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Coupled Quadrature Based Moment Models and OpenFOAM® for Spray Applications

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Introduction

Models for Multiphase Systems

Particle scale

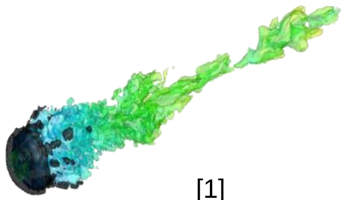
- VoF
- Level-set

Population scale

- LPT
- Method of classes

Integral scale

- Multi fluid aver.
- QBMM



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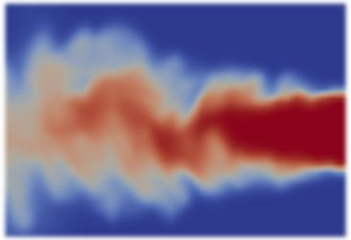
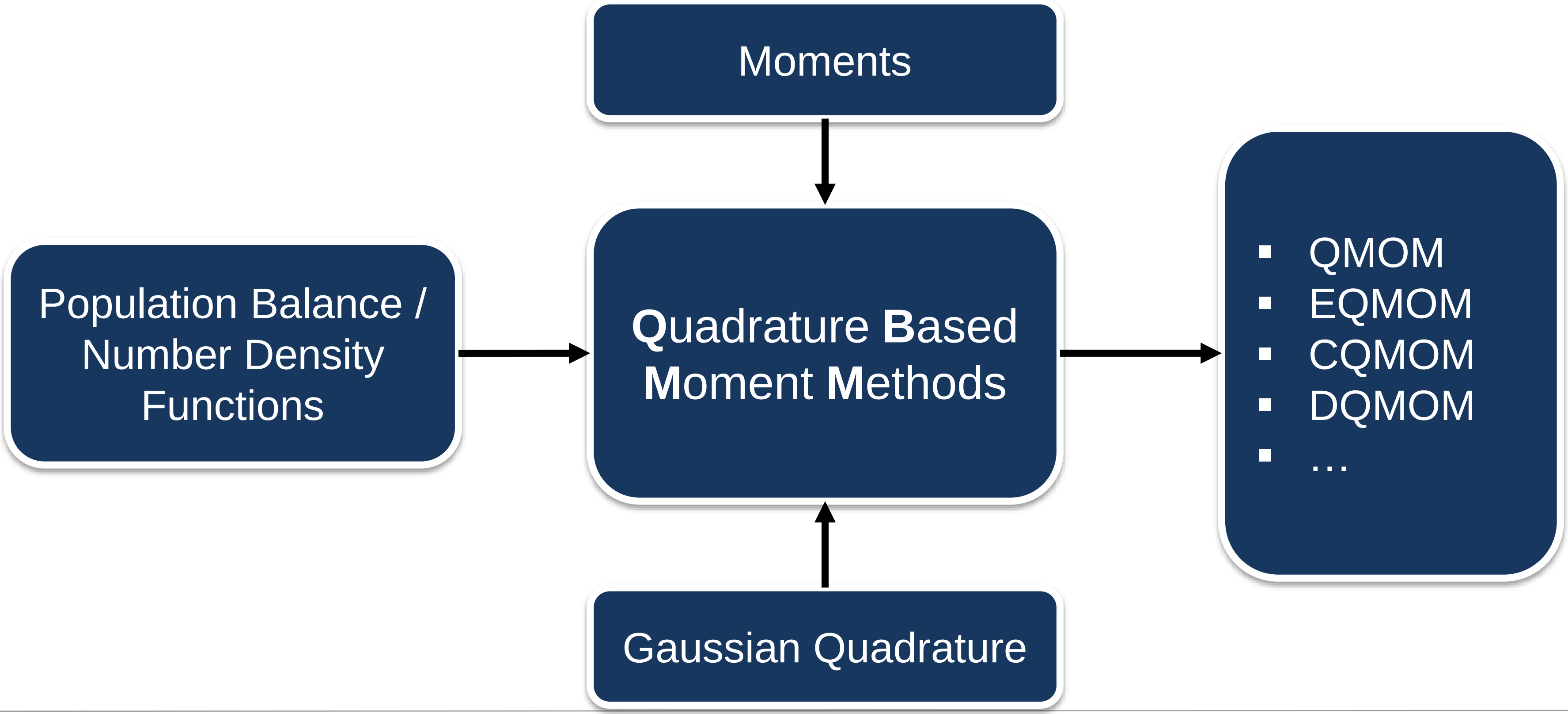


Computational costs

[1] Simulation of Binary Mixture Droplet Evaporation using VOF Methods, Keller, Hasse, 2011

Quadrature Based Moment Methods: An Overview



Population Balance Equations

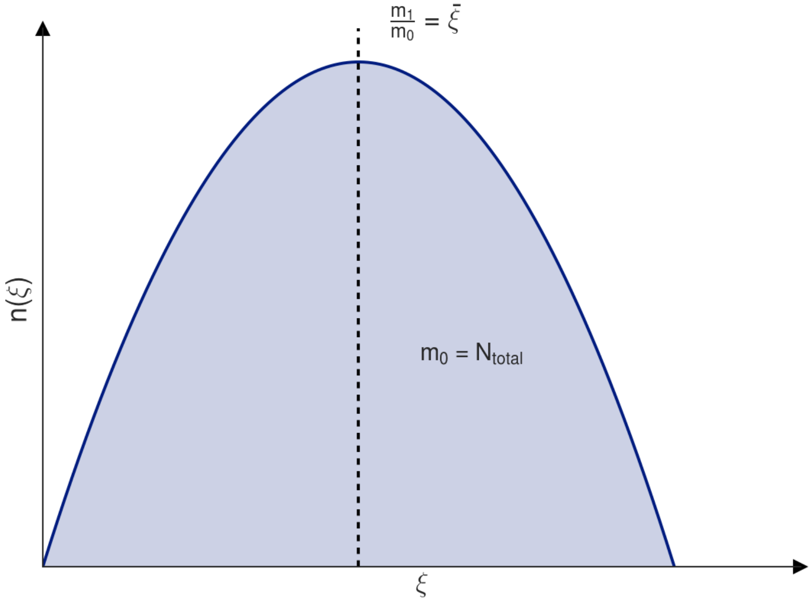
- Basis: Number density functions (NDF)

$$n_{\boldsymbol{\xi}} = n(t, \mathbf{x}, \boldsymbol{\xi}), \qquad \boldsymbol{\xi} = \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} d^2 \\ T \\ u \\ \vdots \end{bmatrix}$$

- Complete description of a particulate polydisperse system
- Solution of a population balance equation (PBE)

$$\frac{\partial n_{\boldsymbol{\xi}}}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \left(\mathbf{v} n_{\boldsymbol{\xi}}\right) + \frac{\partial}{\partial \boldsymbol{\xi}} \cdot \left(\dot{\boldsymbol{\xi}} n_{\boldsymbol{\xi}}\right) = h_{\boldsymbol{\xi}}$$

- High dimensional, numerically expensive



Moments

- A NDF is characterized by its moments

$$m_{\xi,k} = \int_{\Omega_\xi} \xi^k n(\xi)\,\mathrm{d}\xi$$

- Basic Idea: Solve for moments, not the NDF

$$\underbrace{\frac{\partial m_{\xi,k}}{\partial t}}_{\text{Transient term}} + \underbrace{\frac{\partial}{\partial \mathbf{x}}\left(\mathbf{v} m_{\xi,k}\right)}_{\text{Moment advection}} = \underbrace{\dot{m}_{\xi,k}}_{\text{Moment source term}} \longrightarrow \underline{\text{Closure needed}}$$

Gaussian Quadrature

- Goal:

$$\dot{\xi}(\xi) \rightarrow \dot{m}_{\xi,k}$$

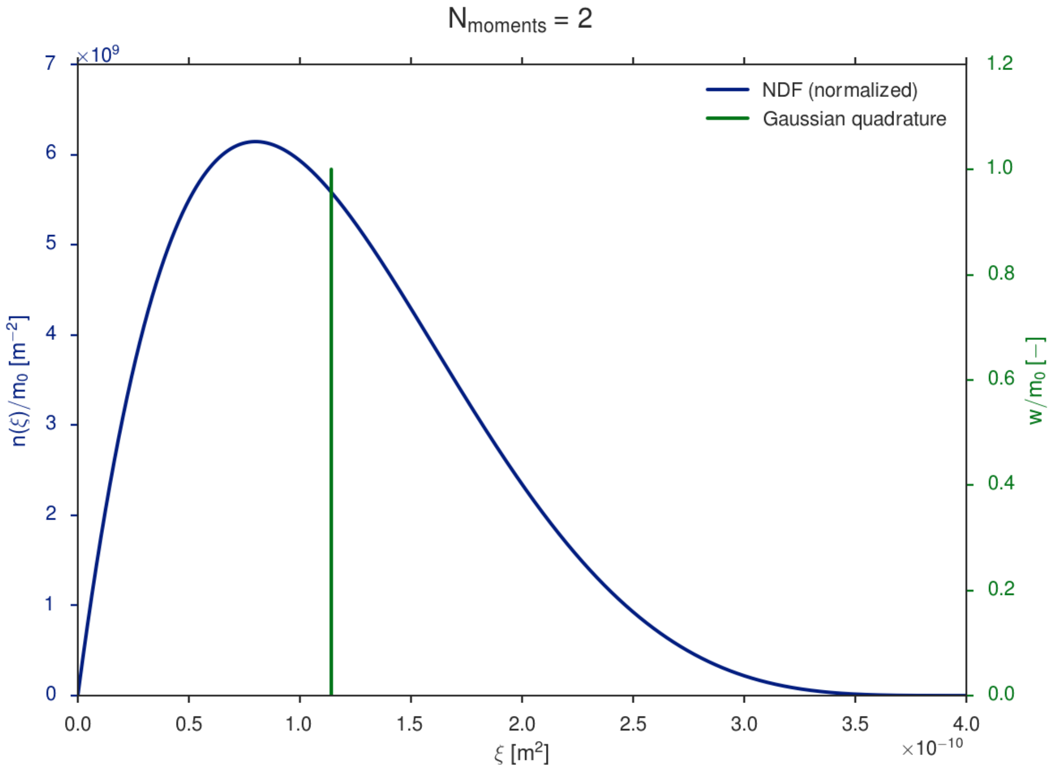
- A suitable tool: A Gaussian quadrature

$$\int_{\Omega_\xi} n(\xi) g(\xi)\,\mathrm{d}\xi \approx \sum_{\alpha=1}^{N} w_\alpha g(\xi_\alpha)$$

➢ **<u>Moments are used for Gaussian quadrature</u>**

$$m_{\xi,k} = \int_{\Omega_\xi} n(\xi) \xi^k\,\mathrm{d}\xi \approx \sum_{\alpha=1}^{N} w_\alpha \xi_\alpha^k$$

The Quadrature Method of Moments (QMOM)



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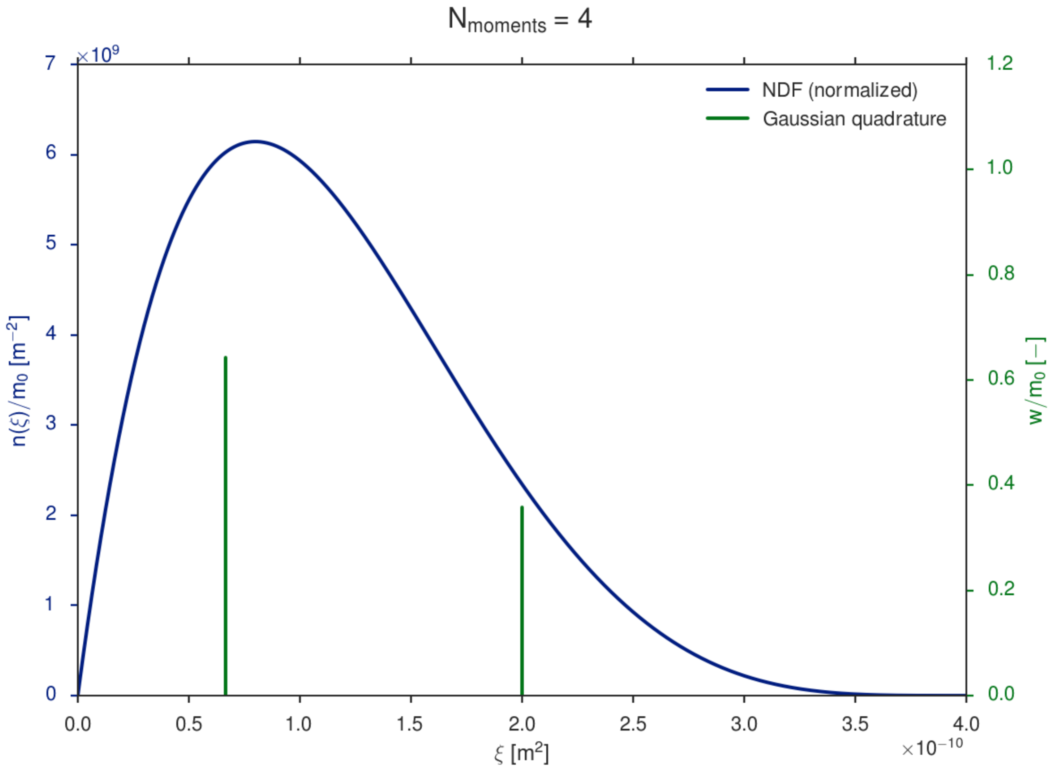

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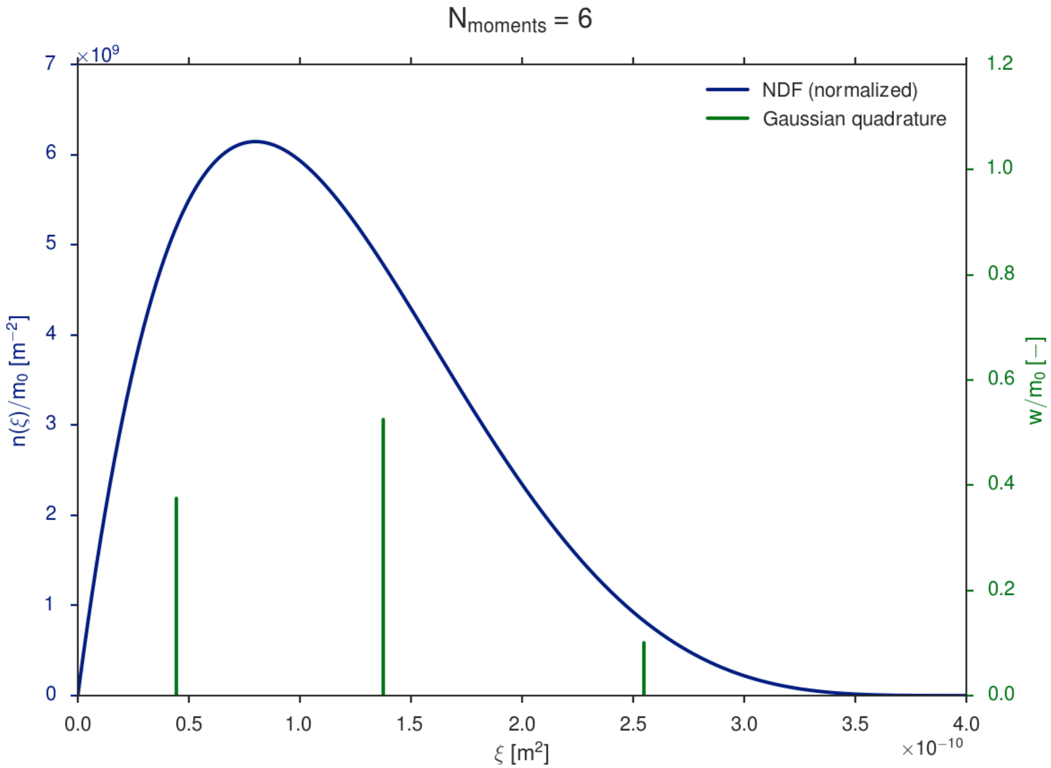

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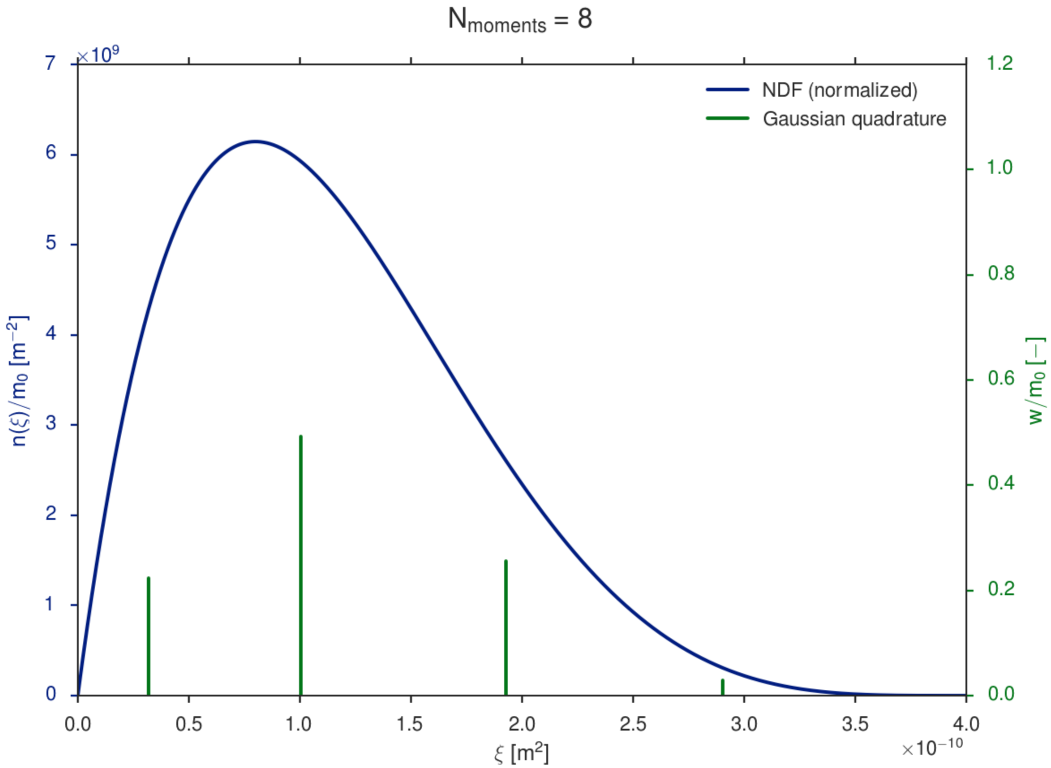

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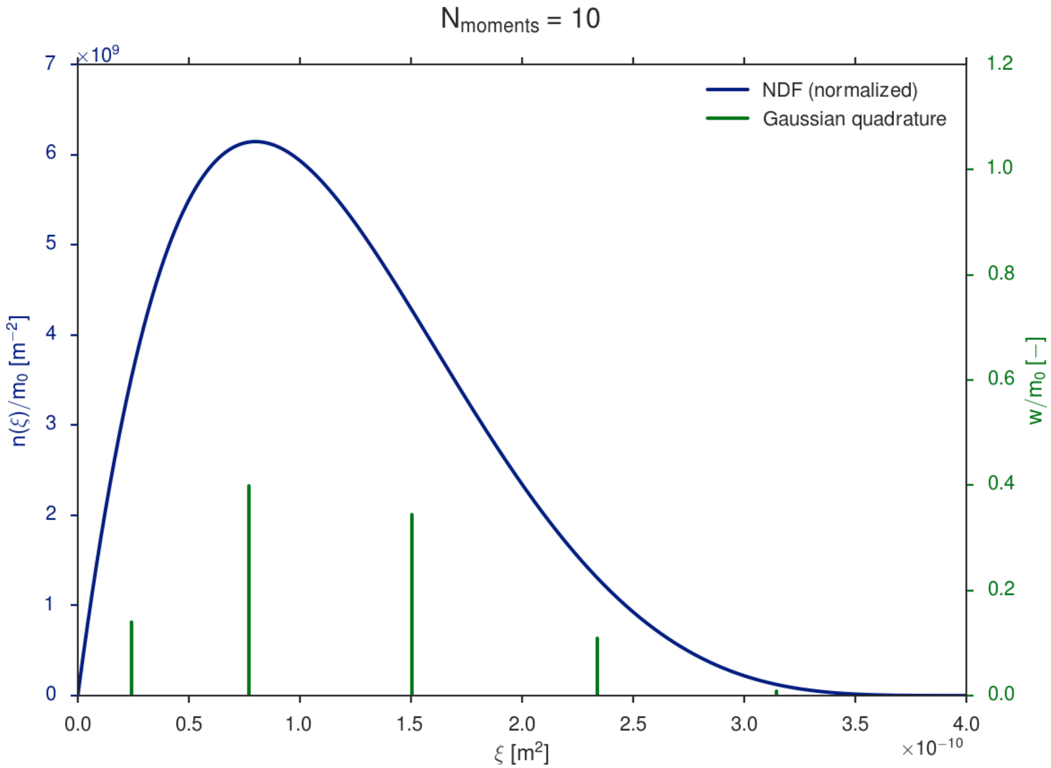

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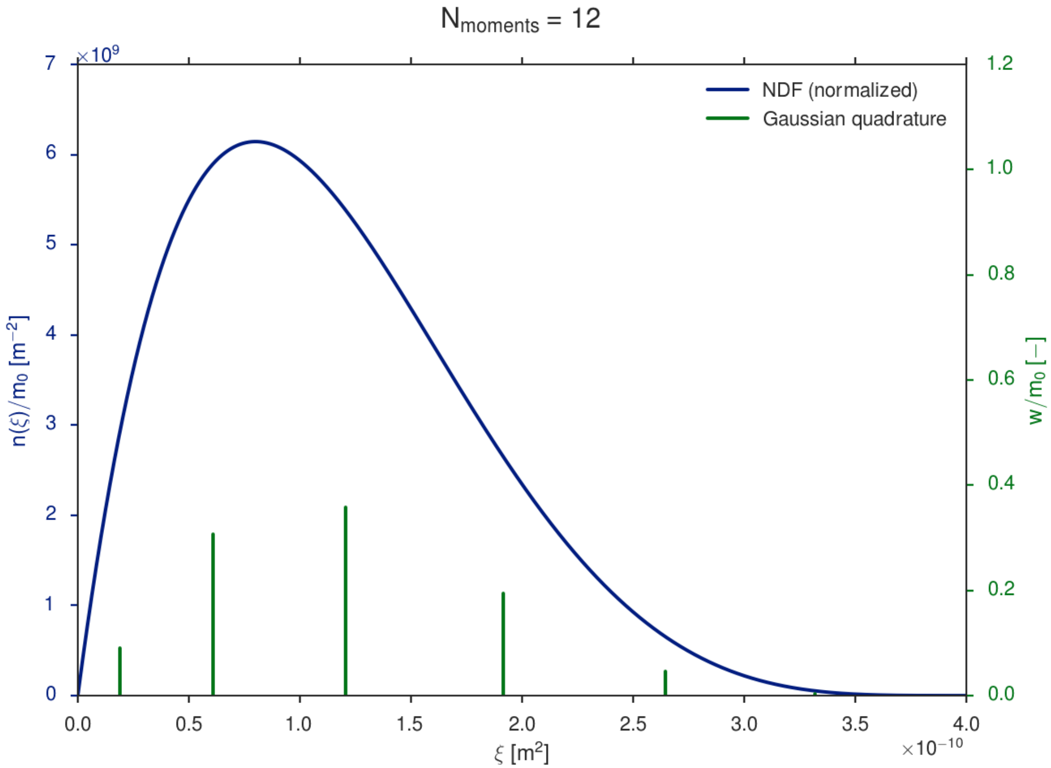

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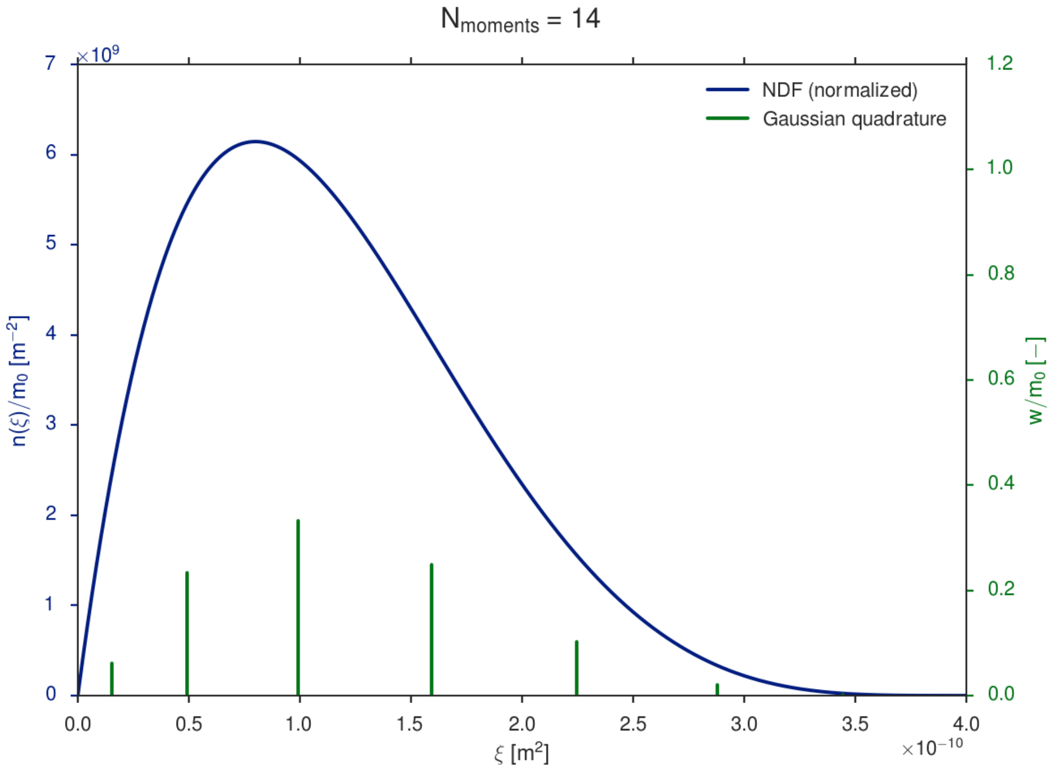

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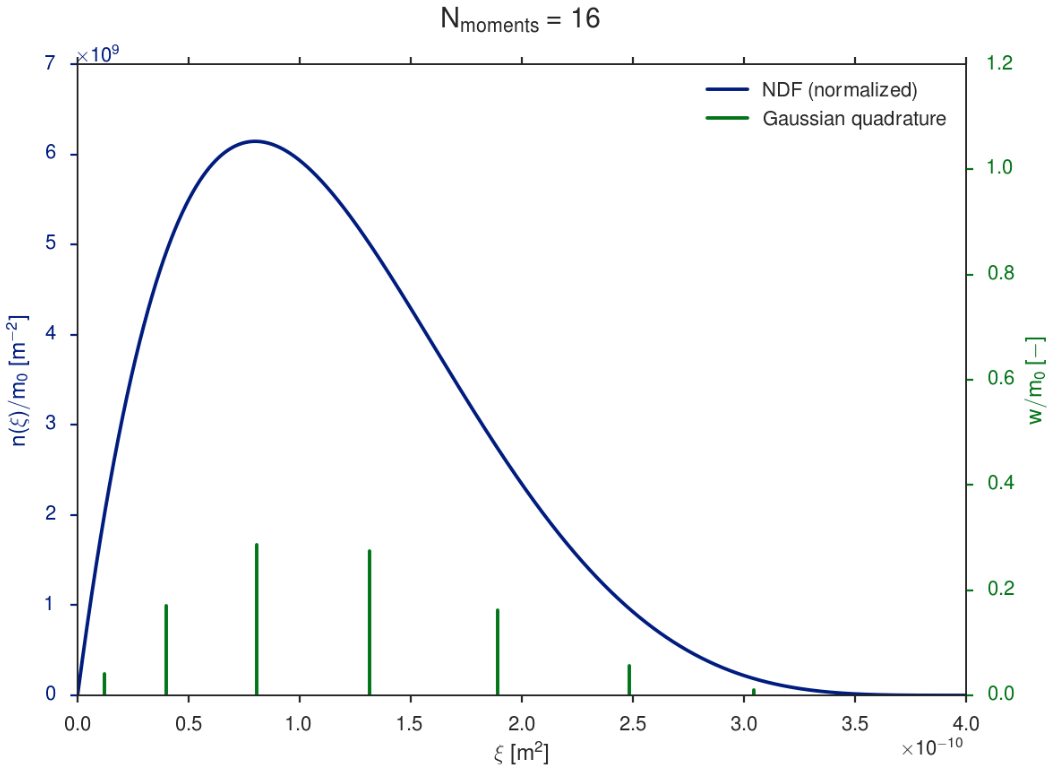

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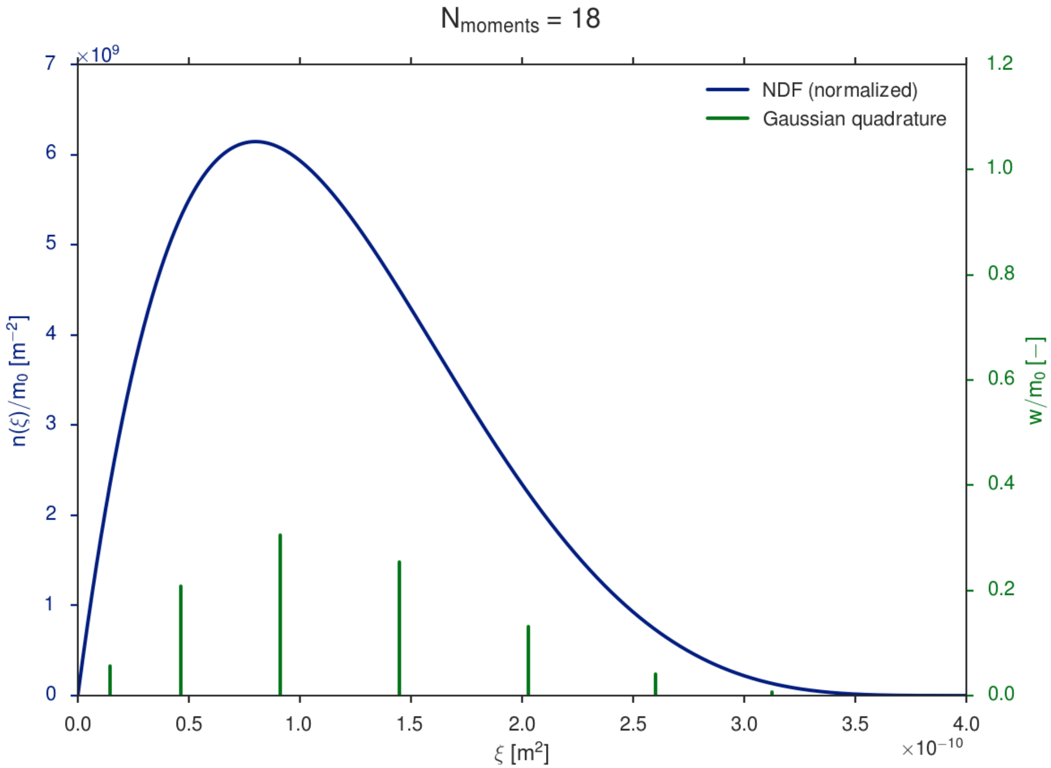

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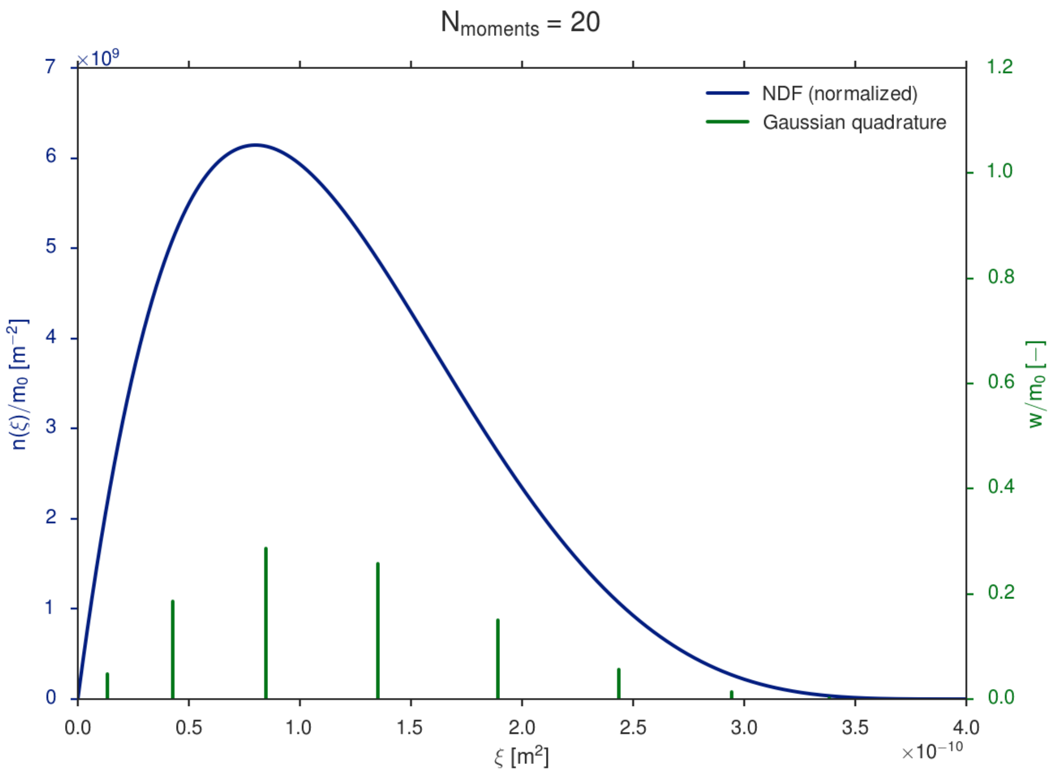

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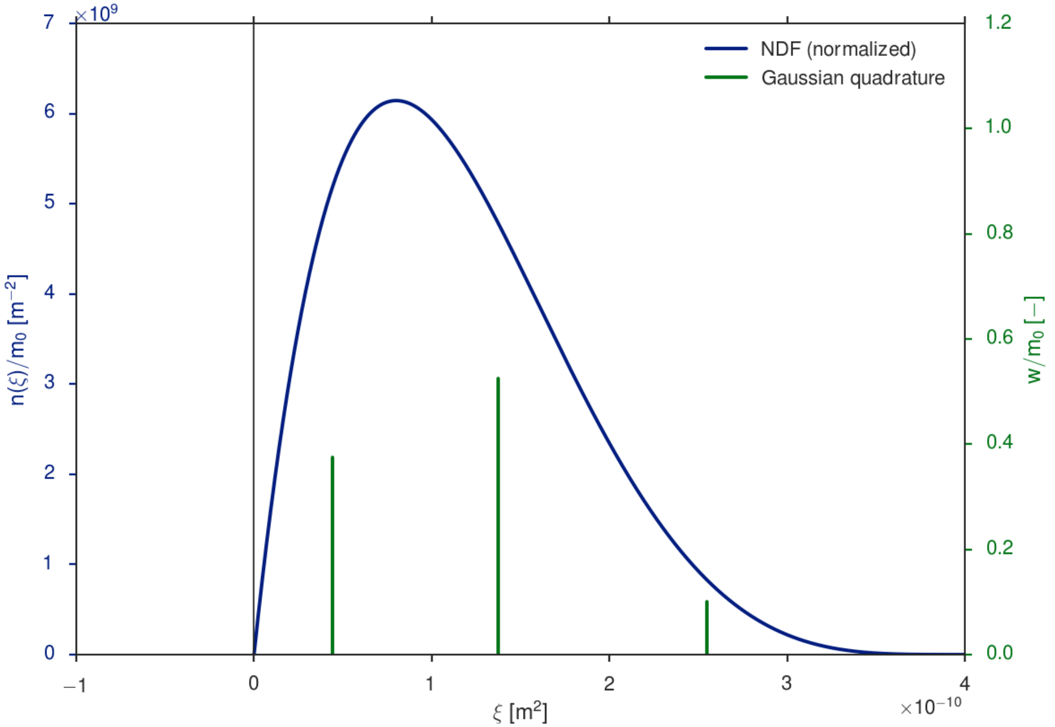
QMOM with Negative Growth Terms

- No information at $n(\xi = 0)$

➢ Accurate evaporation modeling impossible using the standard QMOM

➢ The Extended Quadrature Method of Moments (EQMOM) [1] allows NDF reconstruction



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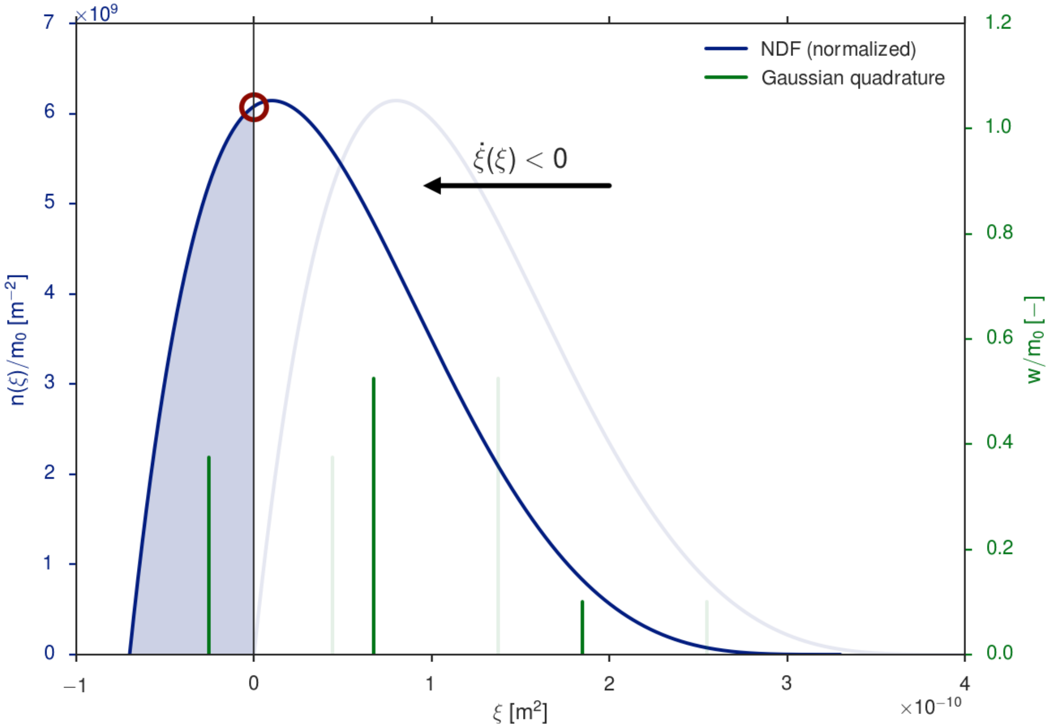

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The Extended Quadrature Method of Moments (EQMOM)

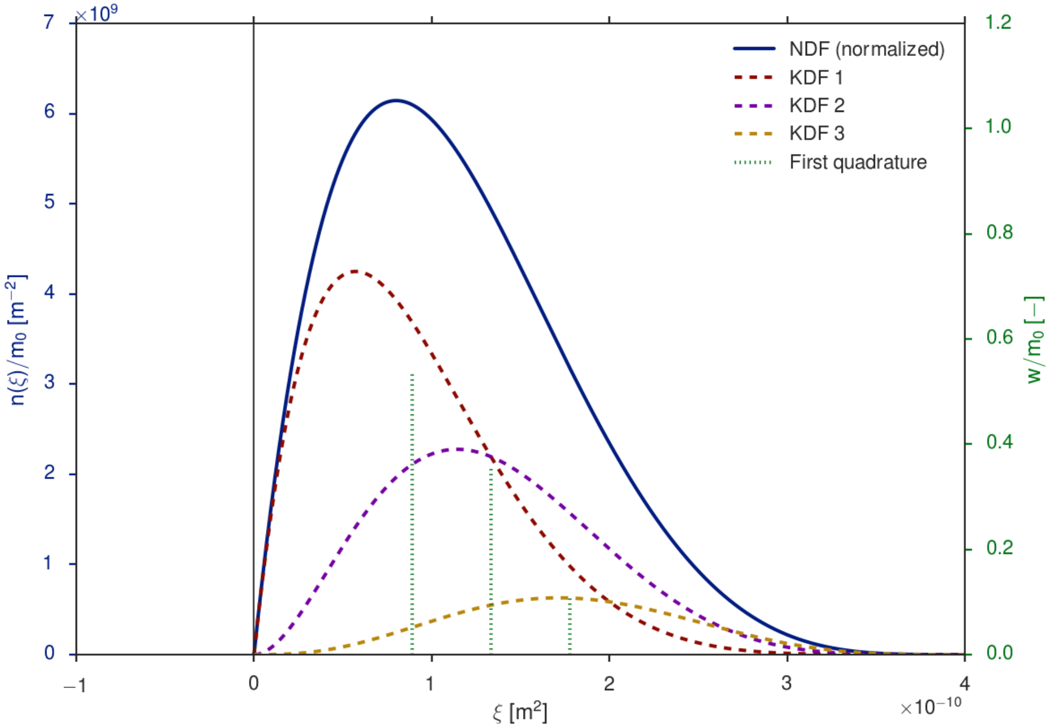
- Reconstruction of the NDF

- Kernel density functions (KDF) of a presumed shape
  - Beta distribution
  - Gamma distribution
  - …

- Additional shape parameter

$$\xi_\alpha, w_\alpha, \sigma$$

➢ 2N+1 moments required



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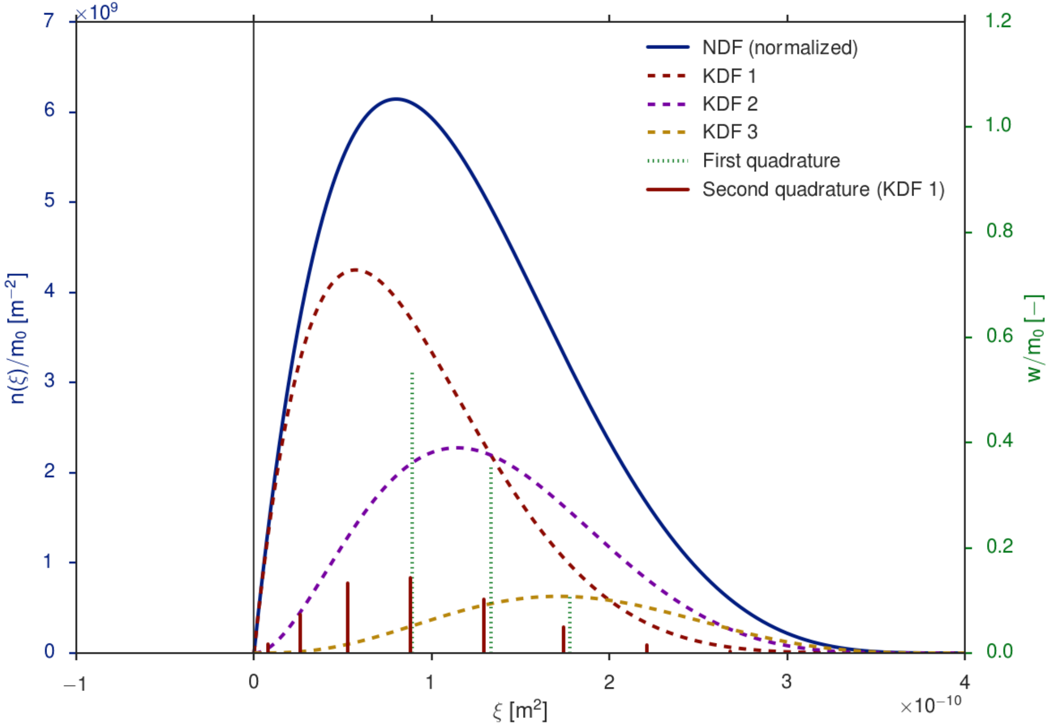

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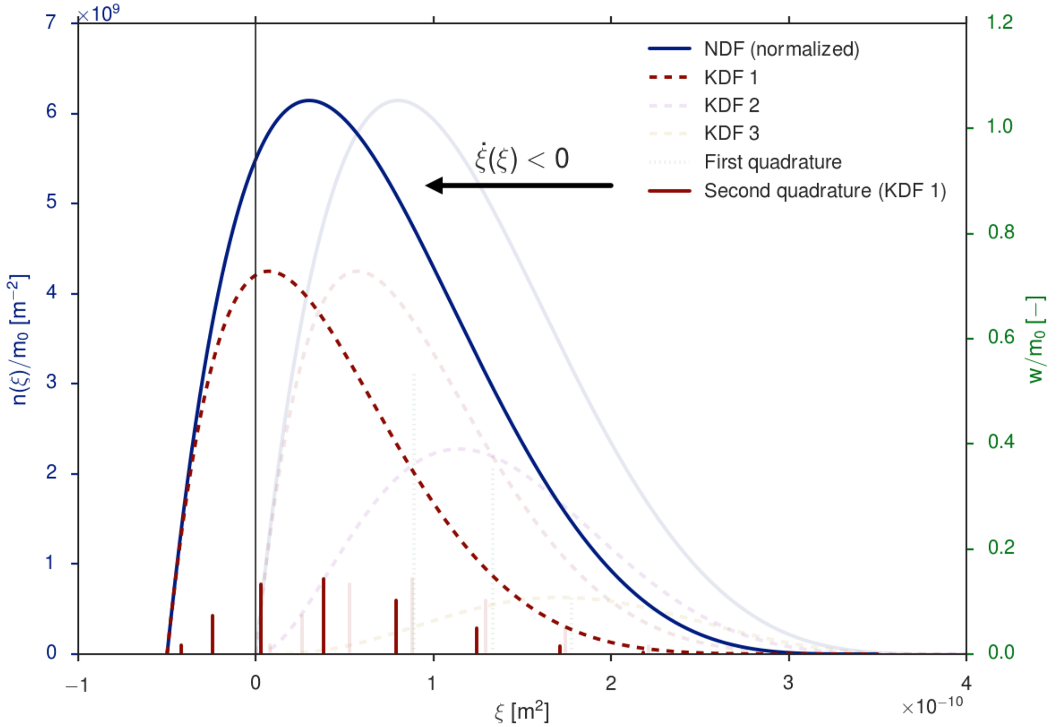


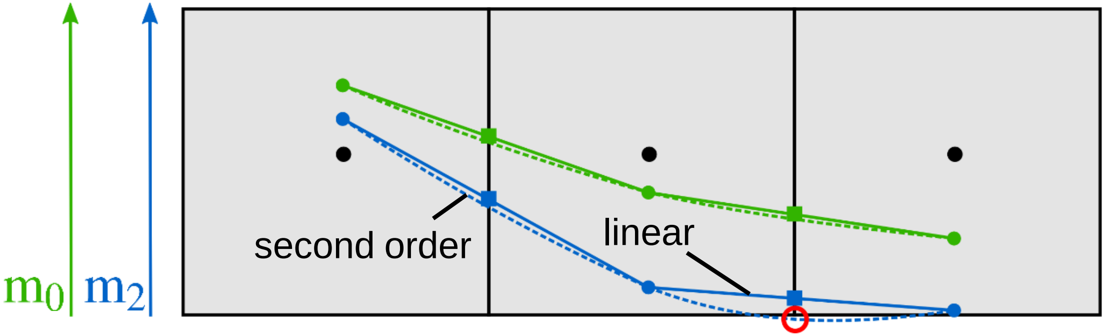
CFD-Coupling: Moment Advection / Interpolation

- Advection term requires interpolation to cell faces

- Moment relation is strongly non-linear

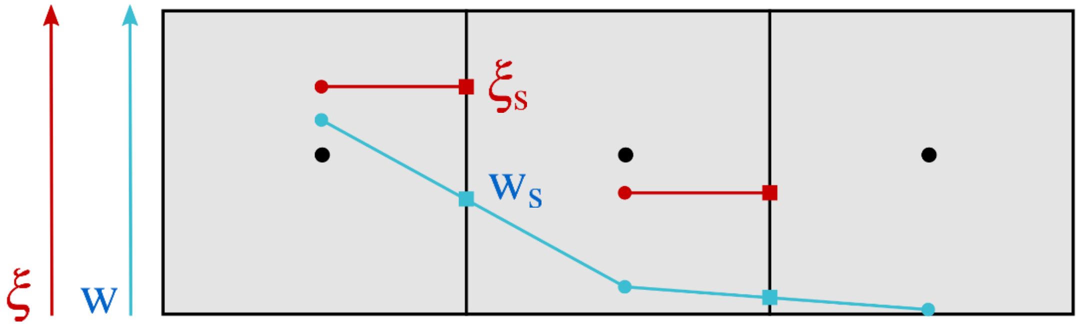
$$m_{\xi,k} = \int_{\Omega_\xi} \xi^k n(\xi)\,\mathrm{d}\xi$$

- Higher order interpolation schemes may lead to invalid moments (inconsistency / realizability problem)



CFD-Coupling: Moment Advection / Interpolation (2)

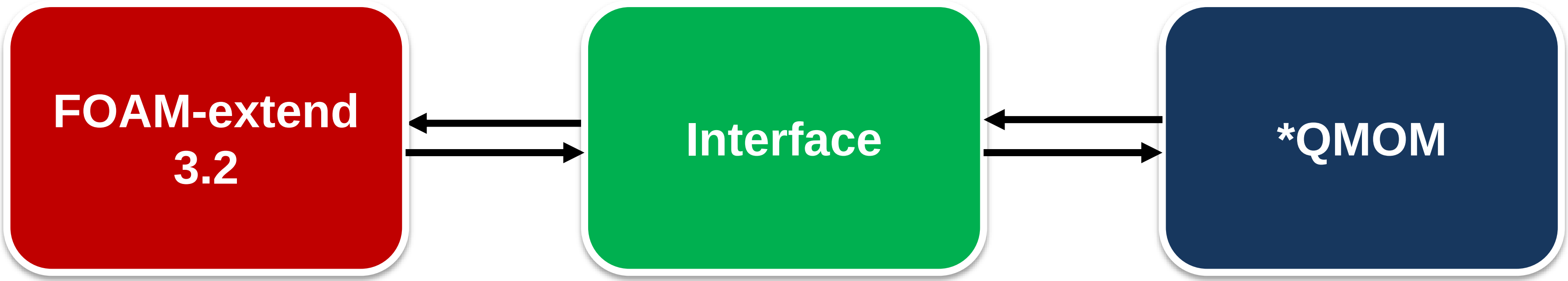
- We use the quadrature nodes and weights instead of interpolating moments directly



- Moment reconstruction at cell faces for flux calculation

$$m_{s,k} = \sum_{i=1}^{N} \xi_{s,i}^{k} w_{s,i}$$

CFD-Coupling: Implementation in OpenFOAM



- Flow equations
- Moment equations
- Field interpolation
- Integration

- Field transfer and conversion
- Moment reconstruction

- Moment inversion
- Source term evaluation
- Gas phase source terms

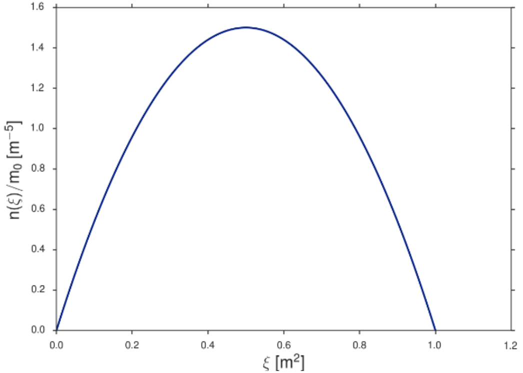
0D Case: Setup

- Univariate Beta-EQMOM
  - $\boldsymbol{\xi} = \xi = d^2$
  - 2 first quadrature nodes (5 moments)
  - 20 second quadrature nodes / KDF
- Solved for mean temperature
- Comparison with Lagrangian Particle Tracking (LPT) simulations

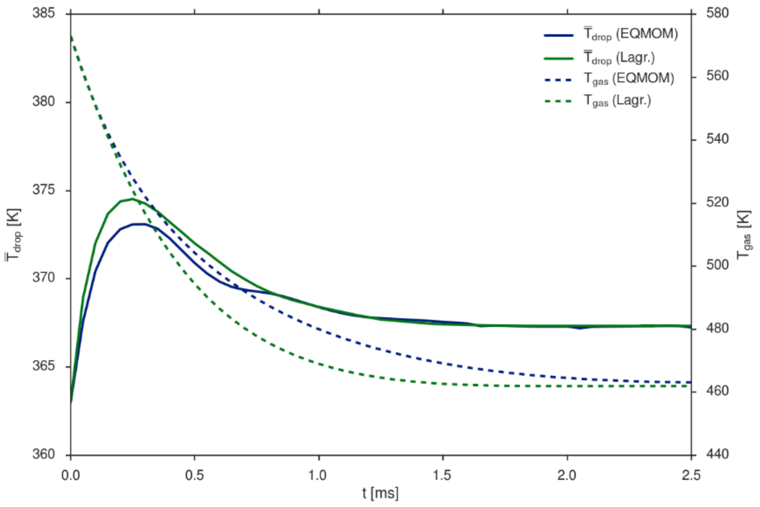
Fuel	Isooctane
Fuel Temperature	90° C (363.15 K)
Ambient Temperature	300° C (573.15 K)
Ambient Pressure	5.97 bar (N_2)

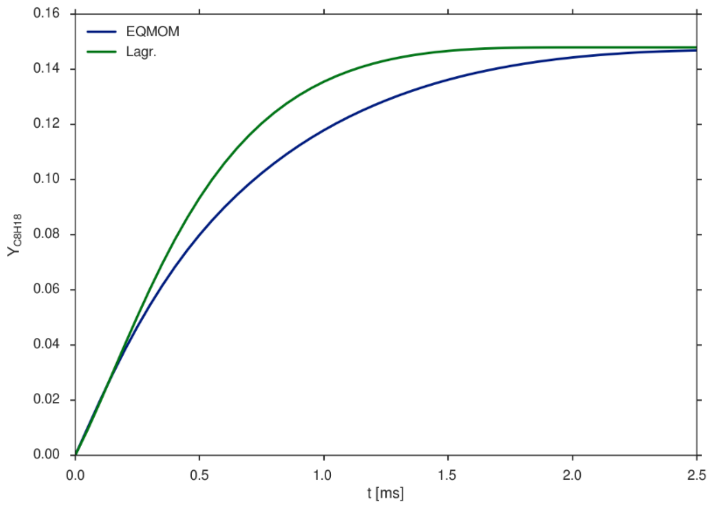
ECN Spray G conditions

$$m_0 \cdot 6(-\xi^2 + \xi),\ \xi \in [0,1]$$



0D Case: Temperatures and Mixture Fraction





- Differences due to homogeneous mean temperature assumption
- Source term formulation in general is correct

1D Case: Setup

- Univariate Beta-EQMOM
  - $\boldsymbol{\xi} = \xi = d^2$
  - 2 first quadrature nodes (5 moments)
  - 20 second quadrature nodes / KDF

- Solved for mean drop velocity (including droplet drag)

- Initial gas velocity 100 m/s

- Comparison with LPT simulations

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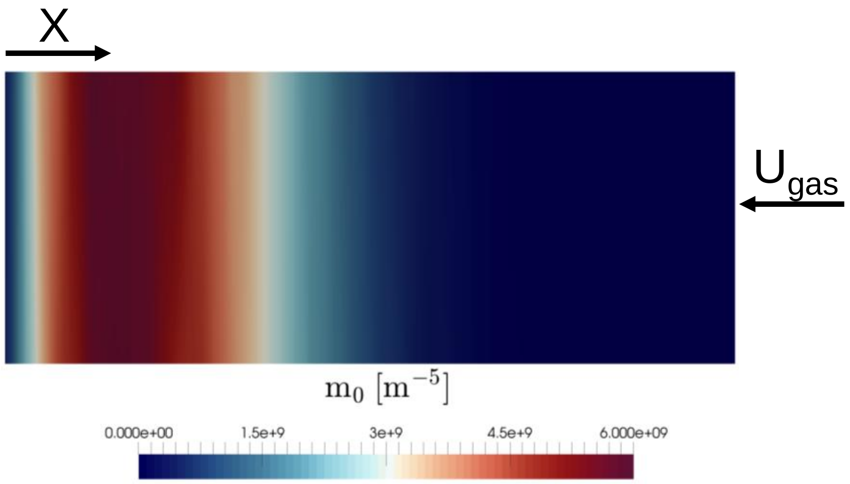
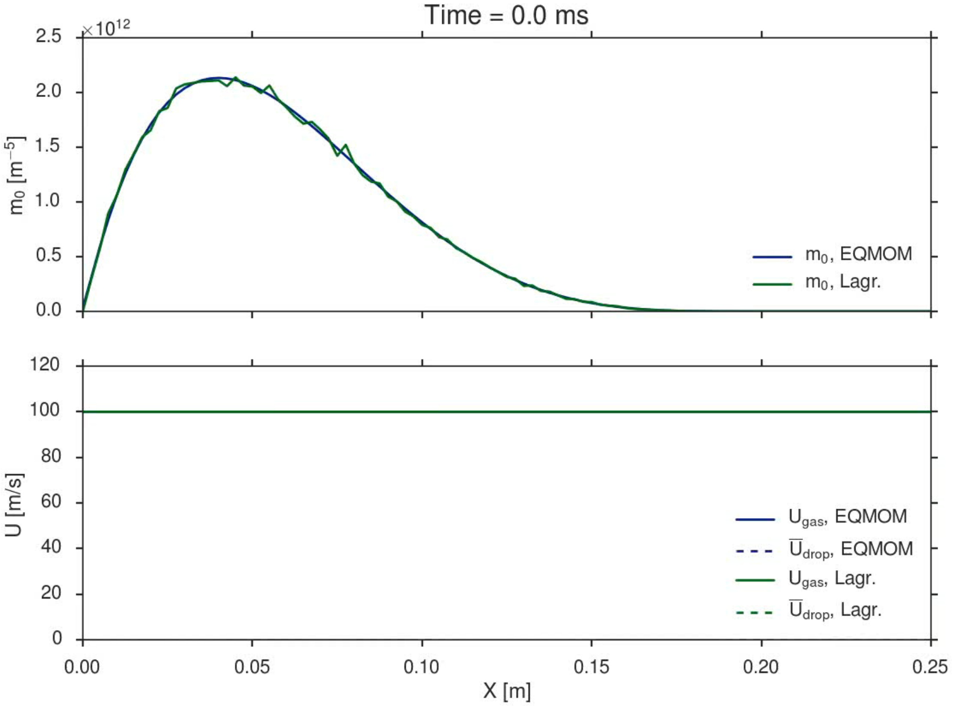


1D Case: 0. Moment and Velocities

- Moment transport works properly with the used advection / interpolation schemes

- There are only small deviations compared to the LPT simulation when solving for the mean velocity

➢ Do we even need the droplet velocity as an internal coordinate?



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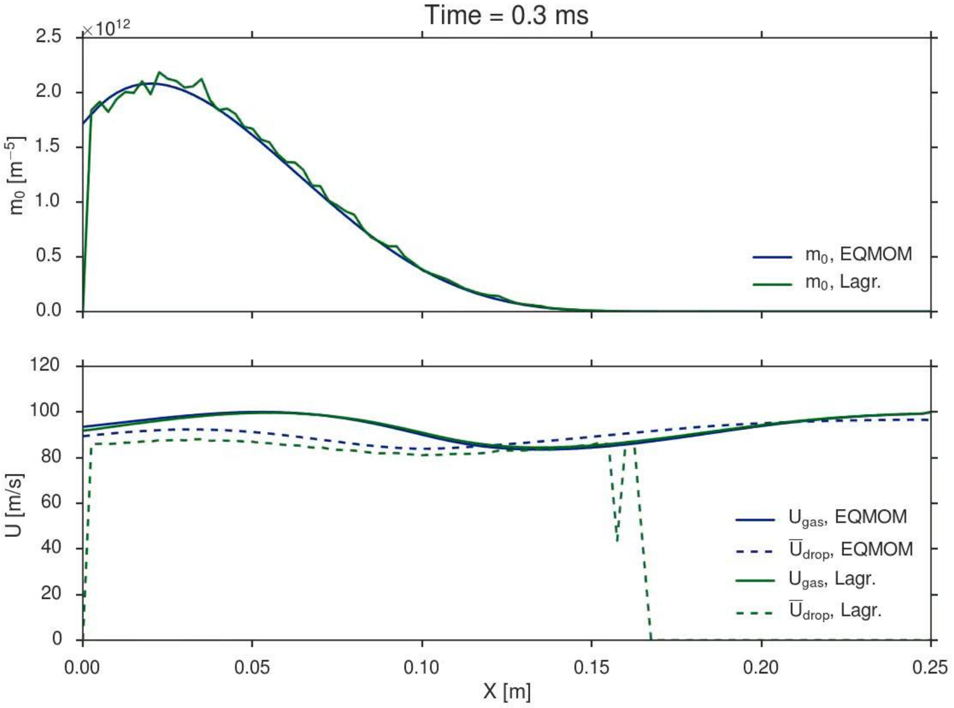

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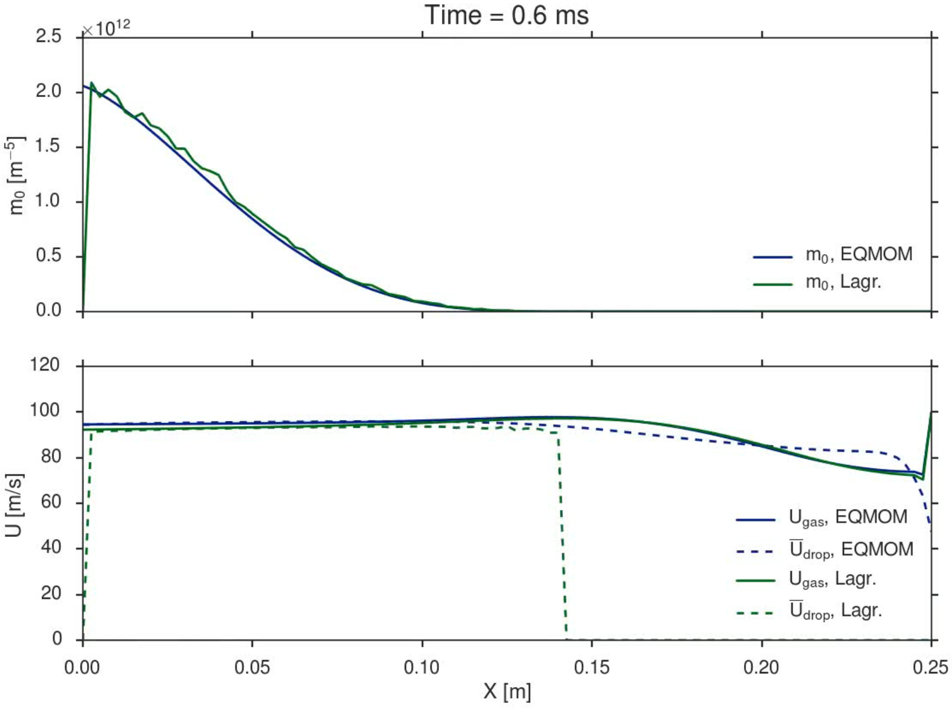

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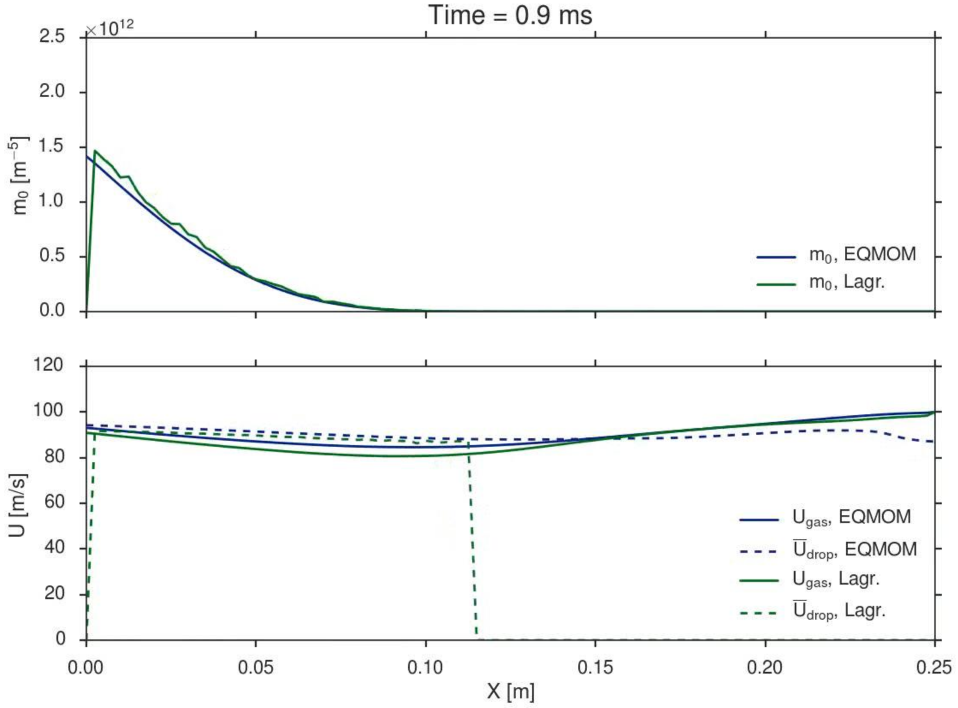

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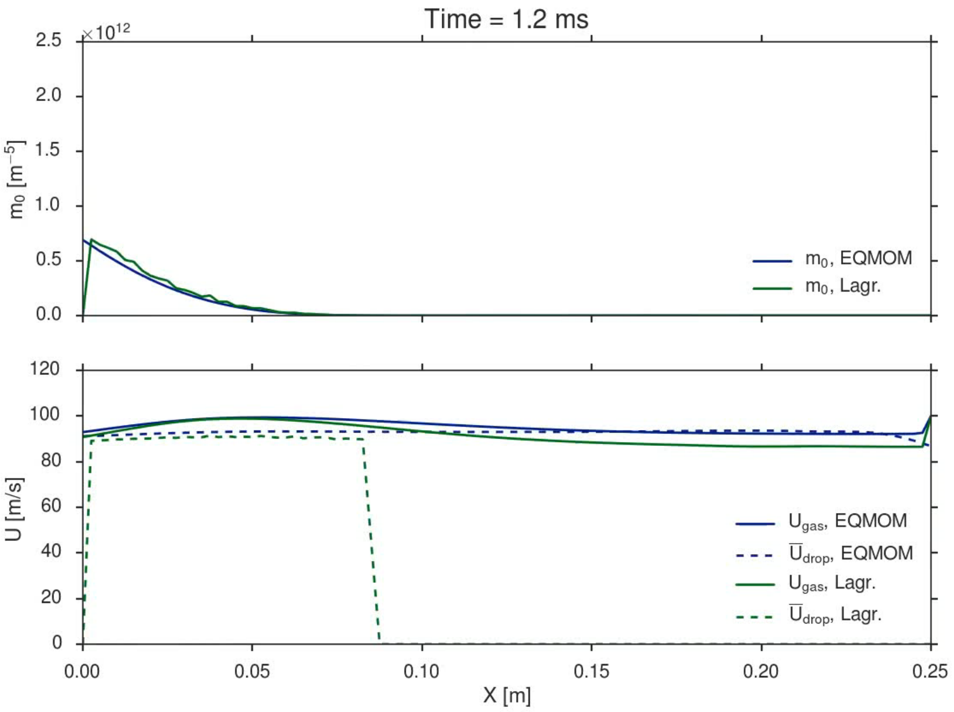

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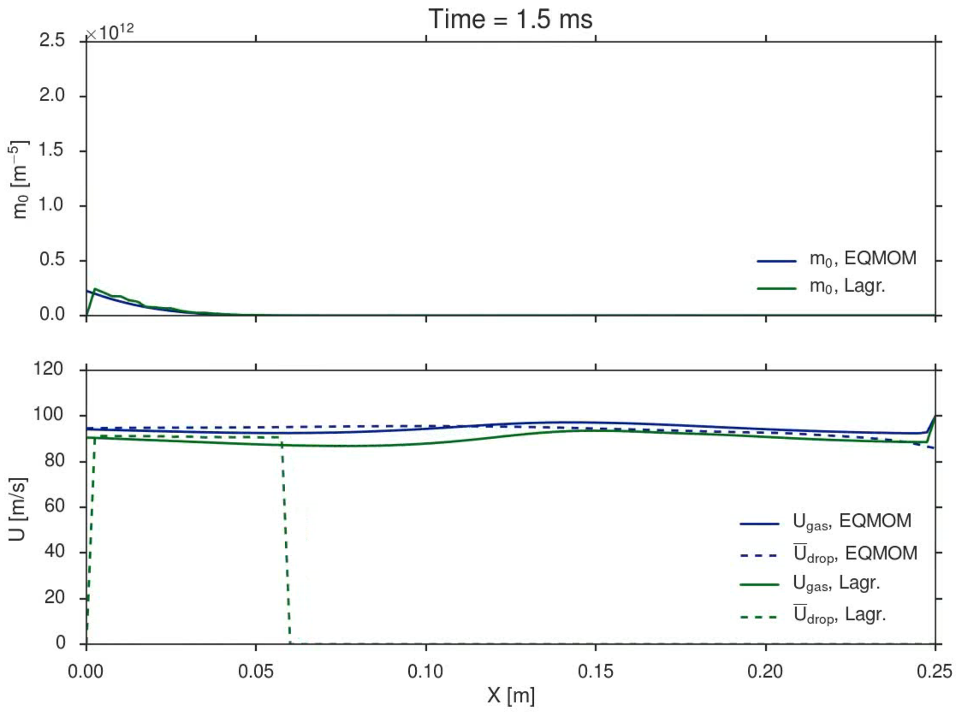

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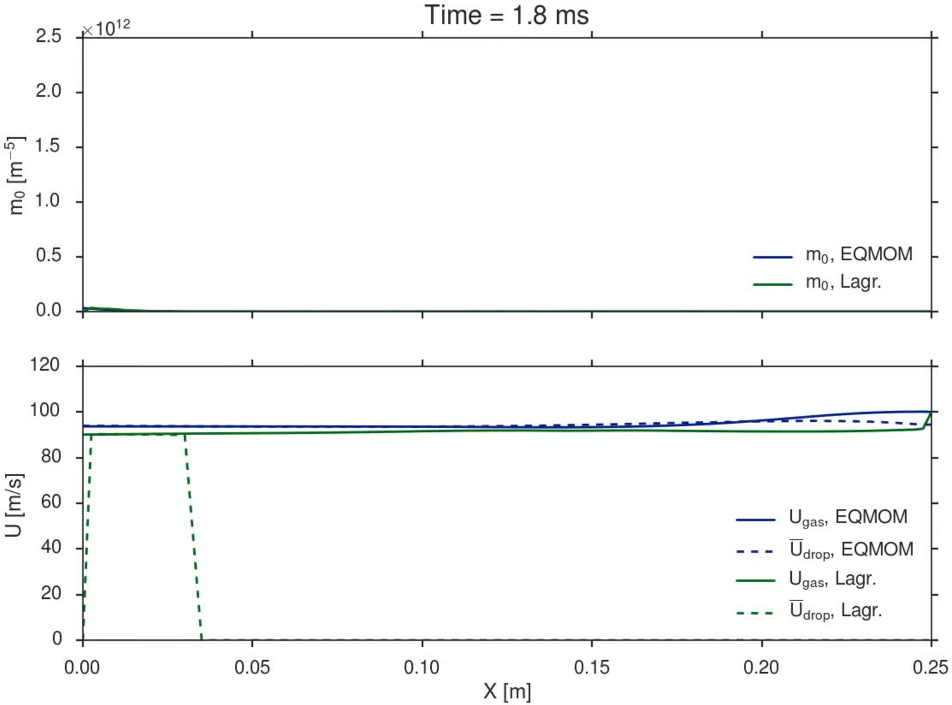

Conclusions and Outlook

- QBMM have the potential to serve as an efficient alternative for spray simulations if we work on
  - Numerical schemes suited to the requirements of QBMM (moment advection)
  - Numerical stability of the EQMOM algorithm
  - Ways to deal with high gradients in droplet concentrations
    - ➢ Injection region
  - Methods to guarantee conservativeness for realistic size distributions

- Next step towards QBMM in engine sprays
  - ➢ ECN Spray G

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