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THE NORMALIZED QUADRATURE METHOD OF MOMENTS COUPLED WITH FINITE POINTSET METHOD

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Abstract. This work reports the numerical performance of the Normalized Quadrature Method of Moments (NQMOM) involving more than one quadrature node (secondary particle) for dispersed phase flows coupled with the Finite Pointset Method (FPM). At first, the model used for the dispersed phase acting in a continuous environment is discussed briefly, followed by a theoretical discussion of NQMOM and FPM. Further sections report the numerical performance for test problems with increasing difficulty.

1 INTRODUCTION

In many situations physical systems are governed by processes in which particles come into existence and die during time. A Population Balance Equation (PBE) is an appropriate mathematical way to formulate the behavior of these particulate processes.The PBE

describes the evolution of the distribution function over one or more extensive physical variables in space and time. In many branches of engineering such modeling approaches led to a deeper understanding of the corresponding processes such as aerosol dynamics and others cf. [6], [7],[5]. Mathematically one usually faces an Integro-PDE or ODE where only in few cases analytical solutions have been found, cf.[4], and hence numerical methods have to be used. Among other schemes the concept of primary and secondary particles has proven to be very promising since many schemes are discovered to be special cases of this method. This concept uses low order moments of the distribution function for reconstruction, cf. [1]. In practice, many implementations suffer from a low overall number of particles. This work reports the numerical performance of a modified version of the concept of primary and secondary particles. Its name is the "Normalized Quadrature Method of Moments" (NQMOM), which has been introduced by [2] and is now extended to two secondary particles and one primary particle while coupled with the Finite Pointset Method (FPM) software package from the Fraunhofer Institute for Industrial Mathematics (ITWM). In the case presented here, the equation models droplets merging and breaking in a continuous fluid. One faces such multiphase flow situations for instance in liquid-liquid-contactors cf. [3].

2 THE MODEL FOR THE DISPERSED PHASE

At first, we will present the model used for the droplets and will give a look on the coupling with the solver for the continuous phase. In the following, we will call the phase consisting of the droplets the dispersed phase. As mentioned before the physical behavior of the dispersed phase, i.e. the change of the physical variables being involved can be described by the PBE. Such physical variables may be the volume of the droplets, their diameter or some solute concentration of the droplets. Here, we involve one physical variable, the volume v. Then, the distribution function $f = f(t, x, v)$ carries the physical information of the droplets in a way such that $f(t, x, v)\mathrm{d}v$ is the number of all droplets at position x having the volume v at time t. f satisfies the following transport equation, called Population Balance Equation

$$\begin{aligned}\partial_t f + \nabla_x \cdot (v_d f) = &+ 1/2 \cdot \int_0^{v_{max}} \omega(v - v', v') f(t, x, v - v') f(t, x, v') \mathrm{d}v' \\ &- f(t, x, v) \int_v^{v_{max}} \omega(v, v') f(t, x, v') \mathrm{d}v' \\ &- \Gamma(v) \cdot f(t, x, v) \\ &+ \int_v^{v_{max}} \Gamma(v') \cdot \beta(v|v') f(t, x, v') \mathrm{d}v'.\end{aligned} \tag{1}$$

v_d denotes the velocity field of the droplets, and Γ, β as well as ω model the breakage and merging behavior of the droplets.

The functions Γ and β in eq. (1) are called breakage functions since they govern the breakage behavior of the droplets. $\beta(v|v')$ is the daughter droplet distribution function.

That means $\beta(v|v')\mathrm{d}v\mathrm{d}v'$ represents the number of droplets of volume v formed by a droplet of volumev' at a breakage event. There are several models for β in literature, but all of them have in common that $\beta(v|v') = 0 \ \forall \ v' < \ v$ since a droplet with volume v' cannot produce a droplet of volume v satisfying $v' < v$ at breakage. $\beta(v|v')$ is a product of $\psi(v|v')$ and $\phi(v')$. $\psi(v|v')$ represents the density of the probability that a mother droplet of volume v' actually produces a daughter droplet of size v at breakage. On the other hand $\phi(v')$ is the average number of daughter droplets which are being born when a mother droplet of size v' is splitting up. Γ is said to be the breakage frequency standing for the number of breakage events per unit time. $\omega(v, v')$ is the aggregation frequency representing the number of aggregation events of a pair of droplets of size v and v' per unit time.
As for the breakage functions Γ and β, there exist several formulas for the aggregation frequency. All of these formulas have to be symmetric with respect to v and v' in order to be capture the aggregation invariance of a pair of droplets having the sizes (v, v') and (v', v). For both types of droplet events, breakage and aggregation, the $\pm$-terms represent the gain and loss numbers of droplets.

The motion of the droplets within the fluid is governed by the balance of the momentum

$$\frac{d}{dt}v_d = -\frac{\nabla p}{\rho_d} + g - \frac{1}{\rho_d \alpha_d}F_{drag} \tag{2}$$

where p denotes the pressure of the continuous liquid and $\frac{d}{dt}$ is meant to be the substantial derivative, i.e. $\frac{d}{dt} := \partial_t + v_d\partial_x$. α_d is the volumetric fraction and follows the conservation law $\frac{d}{dt}\alpha_d = -\alpha_d \nabla \cdot v_d$. In contrast, ρ_d is the density of the dispersed phase. The model for the velocity of the dispersed phase respects the buoyancy force, influence of gravity and the drag force acting on the surface of the droplets according to a non-vanishing relative velocity $v_d - v_l$, v_l being the velocity of the continuous liquid. For the drag force, the well-known model from Schiller & Naumann [8]

$$F_{drag} = \frac{3}{4}\alpha_d \rho_l \frac{C_D}{d_{30}}|v_d - v_l|(v_d - v_l)$$

has been taken. Here ρ_l is the density for the continuous fluid, in analogy to ρ_d, and C_D is given by

$$C_D = \begin{cases} \frac{24}{\mathrm{Re}}(1 + 0.15\ \mathrm{Re}^{0.687}) & \text{if Re } \leq \ 1000 \\ 0.44, & \text{otherwise} \end{cases}$$

Re is supposed to be the relative Reynolds number $\mathrm{Re} = \dfrac{\rho_l |v_d - v_l| d_{30}}{\mu_l}$, where μ_l is the dynamic viskosity of the continuous fluid. Note, that the intermediate diameter of the droplets, d_{30}, can be expressed with the help of f. This is the major reason for the introduction of (1). This issue will be revisited later, cf. (16) .

The equation for v_d is also the point of intersection for the model of the continuous phase since F_{drag} involves quantities from the liquid phase and the pressure gradient ∇p itself comes from the continuous phase. Details follow in section 7.

3 THE DISCRETIZATION OF THE PHYSICAL VARIABLE

In this section we discuss the discretization of (1) with respect to v. In the following, the right-hand-side of (1) will be abbriviated by $s(t, x, v)$.
We perform the approach

$$f(t, x, v) = \sum_{i=1}^{N_{pp}} N_i(t, x)\delta(v - v_i(t, x)) \tag{3}$$

where δ denotes the dirac delta distribution. The tupels (N^i, v^i) are called primary particles with weight N^i and volume v^i and have to be computed. This is done in the following way: The range of v is divided into N_{pp} intervals $I_i = [v_{i-1/2}, v_{i+1/2}]$, each of them associated with one primary particle. So, N_{pp} is the number of primary particles. On this interval, we place N_{sp} secondary particles (N_j^i, v_j^i) that means we do the ansatz

$$f|_{I_i} = \sum_{j=1}^{N_{sp}} N_j^i(t, x)\delta(v - v_j^i(t, x)). \tag{4}$$

Now the average weights and volumes of the secondary particles is the primary particle, i.e.

$$N_i = \frac{\sum_{j=1}^{N_{sp}} N_j^i}{(v_{i+1/2} - v_{i-1/2})},\ v_i = \frac{\sum_{j=1}^{N_{sp}} N_j^i v_j^i}{\sum_{j=1}^{N_{sp}} N_j^i}$$

and the secondary particles remain to be computed.
In order to compute the secondary particles we need $2N_{sp}$ equations for each primary particle to obtain a solution for the $2N_{sp}$ unknowns $(v_j^i, N_j^i),\ j = 1, \cdots, N_{sp}$.
Therefore we plug in the ansatz for $f|_{I_i}$ in (1), multiply by $v^r,\ r = 0, \cdots, 2N_{sp} - 1$ and integrate with respect to v.
In this way, we obtain a set of $2N_{sp}$ equations of moments

$$\partial_t \eta_i^r + \nabla_x \cdot (v_d \eta_i^r) = S_i^r,\ r = 0, \cdots, 2N_{sp} - 1 \tag{5}$$

using the definitions $\eta_i^r := \int_{v_{i-1/2}}^{v_{i+1/2}} v^r f \mathrm{d}v,\ S_i^r := \int_{v_{i-1/2}}^{v_{i+1/2}} v^r s(t, x, v) \mathrm{d}v$.
These equations have to be evaluated in space and time and after each time step the secondary particles are to be reconstructed.

For the reconstruction of the secondary particles, we use (4) and obtain the identities

$$\eta_i^r = \sum_{j=1}^{N_{sp}} v_j^{i^r} N_j^i,\ r = 0, \cdots, N_{sp}. \tag{6}$$

The left hand side results from the numerical solution of (5) which puts us in the need to solve (6) in each time step.

4 THE DISCRETIZATION OF SPACE

The set of equations (5) resulting from the concept of primary and secondary particles are standard advection-reaction-equations and several schemes for hyperbolic equations can be used to resolve these equations.
Here, we use the Finite Pointset Method (FPM) to discretize the problem with respect to x, as it is implemented in the homonymous software package of the ITWM.

The key idea of FPM is to approximate differential operators like $\Delta,\ \nabla\cdot,$ or ∂_x on a set of finitely many points without grid structure.
Let

$$\Omega^p := \{x_i : i = 1, \cdots, N\} \tag{7}$$

be the cloud of points where the computations are intended to be transacted.
Furthermore, let

$$\Omega^p \supset \Omega^p_\xi := \{x\ \in\ \Omega^p : r(\xi, x) < 1\} = \{x_l\ \in \Omega^p, l = 1, \cdots, m < N\} \tag{8}$$

be the set of neighbor particles of $\xi \in \Omega^p$ where $r(x, y)$ is a general distance function for two points x and y.
In FPM a function $u(t, x)$ is assumed to live on Ω^p which means it uses the ansatz

$$u(t, x) = (u_1 \cdots u_N),\ u_i = u(t, x_i),\ x_i\ \in \Omega^p. \tag{9}$$

Using the following notation for a differential operator T on Ω^p

$$T[u](t, \xi) :=< c^\xi, u(t, x) >= \sum_{l=1}^{m} c^\xi_l u(t, x_l)$$

the two major criterions for the stencils c^ξ read

$$\text{least squares criterion: } \min \frac{1}{2}\|W_\xi^{-1} \cdot c_\xi\|^2$$
$$\text{consistency criterion: } K_\xi^T \cdot c^\xi = b$$

where

$$\mathbb{R}^{m\times m} \ni W_\xi = \operatorname{diag}\left(w^1_\xi, \cdots, w^m_\xi\right), w^l_\xi = w(r(\xi, x_l))$$
$$\mathbb{R}^{m\times S} \ni K_\xi = \left(k^0_\xi|, \cdots, |k^S_\xi\right).$$

$k^j_\xi,\ j = 0, \cdots,\ S$ are polynomial test functions on Ω^p_ξ. They read $k^j_\xi = ((x_1 - \xi)^j, \cdots, (x_m - \xi)^j)$ and $w(r)$ is a weight function for the distance r.

The vector b in the consistency criterion controls, which operator is approximated by T and is obtained from a taylor expansion.

The FPM implementation from ITWM is designed as a Lagrangean method which tracks the solution of (5) along curves $x(t) \in \mathbb{R}^3$ with $\dot{x} = v_d$ (streamlines). Using simple computational steps (5) can be brought in a form, which is much more appropriate for Lagrangean methods since there are no more spatial differential operators to discretize: Let $\hat{\eta}_i^r := \frac{\eta_i^r}{\eta_i^0}$ and $\hat{S}_i^r := \frac{S_i^r}{\eta_i^0}$. Then, (5) comes into

$$\frac{d}{dt}\hat{\eta}_i^r + \hat{S}_i^0\hat{\eta}_i^r = \hat{S}_i^r,\ r = 0,\ \cdots,\ 2N_{sp} - 1 \tag{10}$$

which are the equations we actually solve for $\hat{\eta}_i^r$. $\hat{\eta}_i^r$ are called normalized moments and these are the objects NQMOM is named after.

5 ONE PRIMARY PARTICLE AND TWO SECONDARY PARTICLE METHOD

If we run the above described method with only one primary particle, and two secondary particles we end up with the following system of equations for the dispersed phase.

$$\frac{d}{dt}v_d = -\frac{\nabla p}{\rho_d} + g - \frac{1}{\rho_d\alpha_d}F_{drag} \tag{11}$$

$$\frac{d}{dt}\alpha_d = -\alpha_d\nabla\cdot v_d \tag{12}$$

$$\frac{d}{dt}\hat{\eta}_1 + \hat{S}_0\cdot\hat{\eta}_1 = \hat{S}_1 \tag{13}$$

$$\frac{d}{dt}\hat{\eta}_2 + \hat{S}_0\cdot\hat{\eta}_2 = \hat{S}_2 \tag{14}$$

$$\frac{d}{dt}\eta^0 + \eta^0\nabla\cdot v_d = S_0 \tag{15}$$

$$d_{30} = \sqrt[3]{\frac{6}{\pi}\hat{\eta}_1}. \tag{16}$$

Equation (16) is the average diameter of the droplets and is needed to evaluate the drag force in the source term for (11).

In general, equations (11)-(16) have to be solved for more than one primary particle, in order to reconstruct f. If the method uses only one primary particle, it is impossible to reconstruct f, but it provides solutions for the moments. However, the physical information is stored in the moments of f and therefore the One-Primary-Two-Secondary-Particle-Method (OP2SP) is described .

Note that the system of equations (13)-(16) is free of a division by η^0 up to the evaluation of the $\hat{S}_r$'s. However, the auxiliary assumption $N_1 = N_2 := N$ that the weights of the two secondary particles $(N_1, v_1), (N_2, v_2)$ are equal changes this into a completely division-free method. This means that the method is stable even for very small numbers of droplets η^0.

The number of normalised moments $\hat{\eta}_r$ and η_0 is exactly the number of unknowns $N,\ v_1,\ v_2$.

6 NUMERICAL RESULTS FOR THE HOMOGENEUOUS PROBLEM

Now, we report the numerical results for cases where analytical solutions have been found. These problems are homogeneuous in space and breakage events are neglected.

$$\begin{aligned}\partial_t f(t,v) = &+ 1/2 \cdot \int_0^{v_{max}} \omega(v-v',v') f(t,v-v') f(t,x,v') \mathrm{d}v' \\ &- f(t,v) \int_v^{v_{max}} \omega(v,v') f(t,v') \mathrm{d}v'.\end{aligned} \tag{17}$$

For the case of a constant aggregation frequency $\omega \equiv$ const and the sum aggregation kernel $\omega(v,v') = v + v'$ solutions are known, cf. figure 1, figure 2. Here, we compare η_0 and η_1 reconstructed from $\hat{\eta}_1$ and η_0.

The major difficulty of solving this problem lies in the evaluation of the source term. However, approach (3), (4) respectively, yields

$$\hat{S}^r = \frac{\eta^0}{2N_{sp}^2} \sum_{i,j=1}^{Nsp} \left[(v_i + v_j)^r - v_i^r - v_j^r \right] \omega\left(v_i, v_j\right), \; r = 0,1,2 \tag{18}$$

Then, the following schemes can be formulated

$$\eta_0^{n+1} = \eta_0^n \left(1 + \Delta t \hat{S}_0^n\right) \tag{19}$$

$$\hat{\eta}_r^{n+1} = \frac{\hat{\eta}_r^n + \Delta t \hat{S}_r^n}{1 + \Delta t \hat{S}_0^n}. \tag{20}$$

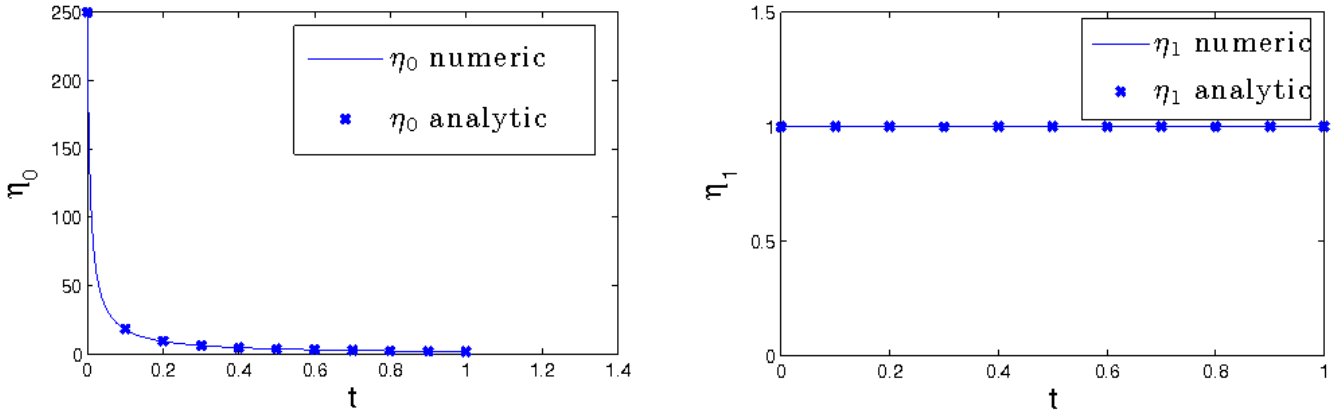

Figure 1: Comparison: Numerical & analytical solutions of η_0, η_1 with $\omega = 1$ no breakage

In both cases η_1 has to be a constant because of conservation of mass whereas η_0 has to be monotonically decreasing since the droplets are only allowed to merge and not to break.

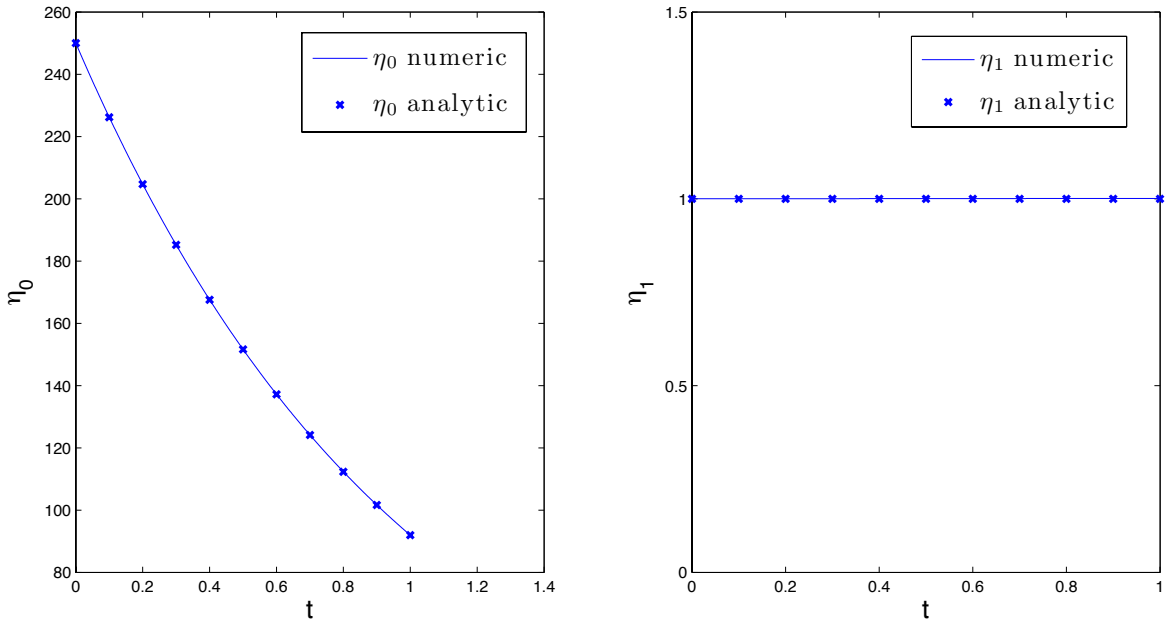

Figure 2: Comparison: Numerical & and analytical solutions of $\eta_0,\ \eta_1$ with $\omega(v, v') = v + v'$, no breakage

7 NUMERICAL RESULTS WITH SPATIAL DEPENDENCE

Next, we encounter a 2D inflow problem with constant aggregation kernel, where the full system (11)-(16) is being solved. In parallel to that, we solve equations for the continuous phase in order to gain the quantities to evaluate the right hand side. For this phase, we consider the following momentum balance

$$\frac{d}{dt}v_l = \frac{1}{\rho_l}(\nabla \cdot S) - \frac{1}{\rho}\nabla p + g + F^l_{drag} \tag{21}$$

v_l being the velocity, p the pressure, g the constant of gravity and S the stress tensor which reads

$$\mu_l \frac{1}{2}\left[\nabla v_l + (\nabla v_l)^T - \frac{1}{3}(\nabla \cdot v_l)\,\mathrm{Id}\right] \tag{22}$$

Supposed v_l to be known one can establish equations for the pressure $p = p_{hyd} + p_{dyn}$

$$\nabla \cdot \left(\frac{1}{\rho_l}\nabla p_{hyd}\right) = \nabla \cdot \left(g + F^l_{drag}\right)$$
$$\nabla \cdot \left(\frac{1}{\rho_l}\nabla p_{dyn}\right) = -\frac{d}{dt}(\nabla \cdot v) - h(v) + \nabla \cdot \left(\frac{1}{\rho_l}\nabla \cdot S\right)$$

where $h(v) = \nabla \cdot \left(\frac{d}{dt}v_l\right) - \frac{d}{dt}\nabla \cdot v_l$. These equations are used to provide the information which are needed to evaluate the dispersed phase equations. Solving equation for p_{dyn} is not

straight forward since for the time step $n+1$ we would need v_l^{n+1}. This problem is solved by a correction technique, where we rework the pressure approximation $\hat{p} = p_{hyd}^{n+1} + p_{dyn}^{n}$. F_{drag}^{l} reads

$$F_{drag}^{l} = C_D \frac{3}{4} |v_d - v_l| \left(v_d - v_l\right) \frac{\alpha_d}{d_{30}} \tag{23}$$

which comes from the overall drag force acting between the continuous and the dispersed phase at position x at time t. In contrast, F_{drag} in (2) is the drag force of a single droplet.

Solving the two phase flow problem now is done in the following way: First, we establish two separated clouds of spatial points. Each of these clouds are associated to one flow phase and moved by the evaluated corresponding velocity field.

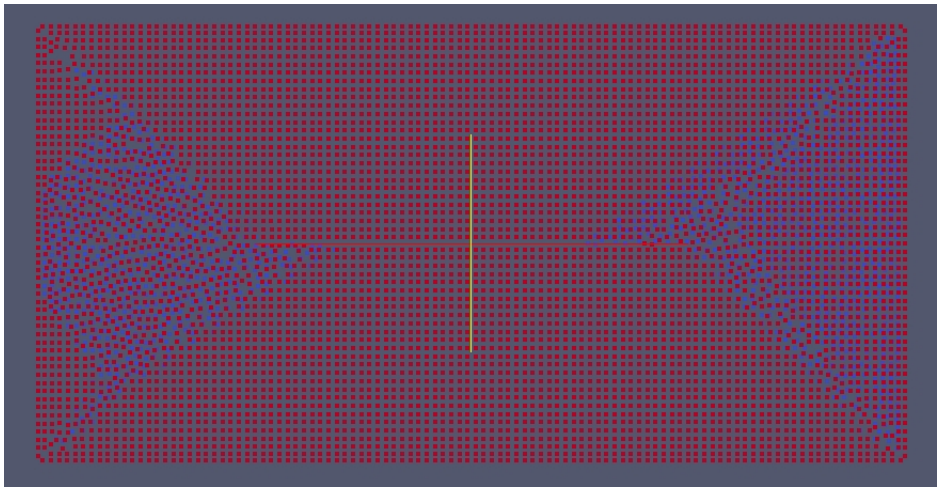

Figure 3: two separated clouds of spatial points (red:dispersed, blue: continuous phase)

These two clouds of points exchange information by interpolating the quantities from one cloud on the other cloud. In this way, we are capable to gather the quantities which are necessary to evaluate the the right hand side of (11).

The additional terms in (15) resulting from a present velocity field are resolved by traditional methods for hyperbolic equations adapted to the meshfree framework (artificial viscosity). The iteration for (11) uses an exponential approach. We rearrange (11) into the general form

$$\frac{d}{dt} v_d + A v_d = B \tag{24}$$

and assume $A,\ B$ to be constant in one time step. Then, we use the analytic solution of (24) to perform a time step dt.

$$v_d^{n+1} = \frac{B}{A} + \left(v_d^n - \frac{B}{A}\right) \exp\left(-A\ dt\right) \tag{25}$$

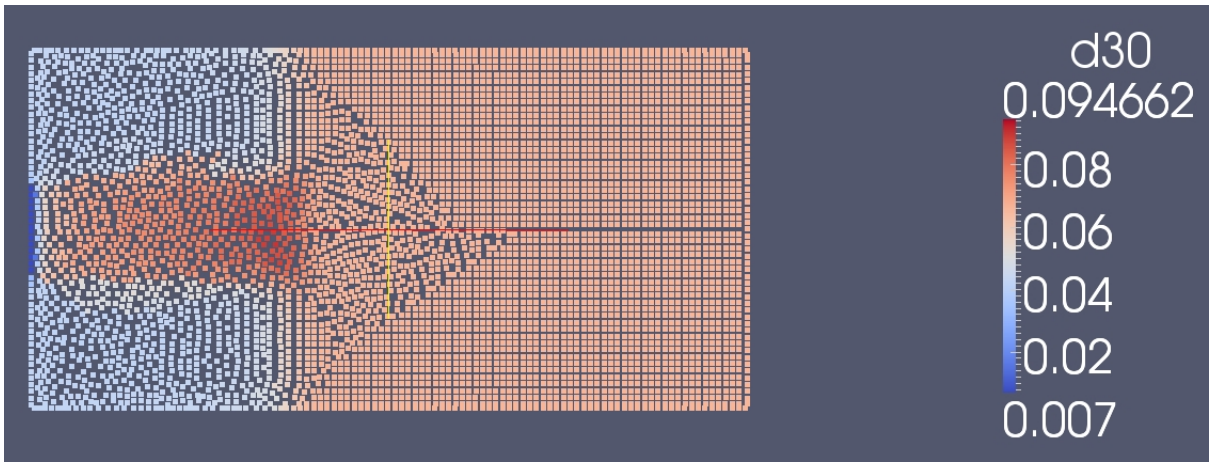

Figure 4: d30 inlet: t=0.99 $\omega \equiv 10^{-8}$, no breakage, gravity acts in direction $\leftarrow$

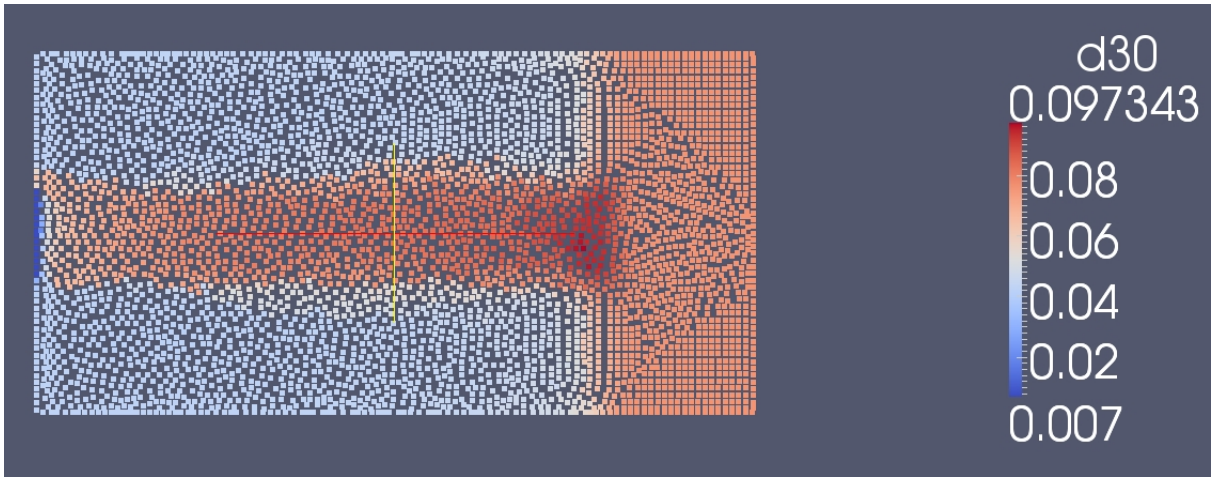

Figure 5: d30 inlet: t=1.50 $\omega \equiv 10^{-8}$, no breakage,gravity acts in direction $\leftarrow$

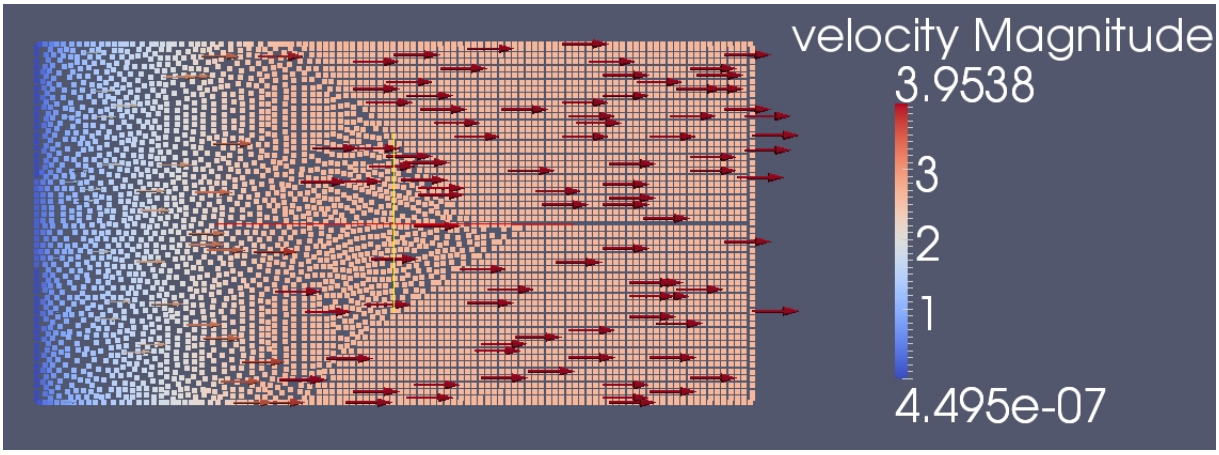

Figure 6: velocity: magnitude and direction, t=0.99 $\omega \equiv 10^{-8}$, no breakage,gravity acts in direction $\leftarrow$

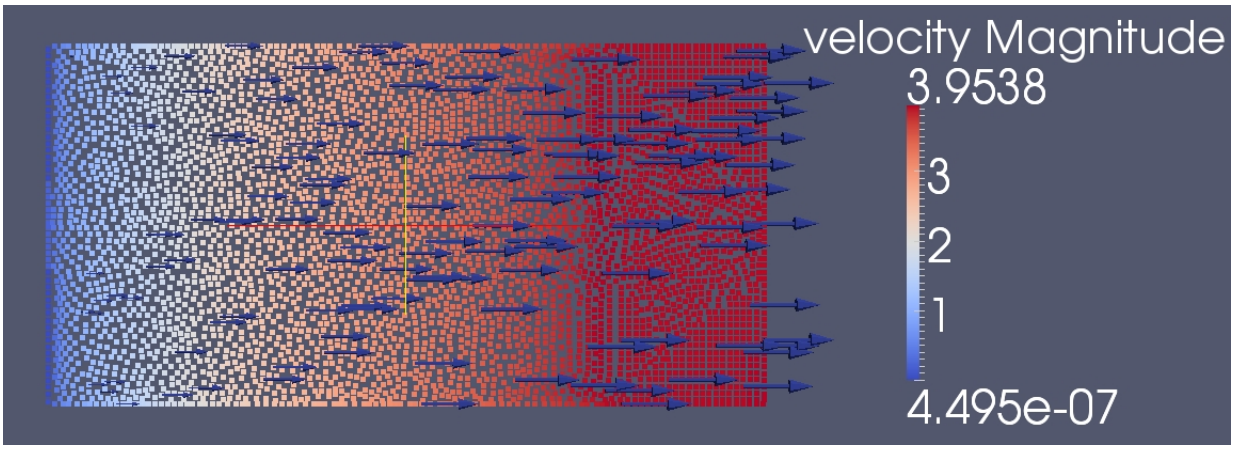

Figure 7: velocity: magnitude and direction, t=1.50 $\omega \equiv 10^{-8}$, no breakage,gravity acts in direction $\leftarrow$

Table 1: Parameters for the numerical results

ρ_c	$1000\frac{kg}{m^3}$
ρ_l	$800\frac{kg}{m^3}$
μ_l	$10^{-3}\frac{\mathrm{Ns}}{m^2}$

The numeric results for d_{30} indicate a qualitative correct behavior. As time proceeds the values are getting transported due to $d_t = \partial_t + v_d \nabla_x$ and increase slightly. This increase happens by virtue of the neglect of breakage events, which means that the droplets are only allowed to merge and not to split up. This implies that the average diameter has to increase.

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