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A dense spray solver for injection LES

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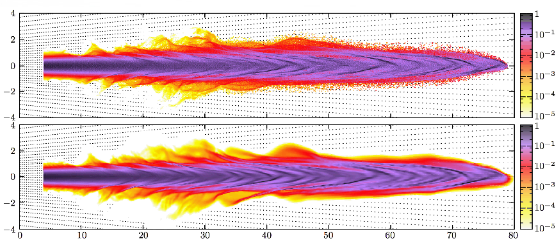

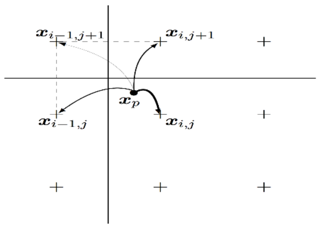

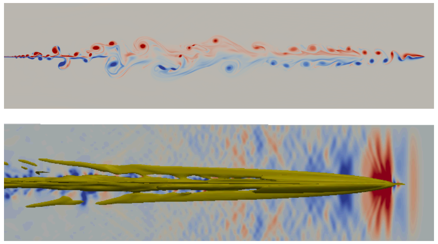

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LDRD – Laboratory Directed Research and Development

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OUTLINE

1 Motivation

2 Model

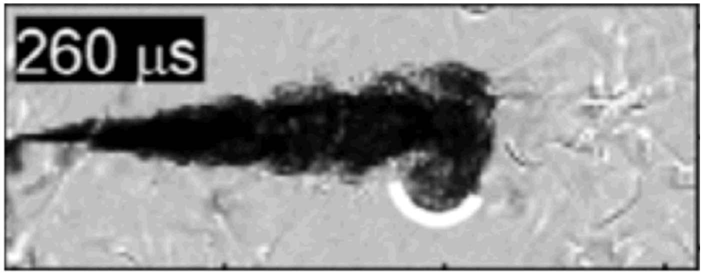
3 Numerics

4 Results

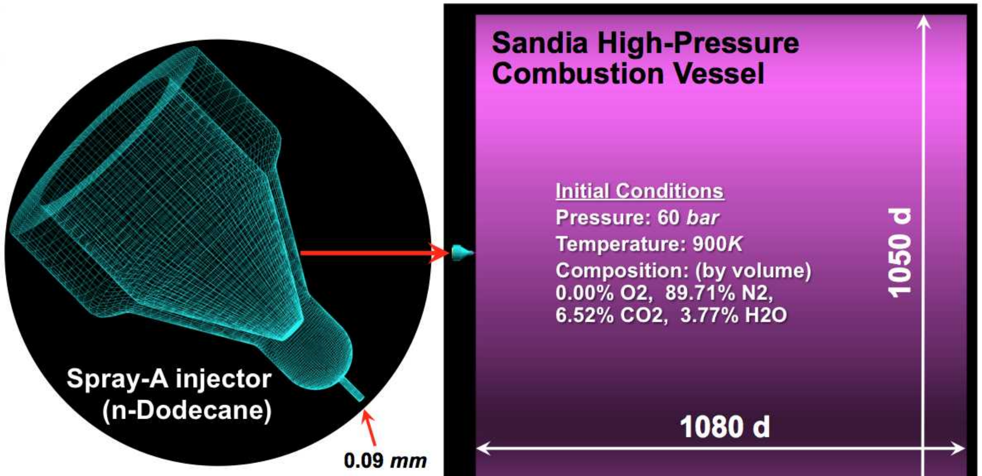
5 Conclusion

MOTIVATION – Liquid fuel injection

- **Inlet is turbulent (+ cavitation)**
- **Chamber flow high pressure and sonic**
- **Atomization process not understood**



=> all these phenomena drive **mixing** and **combustion**



Computational Domain

Injection Conditions

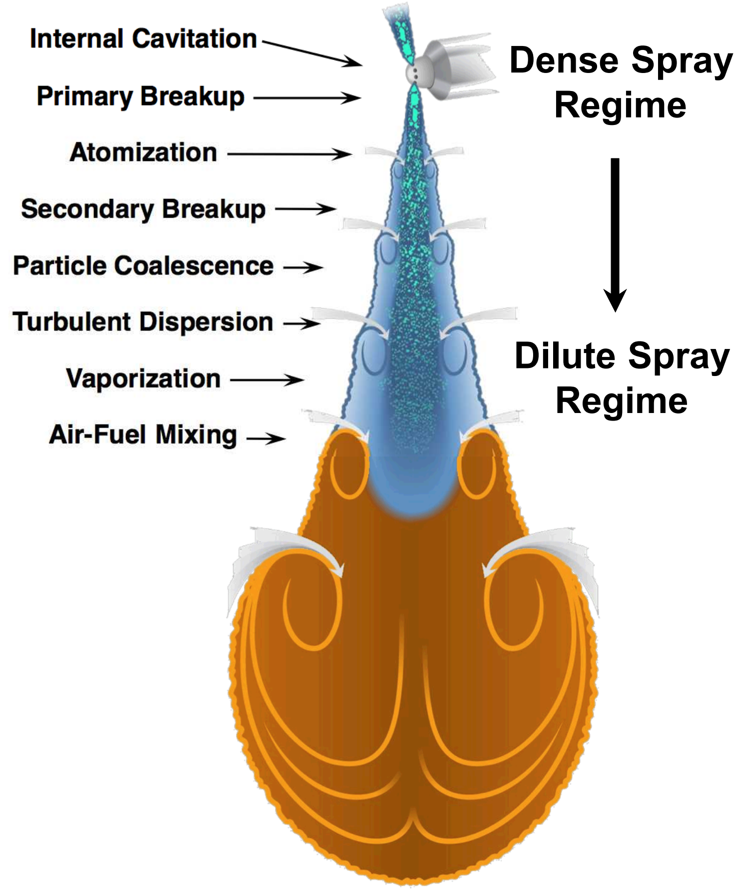
Peak Velocity:	600 *m/s*
Peak Re_d:	117,000
Density:	650 *kg/m*^{3}
Temperature:	363 *K*

Need
a **high fidelity** though
affordable simulation

MODEL – Euler-Euler spray

A simplified but promising approach

- **Coupled NS-PGD** (Pressureless Gas Dynamics) 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**

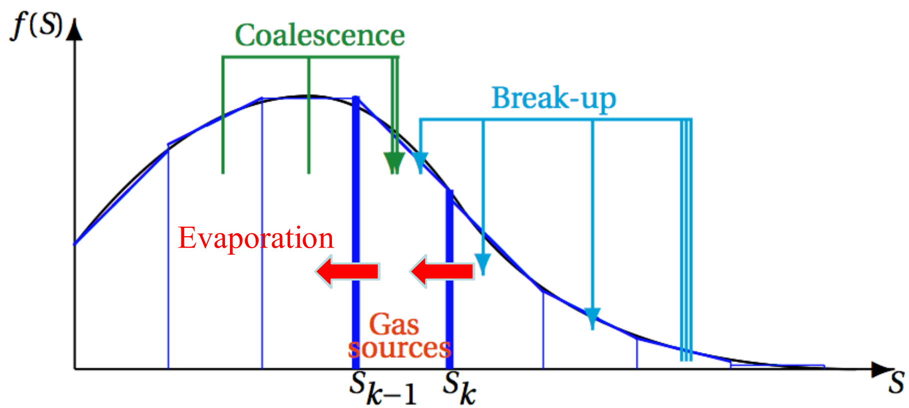


- …provided some modeling
  = need **closures**!

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

MODEL – Euler-Euler spray (E-ES)

Pressureless Gas Dynamics (PGD) decouples Lagrangian advection

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

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

pressureless

sections

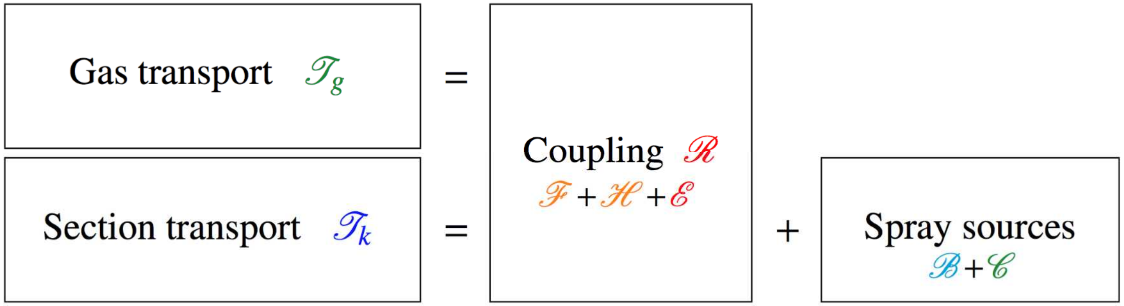
*obtained from kinetic theory or conservation principles

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

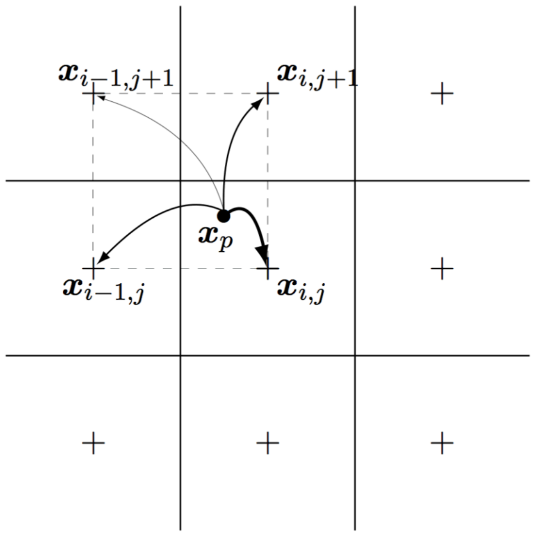
NUMERICS

Outline

- **1) Time integration**
  tailored splitting



- **2) PGD 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

Gas transport $\mathscr{T}_g$ = Coupling $\mathscr{R}$ ($\mathscr{F}+\mathscr{H}+\mathscr{E}$)

Section transport $\mathscr{T}_k$ = Coupling $\mathscr{R}$ ($\mathscr{F}+\mathscr{H}+\mathscr{E}$) + Spray sources $\mathscr{B}+\mathscr{C}$

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

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

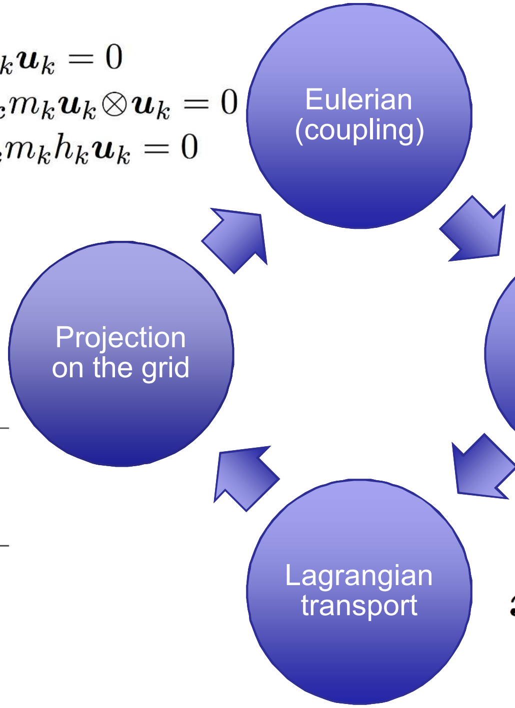
- to integrate spray sources $\mathscr{B}+\mathscr{C}$
  - Realizability and convergence
  - Strong particle-particle coupling

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

NUMERICS – PGD transport

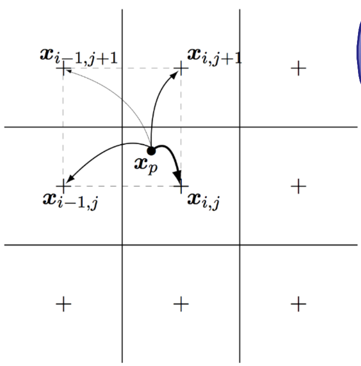
A robust and accurate answer to PGD peculiarities

$$\begin{cases} \partial_t m_k + \partial_{\boldsymbol{x}} m_k \boldsymbol{u}_k = 0 \\ \partial_t m_k \boldsymbol{u}_k + \partial_{\boldsymbol{x}} m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k = 0 \\ \partial_t m_k h_k + \partial_{\boldsymbol{x}} m_k h_k \boldsymbol{u}_k = 0 \end{cases}$$



$$\begin{pmatrix} m_k \\ m_k \boldsymbol{u}_k \\ m_k T_k \end{pmatrix} (t, \boldsymbol{x}) \rightarrow \begin{pmatrix} \boldsymbol{x}_p \\ m_p \\ \boldsymbol{u}_p \\ T_p \end{pmatrix} (t)$$

$$\boldsymbol{x}_p^{n+1} = \boldsymbol{x}_p^n + \boldsymbol{u}_p^n \Delta t$$

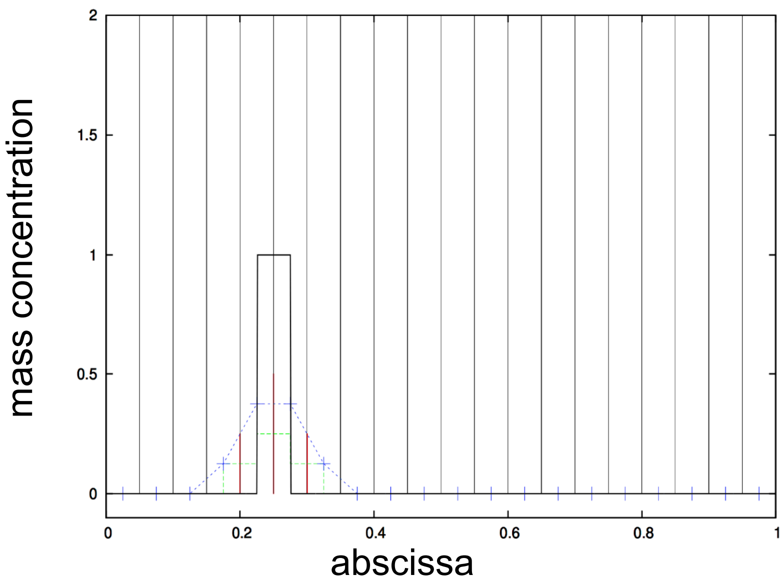


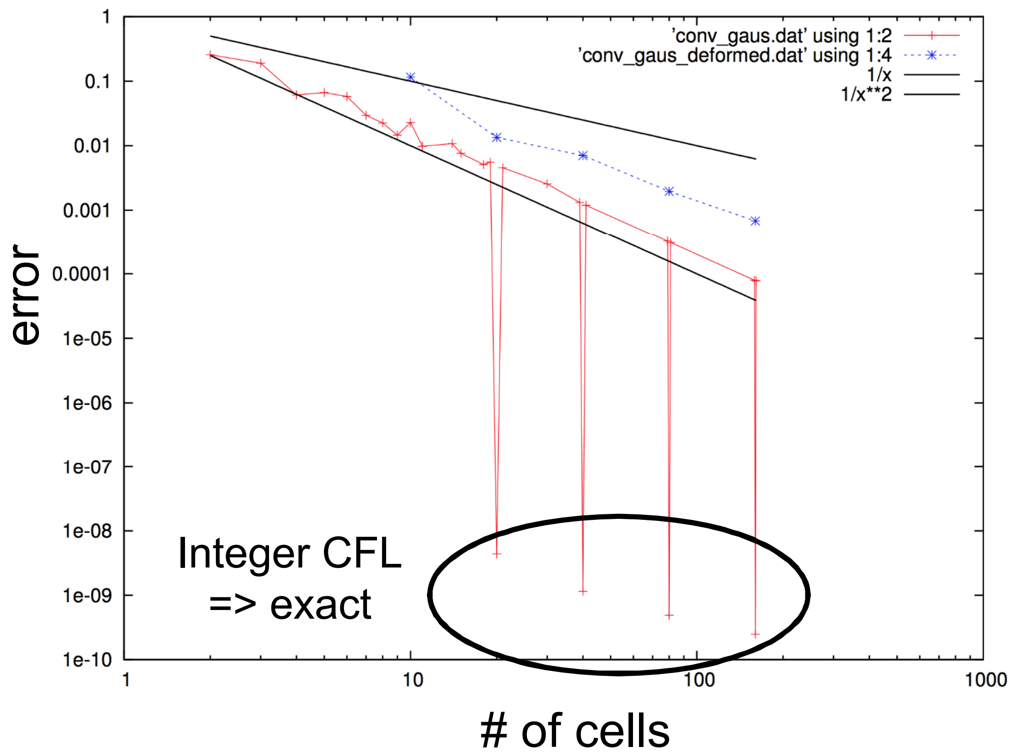
- **Novel semi-Lagrangian PGD transport scheme**
  - **Deterministic: no noise**
  - **Localizes spray info at mesh nodes: good for coupling**
  - **Easier load balancing**
  - **No fluxes to be computed: reduce cost and numerical diffusion**

NUMERICS – PGD transport

Transport is 2nd order in space

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

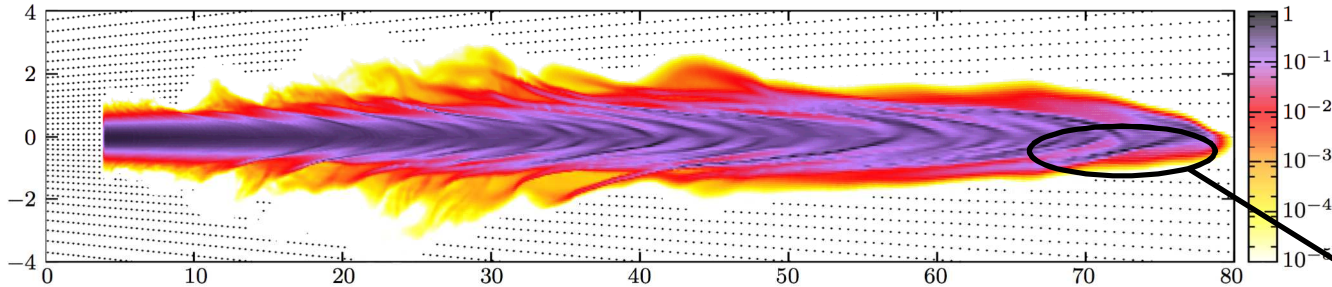




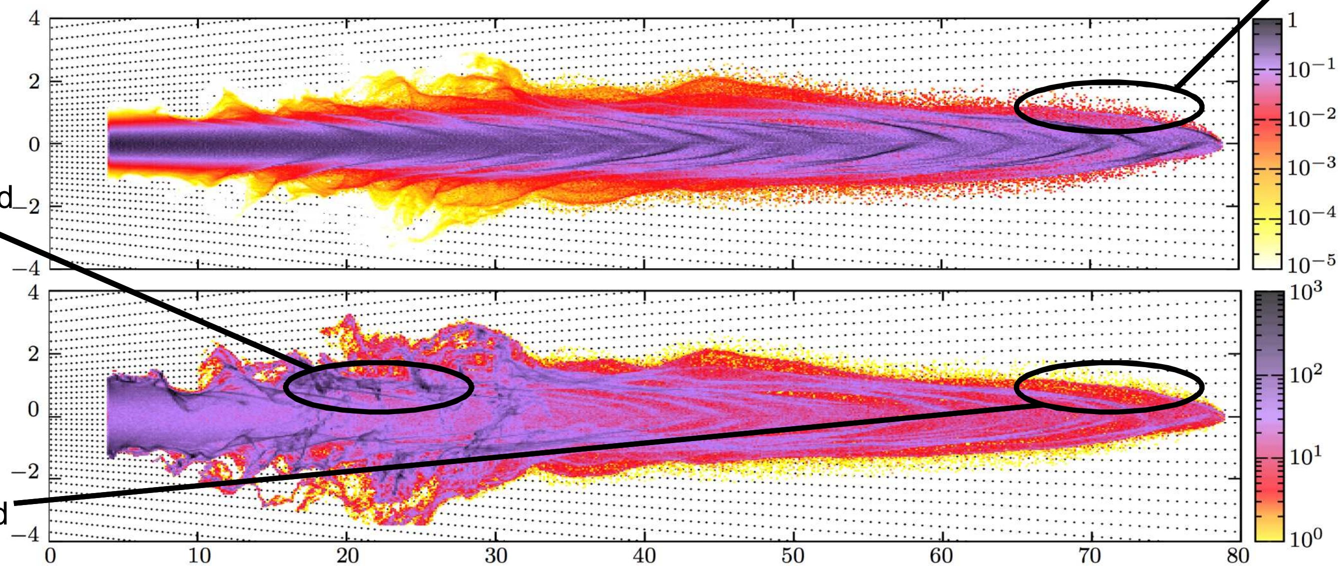
RESULTS – PGD transport

2D test with prescribed flow field

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



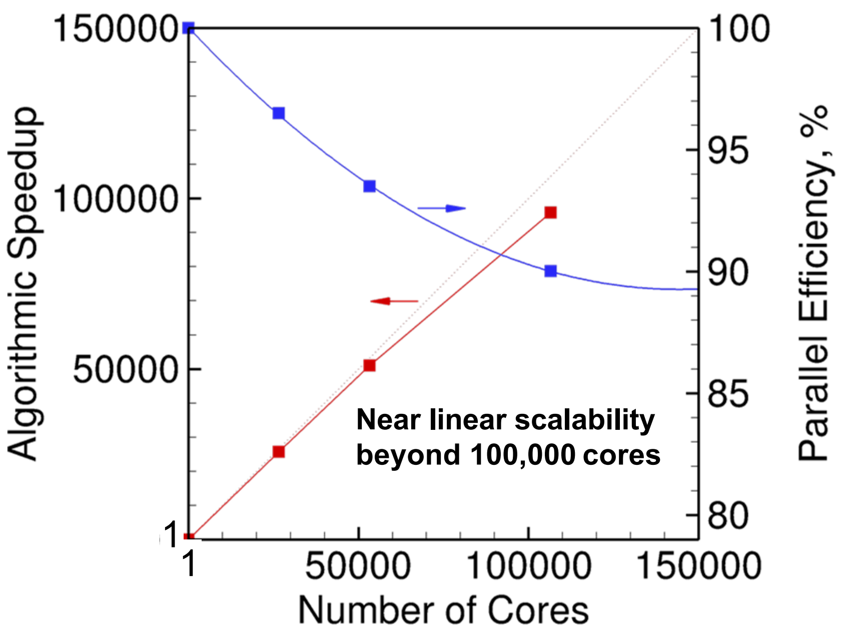
… compared to stochastic Lagrangian



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

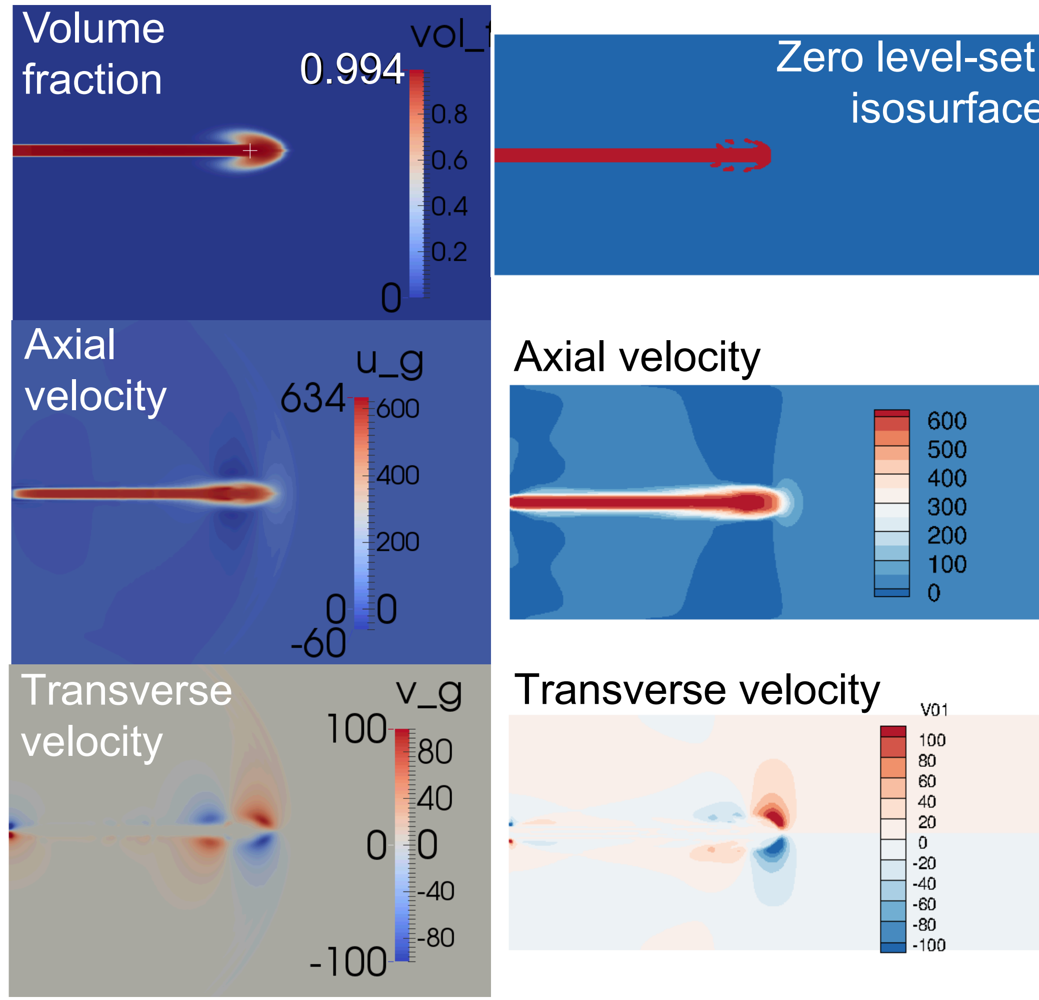
- **High-performance computing framework (Advanced parallel programming model that makes optimal use of advanced MP-computer architectures)**
- **Results from strong and weak scaling on Oak Ridge National Laboratory CRAY XK7 (Titan), June 2013**
  - Test case – jet-in-cross-flow, 500-million cells
  - 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)**

RESULTS – Momentum Coupling

Comparison between E-ES and CLSVOF

- ✓ Supersonic injection
  - – velocity plug-flow boundary
  - – no thermal transfer
- ✓ Agreement on **gas entrainment**
- ✸ Liquid density discrepancy results from **pressureless** assumption
- ✸ Jet tip is different because of **lack of surface tension**

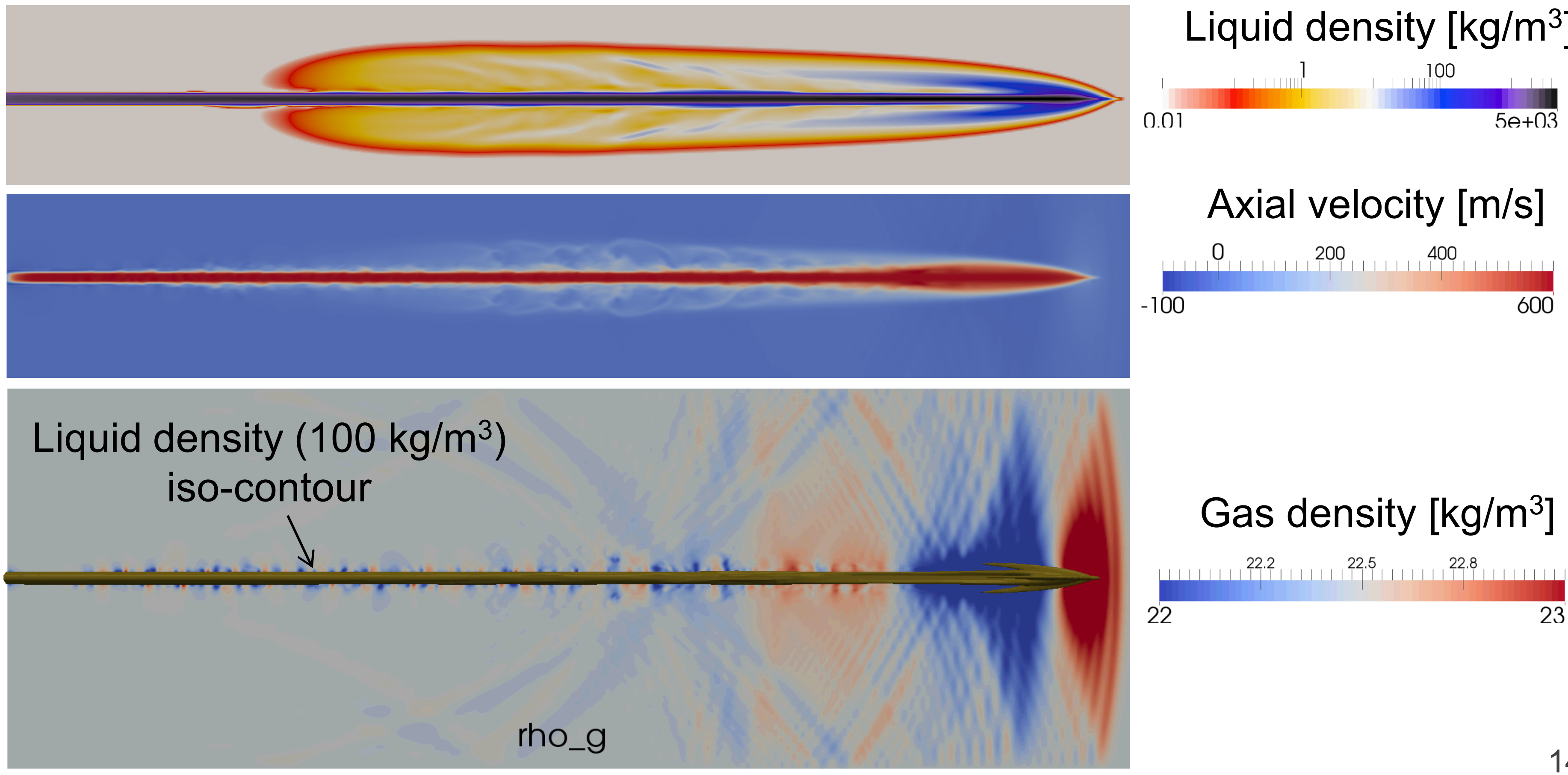
Raptor with E-ES	**CLSVOF**
$\Delta x = 12.5\ \mu m$, $\Delta t = 8$ ns	$\Delta x = 13.3\ \mu m$, $\Delta t \sim 6$ ns



RESULTS – Momentum coupling

Entrainment and induced turbulence by jet injection

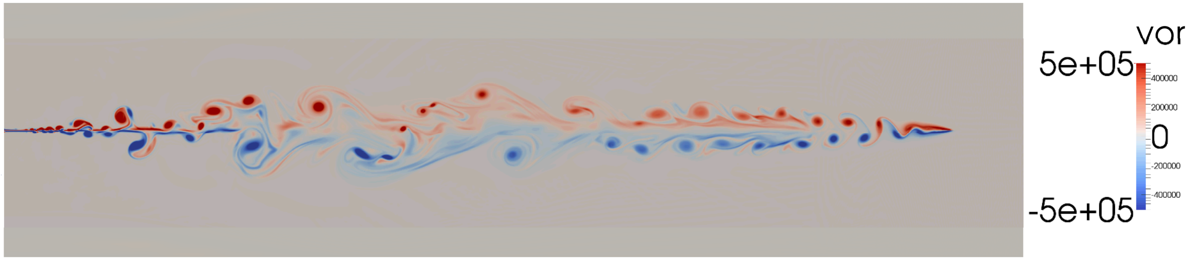
- Executed with **RAPTOR + E-ES**



CONCLUSION

Spray tools

- **kinetic theory**
- **microscopic closure**
- **dedicated numerics**



… are promising to efficiently handle injection.

Perspectives (1 year)

- **Dense core dynamics**
  - pressure
  - turbulence
  - surface tension
- **High-pressure mixing**
  - atomization
  - “evaporation”
  - LES closure
- **Combustion**
  - chemistry
  - LES closure
  - numerics