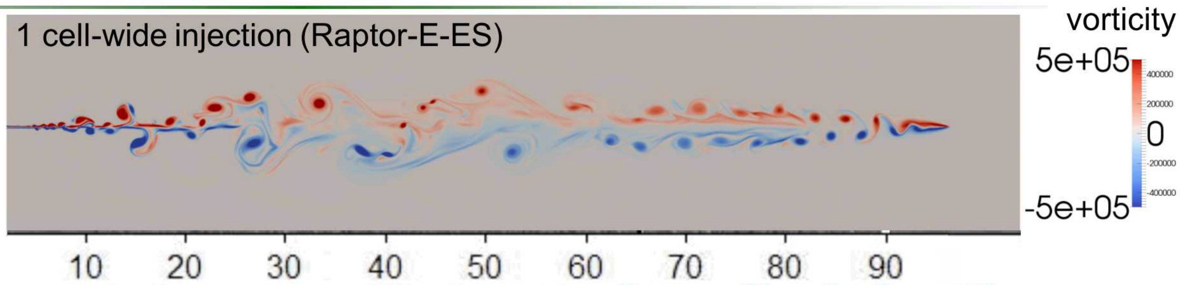
- Executed with **RAPTOR E-ES**
  - **Box 3x3x10mm**
  - **d_{inj}=90μm, T_{end}=40μs**
  - **quiescent gas at 60bar, 900K**
  - **n-dodecane at 702kg/m^3, 600m/s**
  - **50Mcells** (cartesian mesh)
  - **Δx=12.5μm, Δt=8ns, T_{end}=40μs**
  - **1 section** (prescribed initial size)
  - **PGD transport** (δ-shocks)
  - **d^2-law**



CONCLUSION

Conclusion

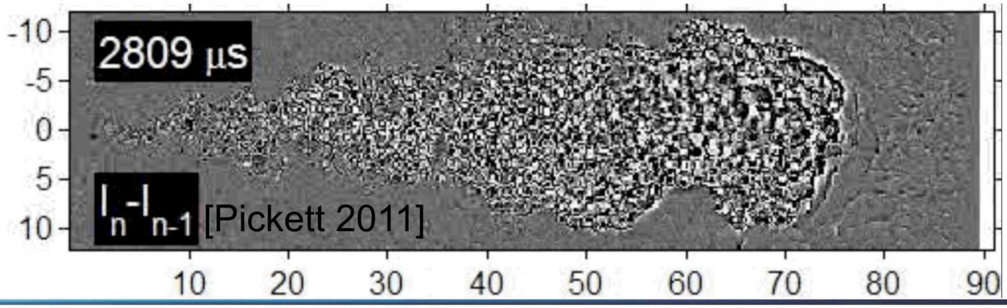
- **Kinetic theory**
- **Two-way coupling**
- **Dedicated numerics**



Spray tools are promising to efficiently handle injection

Perspectives

- **Dense core dynamics**
  - pressure/crossings
  - turbulence
  - surface tension
- **High-pressure mixing**
  - atomization
  - "evaporation"
  - LES closure
- **Combustion**
  - chemistry
  - LES closure
  - numerics
- **Verification**
  - vs CLSVOF
  - vs stochastic Lagrangian
  - vs Real-Gas solver
- **Validation** vs ECN results (spray A)



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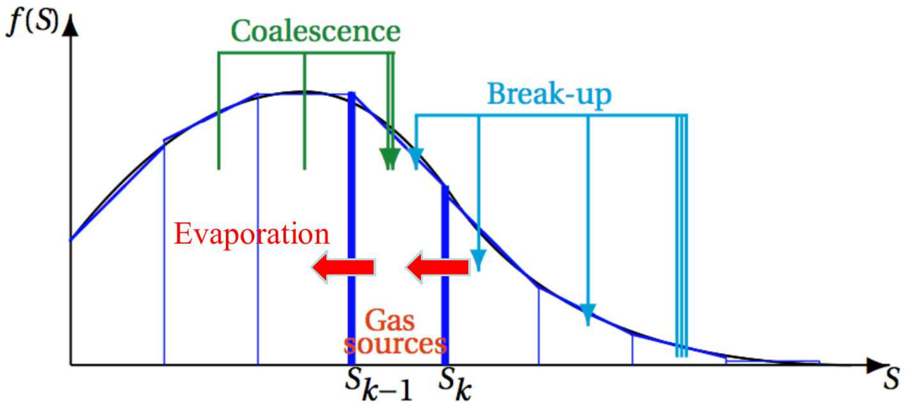
BACK-UP

MODEL – Sectional method

A cost-efficient way to capture polydispersity

- **Various drop sizes are treated as a continuum**



N_{sec} systems

$$\begin{cases} \partial_t n_k + \partial_{\boldsymbol{x}} \cdot (n_k \boldsymbol{u}_k) = {}^2C_k^n + {}^2B_k^n + {}^2E_k^n \\ \partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = {}^2C_k^m + {}^2B_k^m + {}^2E_k^m \\ \partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k + {}^2\boldsymbol{C}_k^u + {}^2\boldsymbol{B}_k^u + {}^2E_k^u \\ \partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = m_k H_k + {}^2C_k^h + {}^2B_k^h + {}^2E_k^h \end{cases}$$

$\rightleftharpoons$ Navier-Stokes with **sources**

…many integral source terms to compute

NUMERICS – PGD transport

Transport is 2nd order in space

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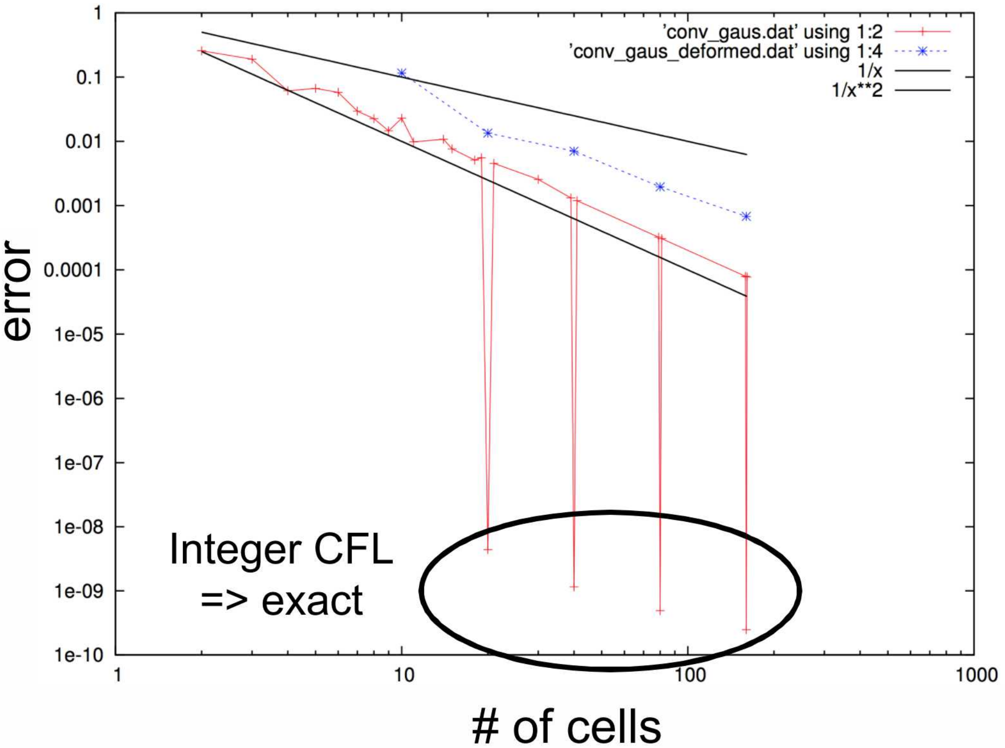
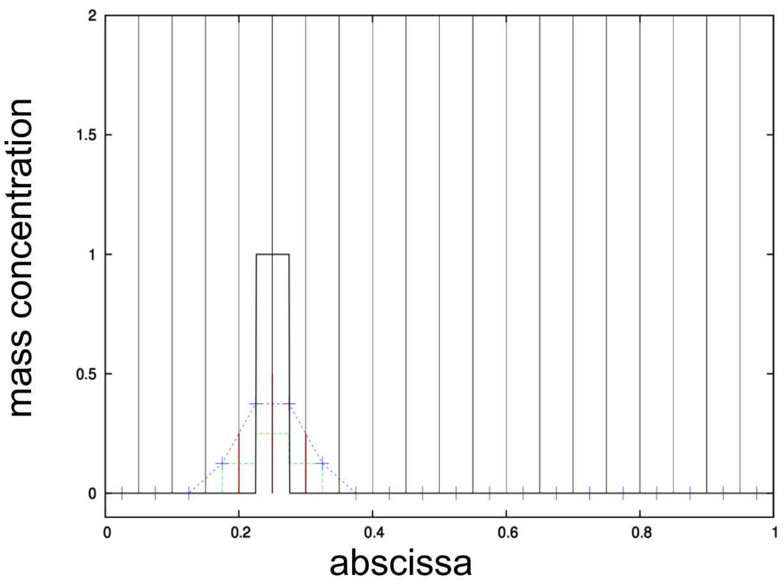
- **Handles vacuum**
- **Handles δ-shocks**

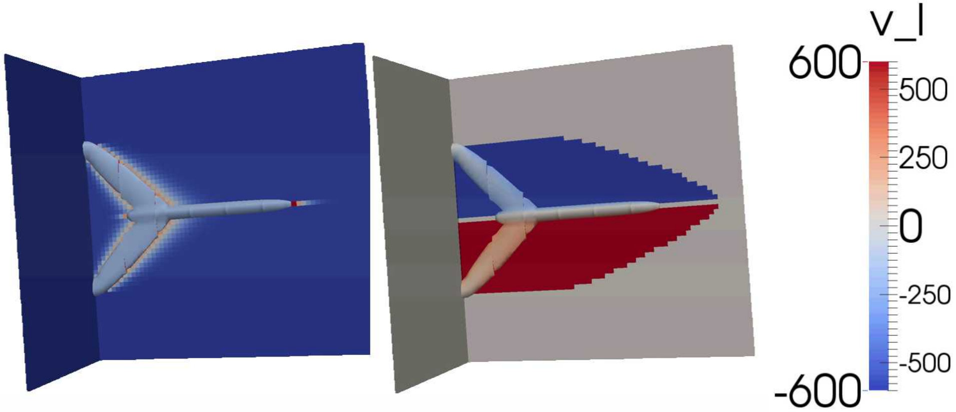




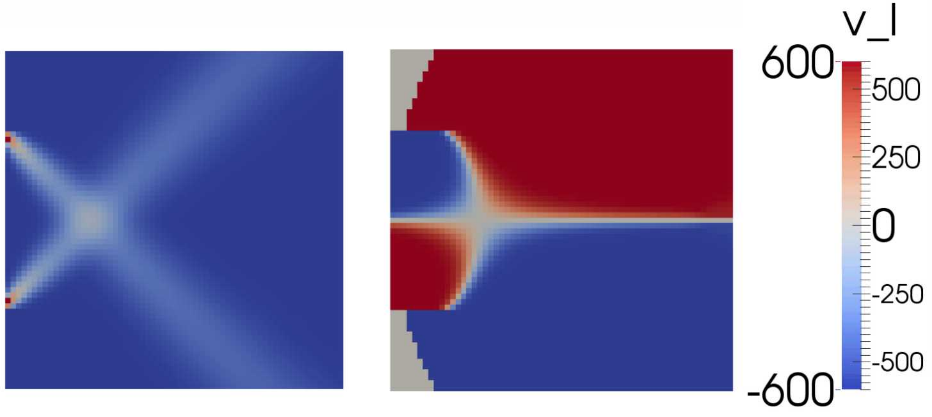
NUMERICS – Beyond PGD transport

Prevention of δ-shocks

- **δ-shocks are an artifact from the PGD assumption**
  - no grid convergence
  - erroneous density and gradients
  - troublesome with two-way coupling



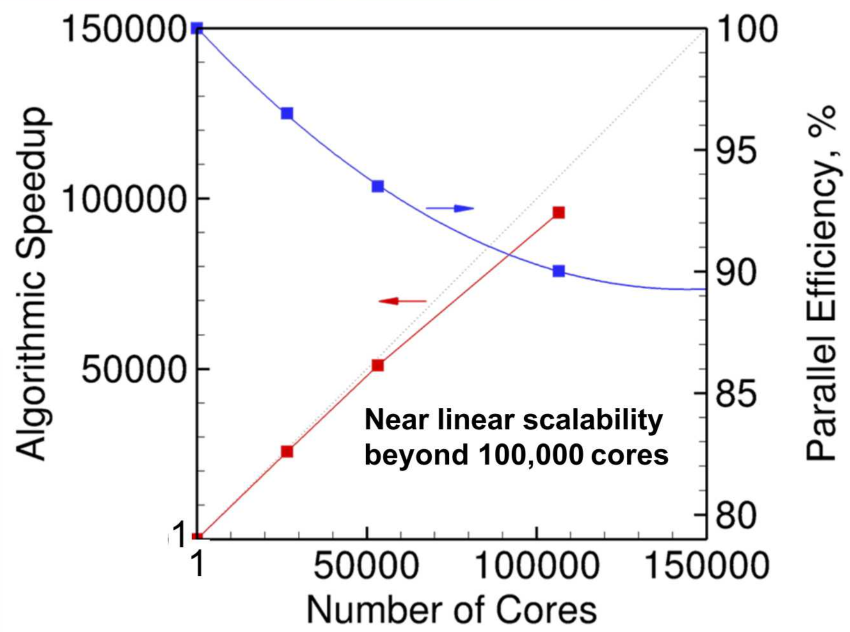
- **Higher order moment methods are developed to solve this**



NUMERICS – Raptor

A general solver optimized for LES

- **Theoretical framework**
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray
  - Dynamic SGS modeling (No Tuned Constants)
  - Advanced UQ methods for error/sensitivity analysis



- **Numerical framework**
  - Staggered finite-volume differencing (non-dissipative, discretely conservative)
  - Dual-time stepping with generalized preconditioning (all-Mach-number formulation)
  - Detailed treatment of geometry, wall phenomena, BC's

- **High-performance computing framework (Advanced parallel programming model that makes optimal use of advanced MP-computer architectures)**
- **Results from strong and weak scaling on Oak Ridge National Laboratory CRAY XK7 (Titan), June 2013**
  - Test case – jet-in-cross-flow, 500-million cells
  - Strong scaling: 24,000 to 120,000 cores, > 90% efficiency
  - Weak scaling: 500-million-cells/24,000-cores to 2-billion-cells/120,000-cores, < 4% increase in CPU time
- **Currently being refactored for hybrid multi-core parallelism and GPU acceleration (MPI/OpenMP/OpenACC)**