

# SUPPLEMENTARY MATERIALS: HIGH ORDER MOMENT MODEL FOR POLYDISPERSE EVAPORATING SPRAYS TOWARDS INTERFACIAL GEOMETRY DESCRIPTION\*

MOHAMED ESSADKI<sup>†</sup>, STEPHANE DE CHAISEMARTIN<sup>‡</sup>, FRÉDÉRIQUE LAURENT<sup>§</sup>,  
AND MARC MASSOT<sup>§</sup>

**Introduction.** In the main paper, a set of fractional moments are used to describe polydisperse evaporating sprays and correspond to physically identified interface geometrical quantities. In these supplementary materials, we present some mathematical elements related to the use of these fractional moments. These elements are already known for integer moments and can be extended in our case. First, the fractional moment space is defined and the notion of canonical moments and quadrature is directly extended from the integer moments case. Then, a complete proof is given for the existence and uniqueness of the Maximum Entropy reconstruction from any moment vector in the interior of the fractional moment space, as well as an algorithm to compute the parameters of this reconstruction. Finally, using the canonical moments, the extension of the realizable transport scheme developed for integer moments in [SM5] is provided.

**SM1. Fractional moment space, canonical moments and quadrature.** The purpose of this part is to extend some definition and relevant properties of the integer moment space to fractional moment space, in order to provide necessary tools to characterize the geometry of this space and thus to design realizable numerical schemes. In the following, we use the normalized fractional moments  $c_{k/2} = m_{k/2}/m_0$ .

## SM1.1. Fractional moment space - link with the integer moment space.

DEFINITION SM1. *We define the Nth fractional moment space as follows:*

$$\mathbb{M}_N^{1/2}([0, 1]) = \{\mathbf{c}_N(\mu), \mu \in \mathcal{P}([0, 1])\}, \quad \mathbf{c}_N(\mu) = (c_0(\mu), c_{1/2}(\mu), \dots, c_{N/2}(\mu))^t,$$

where  $\mathcal{P}([0, 1])$  denotes the set of all probability density measures defined on the interval  $[0, 1]$  and  $c_{k/2} = \int_0^1 x^{k/2} d\mu(x)$ .

The fractional moments can be expressed as integer moments by using the following mapping  $r^2 = x$  for  $x \in [0, 1]$ . Let us then denote  $\tilde{\mu}$  the measure on the interval  $[0, 1]$ , which is in a one to one correspondence with the measure  $\mu$  on  $[0, 1]$  through the above transformation, that is:  $\tilde{\mu}([0, r]) = \mu([0, r^2])$ . The moments can then be written:

$$(SM1) \quad c_{k/2}(\mu) = \int_0^1 x^{k/2} d\mu(x) = \int_0^1 r^k d\tilde{\mu}(r).$$

---

\*Supplementary materials for SIAP MS#M110836.

<sup>†</sup>IFP Energies nouvelles, 1-4 avenue de Bois-Préau, 92852 Rueil-Malmaison Cedex and Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay, Grande Voie des Vignes, 92295 Châtenay-Malabry, Cedex - France ([mohamed.essadki@centralesupelec.fr](mailto:mohamed.essadki@centralesupelec.fr)).

<sup>‡</sup>IFP Energies nouvelles, 1-4 avenue de Bois-Préau, 92852 Rueil-Malmaison Cedex - France ([stephane.de-chaisemartin@ifpen.fr](mailto:stephane.de-chaisemartin@ifpen.fr)).

<sup>§</sup>Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay, Grande Voie des Vignes, 92295 Châtenay-Malabry, Cedex - France and Fédération de Mathématiques de l'Ecole Centrale Paris, CNRS 3487 France ([frederique.laurent@centralesupelec.fr](mailto:frederique.laurent@centralesupelec.fr), [marc.massot@centralesupelec.fr](mailto:marc.massot@centralesupelec.fr)).

This relation expresses an identification between the fractional moment  $c_{k/2}(\mu)$  of the measure  $\mu$  and the integer moment  $\tilde{c}_k = c_k(\tilde{\mu})$  of the measure  $\tilde{\mu}$ . In the following, we use these notations to differentiate between the two natures of the moments, even if they are equal. With this simple identification, we will take benefit from the already existing results of integer moment space to extend them to the case of fractional moment space.

**SM1.2. Canonical moments.** For a fractional moment vector  $\mathbf{c}_N \in \mathbb{M}_N^{1/2}([0, 1])$ , we denote by  $P_N(\mathbf{c}_N)$  the set of all measure  $\mu \in \mathcal{P}([0, 1])$ , which are the solution of the following finite Hausdorff moment problem:

$$(SM2) \quad c_{k/2} = \int_0^1 x^{k/2} d\mu(x), \quad k = 0, 1, \dots, N.$$

If  $\mathbf{c}_N = (c_0, \dots, c_{N/2})^t$  belongs to the interior of  $\mathbb{M}_N^{1/2}([0, 1])$ , we can show that the set  $P_N(\mathbf{c}_N)$  is infinite. Indeed, these results were shown in [SM3] for integer moments, and its generalization for fractional is straightforward through the identification (SM1). Furthermore, the set of  $c_{(N+1)/2}(\mu)$ , where  $\mu \in P(\mathbf{c}_N)$ , is infinite and the maximum and the minimum of this set are different:

$$(SM3) \quad c_{(N+1)/2}^-(\mathbf{c}_N) = \min_{\mu \in P(\mathbf{c}_N)} \{c_{(N+1)/2}(\mu)\}, \quad c_{(N+1)/2}^+(\mathbf{c}_N) = \max_{\mu \in P(\mathbf{c}_N)} \{c_{(N+1)/2}(\mu)\}.$$

We define the canonical fractional moments as follows:

$$(SM4) \quad p_k = \frac{c_{k/2} - c_{k/2}^-(\mathbf{c}_{k-1})}{c_{k/2}^+(\mathbf{c}_{k-1}) - c_{k/2}^-(\mathbf{c}_{k-1})}.$$

The canonical moment vector belongs to  $[0, 1]^N$ , which has a simple geometry compared to the moment space. By using the results obtained on canonical integer moments [SM3], we can write the algebraic relation between fractional moments and their corresponding canonical moments, in the case of  $N = 3$ , by using the identification (SM1):

$$(SM5) \quad p_1 = \frac{m_{1/2}}{m_0}, \quad p_2 = \frac{m_0 m_1 - m_{1/2}^2}{(m_0 - m_{1/2}) m_{1/2}}, \quad p_3 = \frac{(m_0 - m_{1/2})(m_{1/2} m_{3/2} - m_1^2)}{(m_0 m_1 - m_{1/2}^2)(m_{1/2} - m_1)}.$$

**SM1.3. Principal representations - Gauss quadrature.** For a moment vector  $\mathbf{c}_N$  in the interior of  $\mathbb{M}_N^{1/2}$ , the vector  $\mathbf{c}_{N+1}^\pm = (m_0, \dots, m_{N/2}, c_{(N+1)/2}^\pm(\mathbf{c}_N))$  belongs to the boundary of the moment space  $\mathbb{M}_{N+1}^{1/2}$ , and the measure set  $P_{N+1}(\mathbf{c}_{N+1}^\pm) = \{\mu_\pm\}$  has only one element. The measure  $\mu_+$  (resp.  $\mu_-$ ) is called the upper (resp. lower) principal representation. In the case of integer moment vector  $\tilde{\mathbf{c}}_N$ , it was shown [SM3] that the lower and upper principal representations ( $\tilde{\mu}_+$  and  $\tilde{\mu}_-$ ) can be expressed as sum of  $n_s \leq (N+1)/2$  weighted delta-Dirac functions (we count the abscissas in the interior  $]0, 1[$  by 1 and the ones in the extremity, 0 or 1, by 1/2):

$$(SM6) \quad \tilde{\mu}_\pm(r) = \sum_{i=1}^{n_s} \tilde{w}_i^\pm \delta_{r_i^\pm}(r).$$

We recall that the subscript  $\tilde{\bullet}$  is used for integer moments and their corresponding measure, which are related to the fractional moments according to the identification (SM1).

In the case where  $N$  is odd (corresponding to an even number of moments), the lower principal representation corresponds to the classical Gauss quadrature. Let us remove the superscripts – to simplify the notations. Then, the weights  $\tilde{w}_i$  and the abscissas  $r_i$  (which are in  $]0,1[$ ) can be computed from the moments  $\tilde{c}_N$ , for example with the Product-Difference algorithm [SM4]. In other words, this algorithm (efficiently) solves the following non-linear system:

$$(SM7) \quad \tilde{c}_k = \sum_{i=1}^{n_s} \tilde{w}_i r_i^k, \quad k = 0, 1, \dots, N.$$

The identification (SM1) allows us to relate the quadrature in terms of fractional moments, to the quadrature in terms of integer moments:

$$(SM8) \quad c_{k/2} = \sum_{i=1}^{n_s} w_i x_i^{k/2}, \quad k = 0, 1, \dots, N,$$

where  $x_i = (r_i)^2$  and  $w_i = \tilde{w}_i$ . Thus, the Product-Difference algorithm allows to determine the weights and abscissas of the quadrature for fractional moments.

**SM2. Reconstruction through Entropy Maximization.** The Maximum Entropy (ME) problem reads as follows:

$$(SM9) \quad \max \left\{ H[n] = - \int_0^1 n(S) \ln(n(S)) dS \right\}, \quad m_{k/2} = \int_0^1 S^{k/2} n(S) dS, \quad k=0, \dots, N,$$

The existence and uniqueness of the ME solution is first shown, before giving an algorithm to compute the parameters of such a reconstruction.

**SM2.1. Existence and uniqueness of the maximum entropy solution.**

The following Theorem is shown here.

**THEOREM SM2.** *If the vector  $\mathbf{m}_N = (m_0, m_{1/2}, \dots, m_{(N)/2})$  belongs to the interior of the  $N$ th fractional moment space, then the constrained optimization (SM9) problem admits a unique solution, which is in the following form:*

$$(SM10) \quad n^{ME}(S) = \exp \left( -\lambda_0 - \sum_{i=1}^N \lambda_i S^{i/2} \right).$$

We mention that the case of the integer moments has been already treated in [SM6]. Here, some ideas of this work are used, but the present proof is completely different and simplified. Indeed, Mead and Papanicolaou [SM6] have used the monotonic properties of the moments, which is a characterization of the integer moment space, to prove existence of the ME solution. In our case, only the definition of the fractional moment space is used. The proof is then done through two Lemmas.

**SM2.1.1. Uniqueness.** The first Lemma allows to show the uniqueness and to give the form of the ME reconstruction.

**LEMMA SM3.** *If the constrained optimization problem (SM9) admits a solution, then this solution is unique and can be written in the following form:*

$$(SM11) \quad n^{ME}(S) = \exp \left( -\lambda_0 - \sum_{i=1}^N \lambda_i S^{i/2} \right),$$

where  $\boldsymbol{\lambda} = (\lambda_0, \dots, \lambda_N)^t \in \mathbb{R}^N$ . Moreover, this problem is equivalent to find an optimum of the potential function:

$$(SM12) \quad G(\lambda_0, \dots, \lambda_N) = \int_0^1 \exp(-\lambda_0 - \sum_{i=1}^N \lambda_i S^{i/2}) dS + \sum_{k=0}^{N-1} \lambda_k m_{k/2}.$$

*Proof.* The Lagrangian function associated to this standard constrained optimization problem is:

$$(SM13) \quad L(n, \boldsymbol{\lambda}) = H[n] - (\lambda_0 - 1) \left( \int_0^1 n(s) ds - m_0 \right) - \sum_{i=1}^N \left[ \lambda_i \left( \int_0^1 s^{i/2} n(s) ds - m_{i/2} \right) \right],$$

where  $\boldsymbol{\lambda} = (\lambda_0, \dots, \lambda_N)$  is the vector of the Lagrange's multipliers.

Let us suppose that, for a given moment vector  $\mathbf{m}_N$ , there exists a density function  $n^{ME}$  which is the solution of the ME problem (SM9). So, there exists a vector  $\boldsymbol{\lambda}^{ME}$  for which the differential of the Lagrange function  $L(n, \boldsymbol{\lambda})$  at the point  $(n^{ME}, \boldsymbol{\lambda}^{ME})$  vanishes:

$$(SM14) \quad \begin{cases} DL(n^{ME}, \boldsymbol{\lambda}) \cdot (h, \mathbf{0}) &= \int_0^1 h(s) \left[ -\ln(n^{ME}(s)) - \sum_{i=0}^N \lambda_i s^{i/2} \right] ds = 0, \\ \frac{\partial L}{\partial \lambda_i}(n^{ME}, \boldsymbol{\lambda}) &= \int_0^1 s^{i/2} n^{ME}(s) ds - m_{i/2} = 0, \end{cases},$$

where  $h$  is a positive distribution. Since the system (SM14) is valid for all  $h$ , it yields:

$$(SM15) \quad \begin{cases} n^{ME}(S) &= \exp(-\lambda_0 - \sum_{i=1}^N \lambda_i S^{i/2}), \\ m_{k/2} &= \int_0^1 s^{k/2} \exp(-\lambda_0 - \sum_{i=1}^N \lambda_i s^{i/2}) ds. \end{cases}$$

The problem then consists in finding a vector  $\boldsymbol{\lambda} = (\lambda_0, \dots, \lambda_N)$  in  $\mathbb{R}^N$  which satisfies the moment equations in the system (SM15). This problem is equivalent to find an optimum of the potential function  $G(\lambda_0, \dots, \lambda_N)$  defined in (SM12).

The Hessian matrix  $H$  defined by  $H_{i,j} = \frac{\partial^2 G}{\partial \lambda_i \partial \lambda_j}$  is a positive definite matrix, which ensures uniqueness of an eventual existing solution.  $\square$

**SM2.1.2. Existence.** The existence of such reconstruction is shown through the following Lemma.

LEMMA SM4. *If the vector  $\mathbf{m}_N = (m_0, m_{1/2}, \dots, m_{(N)/2})$  belongs to the interior of the  $N$ th fractional moment space, then the function  $G$ , defined in (SM12), is a continuous function in  $\mathbb{R}^N$ , and goes to infinity when  $\|\boldsymbol{\lambda}\| \rightarrow +\infty$ .*

*Proof.* Let us suppose that the last assertion is wrong, so there exists a sequence  $(\boldsymbol{\lambda}^{(n)})_{n=0,1,\dots}$  such that  $\|\boldsymbol{\lambda}^{(n)}\| \rightarrow +\infty$  when  $n \rightarrow +\infty$  and  $\sup_n \{G(\boldsymbol{\lambda}^{(n)})\} < +\infty$ .

Hence, there exists  $A \in \mathbb{R}$  such that:

$$(SM16) \quad G(\boldsymbol{\lambda}^{(n)}) = \int_0^1 \exp(-\sum_{i=0}^N \lambda_i^{(n)} S^{i/2}) dS + \sum_{k=0}^N \lambda_k^{(n)} m_{k/2} < A.$$

We write for each  $n \in \mathbb{N}$ ,  $\boldsymbol{\lambda}^{(n)} = \lambda^n (\alpha_0^{(n)}, \alpha_0^{(n)}, \dots, \alpha_N^{(n)})$ , such that  $\sum_{i=0}^N (\alpha_i^{(n)})^2 = 1$  and  $\lambda^{(n)} \rightarrow +\infty$ .

Since the sequence  $(\boldsymbol{\alpha}^{(n)})_{n=0,1,\dots}$  is a bounded sequence, we can extract a convergent subsequence  $(\boldsymbol{\alpha}^{\phi(n)})_n$ , where  $\phi: \mathbb{N} \rightarrow \mathbb{N}$  is an increasing function and:

$$(SM17) \quad \lim_{n \rightarrow +\infty} \alpha_i^{\phi(n)} = \alpha_i.$$

To simplify the notations, we can directly consider that  $\alpha_i^{(n)} \rightarrow \alpha_i$  when  $n \rightarrow +\infty$ . We note by  $Q^{(n)}(x) = \sum_{i=0}^N (\alpha_i^{(n)} x^{i/2})$  and  $Q(x) = \sum_{i=0}^N \alpha_i x^{i/2}$ .

Since the vector  $\mathbf{m}_N = (m_0, m_{1/2}, \dots, m_{(N)/2})$  is a moment vector, there exists a non-negative distribution function  $f$  such that  $m_{k/2} = \int_0^1 s^{k/2} f(s) ds$  for  $k = 0, \dots, N$ , and

$$(SM18) \quad G(\boldsymbol{\lambda}^{(n)}) = \int_0^1 \exp(-\lambda^{(n)} Q^{(n)}(s)) ds + \int_0^1 \lambda^{(n)} Q^{(n)}(s) f(s) ds \leq A.$$

Since the first integral is positive

$$(SM19) \quad \int_0^1 Q^{(n)}(s) f(s) ds \leq \frac{A}{\lambda^{(n)}}.$$

When  $n$  tends to infinity, we get:

$$(SM20) \quad \int_0^1 Q(s) f(s) ds \leq 0.$$

We have  $Q \neq 0$ ,  $f \geq 0$  and  $f \neq 0$ , and since  $Q$  is a continuous function, it follows from the inequality (SM20) that there exists  $[a, b] \subset [0, 1]$  in which  $Q(s) \leq -B$  and  $B > 0$ . Since  $Q^{(n)}$  converges uniformly to  $Q$  in  $[0, 1]$ , then, for all  $s \in [a, b]$  and for the large enough values of  $n$ :

$$(SM21) \quad Q^{(n)}(s) < -B/2.$$

Using these results in the inequality (SM18), as well as  $\alpha_k^n m_{k/2} \geq -m_0$ , we get:

$$(SM22) \quad \begin{aligned} A &\geq \int_a^b (\exp(-\lambda^{(n)} Q^{(n)}(s))) ds + \sum_{i=0}^N \lambda_i^{(n)} m_{i/2}, \\ &\geq (b-a) \exp(\lambda^{(n)} (B/2)) - \lambda^{(n)} N m_0, \end{aligned}$$

In the limit when  $n$  goes to infinity, we get the contradiction  $+\infty \leq A$ , thus concluding the proof.  $\square$

**SM2.2. Algorithm of the NDF reconstruction through the Entropy Maximization.** The reconstruction of the NDF through the maximization of Shannon entropy goes back to finding the Lagrange's multipliers  $\lambda_0 \dots \lambda_N$  such that:

$$(SM23) \quad m_{k/2} = \int_0^1 S^{k/2} \exp(-(\lambda_0 + \sum_{i=1}^N \lambda_i S^{i/2})) dS, \quad k = 0, \dots, N.$$

Solving this nonlinear system is equivalent to optimize the convex function  $G(\boldsymbol{\lambda})$ . We solve the problem by using the Newton iterations as proposed in [SM6]. The ME reconstruction is then done thanks to the Algorithm SM1.

The integral computations are done by using Gauss-Legendre quadrature. In [SM6], it is shown that 24-point quadrature allows to accurately compute the different integral expressions involved in the Algorithm SM1.

**Algorithm SM1** ME algorithm

---

Choose initial guess of the vector  $\lambda$ .

$$\delta_{k/2} \leftarrow m_{k/2} - \int_0^1 S^{k/2} \exp\left(-\sum_{i=0}^N \lambda_i S^{i/2}\right) dS$$

**while**  $\|\delta\| > \epsilon m_0$  **do**

**for**  $i, j < N$  **do**

$$H_{i,j} \leftarrow \int_0^1 S^{(i+j)/2} \exp\left(-\sum_{i=0}^N \lambda_i S^{i/2}\right) dS$$

**end for**

$$\lambda \leftarrow \lambda - H^{-1} \cdot \delta$$

**for**  $k < N$  **do**

$$\delta_{k/2} \leftarrow m_{k/2} - \int_0^1 S^{k/2} \exp\left(-\sum_{i=0}^N \lambda_i S^{i/2}\right) dS$$

**end for**

**end while**

---

**SM3. Transport scheme.** Here, first and second order schemes are given, which are directly extended from the schemes developed by Kah et al [SM5] for the transport of integer moments. For that, the canonical moments defined for fractional moments in section SM1 are used.

We choose to present the scheme in a two dimensional space to lighten the notations and we note  $\mathbf{U} = (u, v)$ . For the transport resolution in physical space, we use a dimensional splitting algorithm. In this context we consider a free transport in one direction (we present the  $x$ -direction here) of the droplets without the evaporation nor the drag force.

$$(SM24) \quad \begin{aligned} \partial_t m_{k/2} + \partial_x(m_{k/2} u) &= 0, & k = 0, \dots, 3, \\ \partial_t(m_1 \mathbf{U}) + \partial_x(m_1 u \mathbf{U}) &= 0, \end{aligned}$$

The mathematical structure of the pressureless gas system leads to some singularities (known as  $\delta$ -shocks). These singularities occur when the monokinetic assumption is violated. This can happen when trajectory crossings take place and lead to particles accumulation in a very small volume. Following the idea of de Chaisemartin [SM2], Kah et al [SM5] developed a finite volume kinetic scheme for the EMSM model. We use the same approach to solve numerically the system (SM24). In the following, we present briefly the main steps to derive the kinetic scheme for the system (SM24):

- A. We write the equivalent kinetic system to the pressureless system (SM24), as it was proposed in [SM1]:

$$(SM25) \quad \begin{cases} \partial_t f + \partial_x(c_x f) = 0, \text{ and} \\ f(t, x, \mathbf{c}, S) = n(t, x, S) \delta(\mathbf{c} - \mathbf{U}), \end{cases}$$

- B. We use the finite volume discretization of the system (SM24):

$$(SM26) \quad \begin{aligned} \mathbf{m}_i^{n+1} &= \mathbf{m}_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2} - F_{i-1/2}), \\ \mathbf{p}_i^{n+1} &= \mathbf{p}_i^n - \frac{\Delta t}{\Delta x} (G_{i+1/2} - G_{i-1/2}), \end{aligned}$$

where the fluxes are expressed as function of the NDF:

$$\begin{pmatrix} F_{i+1/2}^{\pm} \\ G_{i+1/2}^{\pm} \end{pmatrix} = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \int_0^1 \int_{\mathbb{R}^{\neq}} \begin{pmatrix} 1 \\ S^{1/2} \\ S \\ S^{3/2} \\ Su \\ Sv \end{pmatrix} f(t, x_{i+1/2}, \mathbf{c}, S) d\mathbf{c} dS dt,$$

- C. We split the fluxes in two integral parts:  $F_{i+1/2} = F_{i+1/2}^+ + F_{i+1/2}^-$  and  $G_{i+1/2} = G_{i+1/2}^+ + G_{i+1/2}^-$ . The first (resp. the second) corresponds to the droplet of positive (resp. negative) velocity in  $x$ -direction. Then, we use the exact solution of the kinetic system (SM25), to express the fluxes as function of the NDF at  $t = t_n$ .
- D. Finally, the fluxes are expressed as function of a spatial reconstruction of the moments and velocities at  $t = t_n$ :

$$(SM27) \quad \begin{pmatrix} F_{i+1/2}^{\pm} \\ G_{i+1/2}^{\pm} \end{pmatrix} = \frac{1}{\Delta t} \int_{x_{i-1/2}}^{x_{i+1/2}} \begin{pmatrix} m_0(t_n, x) \\ m_{1/2}(t_n, x) \\ m_1(t_n, x) \\ m_{3/2}(t_n, x) \\ m_1 u(t_n, x) \\ m_1 v(t_n, x) \end{pmatrix} \mathbb{1}_{\Sigma^{\pm}}(x) dx,$$

$$\text{where } \Sigma^{\pm} = \left\{ x' , \pm(x_{i+1/2} - \Delta t u(t_n, x')) < \pm x' \right\}$$

Here, we present two numerical kinetic schemes of first and second order, which follow this strategy.

**SM3.1. First order scheme.** For a first order scheme, we consider a constant piecewise reconstruction for the moments and the velocity. Then the fluxes become:

$$(SM28) \quad \begin{pmatrix} F_{i+1/2} \\ G_{i+1/2} \end{pmatrix} = \begin{pmatrix} m_{0,i}^n \\ m_{1/2,i}^n \\ m_{1,i}^n \\ m_{3/2,i}^n \\ m_{1,i}^n u_{0,i}^n \\ m_{1,i}^n v_i^n \end{pmatrix} \max(u_i^n, 0) + \begin{pmatrix} m_{0,i+1}^n \\ m_{1/2,i+1}^n \\ m_{1,i+1}^n \\ m_{3/2,i+1}^n \\ m_{1,i+1}^n u_{0,i+1}^n \\ m_{1,i}^n v_{i+1}^n \end{pmatrix} \min(u_{i+1}^n, 0),$$

**SM3.2. Second order scheme.** Kah et al [SM5] developed a realizable second order kinetic scheme. They showed that the canonical moments (in the context of integer moments) are transported variables. Therefore, these quantities satisfy a maximum principle. Since, the canonical moments live in the simple space  $[0, 1]^N$  ( $N = 3$  in our case). The authors proposed to use linear reconstruction of the canonical moments to design a high order scheme, instead of reconstructing directly the moments, which belong to a complex space. We adopt the same approach with some adaptations for the fractional moments. After reconstructing the variables (velocity and canonical moments) the fluxes are computed by a simple integration.

**SM3.2.1. Reconstruction.** The reconstructed variables are the moment  $m_0$ , the canonical moments (defined in part [SM1](#))  $p_1, p_2, p_3$  and the velocity.

$$(SM29) \quad \begin{cases} m_0(x) &= m_{0,i} + Dm_{0,i}(x - x_i), \\ p_1(x) &= \overline{p_{1,i}} + Dp_{1,i}(x - x_i), \\ p_2(x) &= \overline{p_{2,i}} + Dp_{2,i}(x - x_i), \\ p_3(x) &= \overline{p_{3,i}} + Dp_{3,i}(x - x_i), \\ u(x) &= \overline{u_i} + Du_i(x - x_i), \\ v(x) &= \overline{v_i} + Dv_i(x - x_i), \end{cases}$$

where  $x \in [x_{i-1/2}, x_{i+1/2}]$ . Generally the quantities with the bar are different from the cell averaged quantities  $p_{k,i}$ ,  $u_{k,i}$  and  $v_{k,i}$  and they are determined depending on the slopes and the following conservation properties:

$$(SM30) \quad \begin{aligned} m_{1/2,i}^n &= \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} m_0(x) p_1(x) dx, \\ m_{1,i}^n &= \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} m_0(x) p_1(x) [(1 - p_1)p_2 + p_1](x) dx, \\ m_{3/2,i}^n &= \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} m_0 p_1 \{ (1 - p_1)(1 - p_2)p_2 p_3 + [(1 - p_1)p_2 + p_1]^2 \} (x) dx, \\ m_{1,i}^n u_i^n &= \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} m_0(x) p_1(x) [(1 - p_1)p_2 + p_1](x) u(x) dx. \end{aligned}$$

Compared to the expressions developed in the case of the EMSM model, only the last integral expression is different. In fact, the velocity is weighted with the moment  $m_1$  for both models, but in the new model,  $m_1$  acts as a second order moment. For this reason, the expression of the moment  $m_1$  as function of the canonical moment is different from the one in the case of integer moments.

Kah et al. [\[SM5\]](#) show that the bar terms can be written as follows:

$$(SM31) \quad \begin{aligned} \overline{p_{k,i}} &= a_{k,i} + b_{k,i} Dp_{k,i}, \\ \overline{u_i} &= a_{u,i} + b_{u,i} Du_i, \end{aligned}$$

where for each  $k$ ,  $a_{k,i}$  and  $b_{k,i}$  are independent of  $Dp_{k,i}$ , and  $a_{u,i}$  and  $b_{u,i}$  are independent of  $Du_i$ .

**SM3.2.2. Slope limitation.** In order to satisfy the maximum principle for the transported quantities (the canonical moment and the velocity) and the positivity of the number density  $m_0$ , the slopes should be calculated carefully. Following the development done in [\[SM5\]](#), the slopes are calculated as follows:

$$(SM32) \quad \begin{aligned} Dm_{0,i} &= \phi(m_{0,i-1}^n, m_{0,i}^n, m_{0,i}^n) \min \left( \frac{|m_{0,i+1}^n - m_{0,i}^n|}{\Delta x}, \frac{|m_{0,i}^n - m_{0,i-1}^n|}{\Delta x}, \frac{2m_{0,i}^n}{\Delta x} \right), \\ Dp_{k,i} &= \phi(p_{k,i-1}^n, p_{k,i}^n, p_{k,i+1}^n) \min \left( \frac{|p_{k,i+1}^n - a_{k,i}|}{\Delta x + 2b_{k,i}}, \frac{|a_{k,i} - p_{k,i-1}^n|}{\Delta x - 2b_{k,i}} \right), \\ Du_i &= \phi(u_{i-1}^n, u_i^n, u_{i+1}^n) \min \left( \frac{|u_{i+1}^n - u_i^n|}{\Delta x + 2b_{u,i}}, \frac{|u_i^n - u_{i-1}^n|}{\Delta x - 2b_{u,i}}, \frac{1}{\Delta t} \right), \end{aligned}$$

where  $\phi(a, b, c) = 1/2(\text{sgn}(b - a) + \text{sgn}(c - b))$ .



Using the equations (SM30), (SM31) and (SM32) the slopes and the bar variables can be expressed as functions of the current and neighbor cell variables. However, these algebra relations are quite heavy. Therefore, their calculation is achieved using Maple software.

**SM3.2.3. Fluxes Computation.** After computing the slopes and the bar variables, the fluxes can be computed as follows:

$$(SM33) \quad \begin{pmatrix} F_{i+1/2}^+ \\ G_{i+1/2}^+ \end{pmatrix} = \frac{1}{\Delta t} \int_{x_{i+1/2}^L}^{x_{i+1/2}^R} m_0 \begin{pmatrix} 1 \\ p_1 \\ p_1[(1-p_1)p_2+p_1] \\ p_1\{(1-p_1)(1-p_2)p_2p_3+[(1-p_1)p_2+p_1]^2\} \\ p_1[(1-p_1)p_2+p_1]u \\ p_1[(1-p_1)p_2+p_1]v \end{pmatrix} dx,$$

and

$$(SM34) \quad \begin{pmatrix} F_{i+1/2}^- \\ G_{i+1/2}^- \end{pmatrix} = -\frac{1}{\Delta t} \int_{x_{i+1/2}^R}^{x_{i+1/2}^L} m_0 \begin{pmatrix} 1 \\ p_1 \\ p_1[(1-p_1)p_2+p_1] \\ p_1\{(1-p_1)(1-p_2)p_2p_3+[(1-p_1)p_2+p_1]^2\} \\ p_1[(1-p_1)p_2+p_1]u \\ p_1[(1-p_1)p_2+p_1]v \end{pmatrix} dx,$$

such that

$$(SM35) \quad \begin{aligned} x_{i+1/2}^L &= x_{i+1/2} - \Delta t \frac{(\bar{u}_i + \frac{\Delta x}{2} Du_i)_+}{1 + \Delta t Du_i}, \\ x_{i+1/2}^R &= x_{i+1/2} - \Delta t \frac{(\bar{u}_{i+1} - \frac{\Delta x}{2} Du_{i+1})_+}{1 + \Delta t Du_{i+1}}. \end{aligned}$$

The expressions inside the integrals are polynomial functions of  $x$  of order up to 6, their calculation can be achieved by using four points of the Gauss-Legendre quadrature.

#### REFERENCES

- [SM1] F. BOUCHUT, S. JIN, AND X. LI, *Numerical approximations of pressureless and isothermal gas dynamics*, SIAM J. Num. Anal., 41 (2003), pp. 135–158.
- [SM2] S. DE CHAISEMARTIN, L. FRÉRET, D. KAH, F. LAURENT, R. FOX, J. REVEILLON, AND M. MASSOT, *Eulerian models for turbulent spray combustion with polydispersity and droplet crossing*, Comptes Rendus Mécanique, 337 (2009), pp. 438–448. Special Issue ‘Combustion for Aerospace Propulsion’.
- [SM3] H. DETTE AND W. J. STUDDEN, *The theory of canonical moments with applications in statistics, probability, and analysis*, John Wiley & Sons Inc., New York, 1997.
- [SM4] R. GORDON, *Error bounds in equilibrium statistical mechanics*, Journal of Mathematical Physics, 9 (1968), pp. 655–663.
- [SM5] D. KAH, F. LAURENT, M. MASSOT, AND S. JAY, *A high order moment method simulating evaporation and advection of a polydisperse spray*, Journal of Computational Physics, 231 (2012), pp. 394–422.
- [SM6] L. R. MEAD AND N. PAPANICOLAOU, *Maximum entropy in the problem of moments*, J. Math. Phys., 25 (1984), pp. 2404–2417.